

Multiwfn: A multifunctional wavefunction analyzer

Journal of Computational Chemistry

33, 580-592

DOI: [10.1002/jcc.22885](https://doi.org/10.1002/jcc.22885)

Citation Report

#	ARTICLE	IF	CITATIONS
1	Hybridization-related correction to the jellium model for fullerenes. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2012, 45, 215101.	0.6	19
2	Four new indole alkaloids from <i>Plantago asiatica</i> . <i>Natural Products and Bioprospecting</i> , 2012, 2, 249-254.	2.0	14
3	Quantum chemical topology investigation on structure, electronic properties and interaction of $CuNg_n + (n=1-3, Ng=He, Ne)$. <i>Structural Chemistry</i> , 2012, 23, 1831-1836.	1.0	5
4	Static and dynamic structure of monomers, dimers and trimers of $HgCl_2$ from density-functional calculations. <i>European Physical Journal D</i> , 2012, 66, 1.	0.6	11
5	Loading Aromatic Six-Membered Carbocyclic Rings with Coinage Metals: Aromatic Metalated Benzenes C_6M_6 and $1,3,5-C_6H_3M_3$ ($M = Cu, Ag, Au$) Exhibiting Intriguing Properties. <i>Organometallics</i> , 2012, 31, 7206-7212.	1.1	10
6	Two-Center Two-Electron Covalent Bonds with Deficient Bonding Densities. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10150-10159.	1.1	18
7	Theoretical Insight into the Origin of Large Stokes Shift and Photophysical Properties of Anilino-Pyridine Boron Difluoride Dyes. <i>ChemPhysChem</i> , 2012, 13, 3714-3722.	1.0	66
8	C library for topological study of the electronic charge density. <i>Journal of Computational Chemistry</i> , 2012, 33, 2526-2531.	1.5	6
9	Ordering of Molecules with π -Conjugated Triangular Core by Switching Hydrogen Bonding and van der Waals Interactions. <i>Journal of Physical Chemistry C</i> , 2012, 116, 17082-17088.	1.5	17
10	Elongation of Planar Boron Clusters by Hydrogenation: Boron Analogues of Polyenes. <i>Journal of the American Chemical Society</i> , 2012, 134, 13228-13231.	6.6	72
11	π -Stacked organic molecular crystals under electric fields as viable storage media for molecular hydrogen. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 11842-11845.	3.8	0
12	On the structures, stabilities, and potential energy surfaces of planar B_nN ($n=1-6$) clusters. <i>Computational and Theoretical Chemistry</i> , 2012, 999, 190-202.	1.1	1
13	Toward panchromatic organic functional molecules: Density functional theory study on the nature of the broad UV-Vis-NIR spectra of substituted tetra(azulene)porphyrins. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 38, 304-313.	1.3	4
14	Quantitative analysis of molecular surface based on improved Marching Tetrahedra algorithm. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 38, 314-323.	1.3	1,449
15	Chelation of a proton by oxidized diphosphines. <i>Journal of Organometallic Chemistry</i> , 2012, 721-722, 124-129.	0.8	4
16	Computational studies of the structure and cation-anion interactions in 1-ethyl-3-methylimidazolium lactate ionic liquid. <i>Science China Chemistry</i> , 2012, 55, 1548-1556.	4.2	13
17	Nature of the Interaction between Natural and Size-Expanded Guanine with Gold Clusters: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24954-24961.	1.5	25
18	Experimental and Computational Study of a New Wheel-Shaped $[W_5O_{21}]^{3-}[(UVO)_2O_2]^{2-}(\frac{1}{4}O_2)_3$ Polyoxyometalate. <i>Inorganic Chemistry</i> , 2012, 51, 8784-8790.	1.5	3

#	ARTICLE	IF	CITATIONS
19	Pseudopeptidic ligands: exploring the self-assembly of isophthaloylbisglycine (H2IBG) and divalent metal ions. Dalton Transactions, 2012, 41, 12501.	1.6	6
20	Electronic structures and optical properties of the IPR-violating C ₆₀ X ₈ (X = H, F, and Cl) fullerene compounds: a computational study. Physical Chemistry Chemical Physics, 2012, 14, 16476.	1.3	5
21	From density functional steric analysis and molecular electrostatic potential to the estimation of etherification rate constant. Journal of Physical Organic Chemistry, 2012, 25, 797-802.	0.9	8
22	Probing the electronic structure, chemical bonding, and excitation spectra of [CuE] ⁺⁰ (E = 14 group element) diatomics employing DFT and <i>ab initio</i> methods. Journal of Computational Chemistry, 2012, 33, 2318-2331.	1.5	6
23	Silicon-Containing Formal 4-Electron Four-Membered Ring Systems: Antiaromatic, Aromatic, or Nonaromatic?. Chemistry - A European Journal, 2012, 18, 7516-7524.	1.7	51
24	The Excess Electron in a Boron Nitride Nanotube: Pyramidal NBO Charge Distribution and Remarkable First Hyperpolarizability. Chemistry - A European Journal, 2012, 18, 11350-11355.	1.7	87
25	A Special Conjugated Model around sp ³ Carbon Atoms: Density Functional Theory Study on the Homoaromatic Electron Delocalization and Applications of Benzo-Fused Tetra(triptycene)porphyrins. ChemPhysChem, 2012, 13, 2046-2050.	1.0	18
26	Design of a Universal Reversible Bidirectional Current Switch Based on the Fullerene-Phthalocyanine Supramolecular System. Journal of Physical Chemistry A, 2012, 116, 6785-6791.	1.1	24
27	Interaction and protection mechanism between Li@C ₆₀ and nucleic acid bases (NABs): Performance of PM6-DH2 on noncovalent interaction of NABs@Li@C ₆₀ . Journal of Computational Chemistry, 2012, 33, 490-501.	1.5	9
28	Effect of metal cations [Li ⁺ , Na ⁺ , K ⁺ , Be ²⁺ , Mg ²⁺ , and Ca ²⁺] on the structure of 2-(3-hydroxy-2-pyridyl)benzoxazole: A theoretical investigation. International Journal of Quantum Chemistry, 2013, 113, 1316-1324.		1
29	Exploring the role of varied-length spacers in charge transfer: a theoretical investigation on pyrimidine-bridged porphyrin dyes. RSC Advances, 2013, 3, 17515.	1.7	25
30	Weak energetic effects between X ^F and X ^N halogen bonds: CSD search and theoretical study. Chemical Physics Letters, 2013, 582, 49-55.	1.2	13
31	The X ^C -Y (X = O/F, Y = O/S/F/Cl/Br/N/P) π -carbon bond TM and hydrophobic interactions. Physical Chemistry Chemical Physics, 2013, 15, 14377.	1.3	289
32	Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds. Journal of Chemical Theory and Computation, 2013, 9, 3872-3877.	2.3	312
33	Describing curved-planar π - π interactions: modeled by corannulene, pyrene and coronene. Physical Chemistry Chemical Physics, 2013, 15, 12694.	1.3	37
34	Exploration on stability, aromaticity, and potential energy surface of planar BnC ₂ (n=3-8). Computational and Theoretical Chemistry, 2013, 1006, 19-30.	1.1	7
35	A promising anchor group for efficient organic dye sensitized solar cells with iodine-free redox shuttles: a theoretical evaluation. Journal of Materials Chemistry A, 2013, 1, 14000.	5.2	62
36	Basis set effect on defect induced spin polarization of a carbon nanotube in density functional theory calculations. Chemical Physics Letters, 2013, 585, 107-111.	1.2	4

#	ARTICLE	IF	CITATIONS
37	Molecular Engineering of Indoline-Based Dye Organic Sensitizers toward High Efficiency Performance from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17382-17398.	1.5	79
38	Synthesis, Characterization, and Photophysical Properties of Heteroleptic Copper(I) Complexes with Functionalized 3-(2-Pyridyl)-1,2,4-triazole Chelating Ligands. <i>Inorganic Chemistry</i> , 2013, 52, 9727-9740.	1.9	92
39	Density functional studies on photophysical properties and chemical reactivities of the triarylboranes: effect of the constraint of planarity. <i>Journal of Molecular Modeling</i> , 2013, 19, 3437-3446.	0.8	11
40	Theoretical study of the thermodynamic and burning properties of oxygen-rich hydrazine derivatives—green and powerful oxidants for energetic materials. <i>Journal of Molecular Modeling</i> , 2013, 19, 2583-2591.	0.8	6
41	Density functional theory study of structure and bonding of water on alumina nanotube. <i>Computational Materials Science</i> , 2013, 79, 781-788.	1.4	6
42	Understanding the Unconventional Effects of Halogenation on the Luminescent Properties of Oligo(Phenylene Vinylene) Molecules. <i>Chemistry - an Asian Journal</i> , 2013, 8, 3091-3100.	1.7	27
43	Noncovalent interaction and its influence on excited-state behavior: A theoretical study on the mixed coaggregates of dicyanonaphthalene and pyrazoline. <i>Chemical Physics Letters</i> , 2013, 556, 230-236.	1.2	14
44	Size-selective effects in the geometry and electronic property of bimetallic Au–Ge nanoclusters. <i>Computational and Theoretical Chemistry</i> , 2013, 1010, 32-37.	1.1	23
45	Revealing the nature of intermolecular interaction and configurational preference of the nonpolar molecular dimers (H ₂) ₂ , (N ₂) ₂ , and (H ₂)(N ₂). <i>Journal of Molecular Modeling</i> , 2013, 19, 5387-5395.	0.8	129
46	A probe on the intermolecular forces in diisopropyl ether–n-butyric acid mixture by dielectric, FTIR studies and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 105, 102-108.	2.0	17
47	Modulating Stepwise Photochromism in Platinum(II) Complexes with Dual Dithienylethene–Acetylides by a Progressive Red Shift of Ring-Closure Absorption. <i>Inorganic Chemistry</i> , 2013, 52, 12511-12520.	1.9	24
48	The impact of intramolecular H-bonding on the aromatic character of substituted penta-fulvenes. <i>Computational and Theoretical Chemistry</i> , 2013, 1017, 31-36.	1.1	5
49	Weak energetic effects between halogen and hydrogen bonds in crystal structures of halo-perfluorobenzenes (X-PFCs) and pyrazine molecules: A computational study. <i>Computational and Theoretical Chemistry</i> , 2013, 1026, 1-6.	1.1	6
50	The electronic structures and charge transfer properties of tetra(naphthalene-dione)porphyrins and tetra(naphthalene-dithione)porphyrins as dye-sensitized solar cell skeleton. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2605-2610.	1.0	8
51	On the Nature of Hypercoordination in Dihalogenated Perhalocyclohexasilanes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3529-3538.	1.1	27
52	Conformational analysis and intramolecular hydrogen bonding of cis-3-aminoindan-1-ol: a quantum chemical study. <i>Journal of Molecular Modeling</i> , 2013, 19, 4837-4847.	0.8	3
53	Strong Adsorption Between Uranium Dicarbide and Graphene Surface Induced by f Electrons. <i>Journal of Physical Chemistry C</i> , 2013, 117, 26849-26857.	1.5	14
54	Face-Capping $\frac{1}{3}$ -BO in B ₆ (BO) ₇ : Boron Oxide Analogue of B ₆ H ₇ with Rhombic 4c ^{2e} Bonds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11587-11591.	1.1	12

#	ARTICLE	IF	CITATIONS
55	Broadband Ultrafast Photoluminescence Spectroscopy Resolves Charge Photogeneration via Delocalized Hot Excitons in Polymer:Fullerene Photovoltaic Blends. <i>Journal of the American Chemical Society</i> , 2013, 135, 18502-18512.	6.6	93
56	Structures and hydrogen bonds of biodegradable naphthenate ionic liquids. <i>Fluid Phase Equilibria</i> , 2013, 360, 169-179.	1.4	24
57	[FAAF] ⁿ (A = O, S, Se, Te) or How Electrostatic Interactions Influence the Nature of the Chemical Bond. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5211-5215.	2.3	11
58	Geometry, stability, and isomerization of B _n N ₂ (n = 1-6) isomers. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2251-2260.	1.0	2
59	Infrared Spectra of NgBeS (Ng = Ne, Ar, Kr, Xe) and BeS ₂ in Noble-Gas Matrices. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1508-1513.	1.1	56
60	A Unique Au-Ag-Au Triangular Motif in a Trimetallic Halonium Dication: Silver Incorporation in a Gold(I) Catalyst. <i>Chemistry - A European Journal</i> , 2013, 19, 12264-12271.	1.7	65
61	Structures and Phosphorescence Properties of Triphosphine-Supported Au ₂ Ag ₂ and Au ₈ Ag ₄ Alkynyl Cluster Complexes. <i>Organometallics</i> , 2013, 32, 5402-5408.	1.1	33
62	A theoretical study on magnetic properties of bis-TEMPO diradicals with possible application. <i>Computational and Theoretical Chemistry</i> , 2013, 1024, 15-23.	1.1	15
63	Complementarity of QTAIM and ELF Partitions: Deeper Understanding of the Anomeric Effect. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4816-4824.	2.3	12
64	Polarization-enhanced bonding process of halogen bond, a theoretical study on H/F-X (X = F, Cl, Br). <i>J. Phys. Chem. A</i> , 2013, 117, 10784-10793.	1.1	3
65	Boron complexes of redox-active diimine ligand. <i>Dalton Transactions</i> , 2013, 42, 7952.	1.6	30
66	Shedding light on the bonding, photophysical and magnetotropic properties of triangular Pt ₃ complexes and their open-face Pt ₃ half-sandwiches. <i>Dalton Transactions</i> , 2013, 42, 2201-2212.	1.6	6
67	Two new uranyl fluoride complexes with UV-Vis-alkali (Na, Cs) interactions: Experimental and theoretical studies. <i>CrystEngComm</i> , 2013, 15, 8041.	1.3	8
68	Oxidation state and covalency in f-element metallocenes (M = Ce, Th, Pu): a combined CASSCF and topological study. <i>Dalton Transactions</i> , 2013, 42, 16428.	1.6	90
69	Face-to-Face Stacks of Trinuclear Gold(I) Trihalides with Benzene, Hexafluorobenzene, and Borazine: Impact of Aromaticity on Stacking Interactions. <i>Inorganic Chemistry</i> , 2013, 52, 1047-1060.	1.9	11
70	On the Covalent Character of Rare Gas Bonding Interactions: A New Kind of Weak Interaction. <i>Journal of Physical Chemistry A</i> , 2013, 117, 207-212.	1.1	96
71	Microwave Spectroscopic and Atoms in Molecules Theoretical Investigations on the Ar-H-C≡C-Propargyl Alcohol Complex: Ar-H ₂ O, Ar-H ₂ N ₂ , and Ar-H ₂ C Interactions. <i>ChemPhysChem</i> , 2013, 14, 754-763.	1.0	34
72	Theoretical investigations on structural, electronic, and magnetic properties of TM ₂ Np ₂ (Np=Naphthalene, TM=Sc-Ni) sandwich clusters. <i>Computational and Theoretical Chemistry</i> , 2013, 1013, 46-51.	1.1	6

#	ARTICLE	IF	CITATIONS
73	Theoretical investigation on the electronic and optical properties of diarylfluorene-based π -stacked molecules as supramolecular semiconductors. <i>Chemical Physics Letters</i> , 2013, 578, 150-155.	1.2	4
74	Weak intramolecular OH \cdots π hydrogen bonding in methallyl- and allyl-carbinol. <i>Chemical Physics Letters</i> , 2013, 582, 31-37.	1.2	13
75	Density functional theory study on the influence of pyrrolidine substituent of C ₆₀ bisadduct on its supramolecular interaction with porphine. <i>Chemical Physics</i> , 2013, 423, 43-48.	0.9	2
76	Jatropholane-Type Diterpenes from <i>Euphorbia sikkimensis</i> . <i>Journal of Natural Products</i> , 2013, 76, 265-269.	1.5	23
77	Bond Order Analysis Based on the Laplacian of Electron Density in Fuzzy Overlap Space. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3100-3108.	1.1	379
78	Theoretical analyses of the host-guest interaction within chlorine hydrate. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2228-2233.	1.0	1
79	Theoretical characterization and design of small molecule donor material containing naphthodithiophene central unit for efficient organic solar cells. <i>Journal of Computational Chemistry</i> , 2013, 34, 1611-1619.	1.5	130
80	A theoretical study of conformational flexibility, magnetic properties, and polarizabilities of trimethylnaphthalenes. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1890-1898.	1.0	7
81	Theoretical Study on the Rectifying Performance of Organoimido Derivatives of Hexamolybdates. <i>ChemPhysChem</i> , 2013, 14, 610-617.	1.0	16
82	A RASSCF study of free base, magnesium and zinc porphyrins: accuracy versus efficiency. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 2197.	1.3	17
83	Efficient photo-driven hydrogen evolution by binuclear nickel catalysts of different coordination in noble-metal-free systems. <i>Dalton Transactions</i> , 2013, 42, 8684.	1.6	40
84	Natures of benzene-water and pyrrole-water interactions in the forms of π and π types: theoretical studies from clusters to liquid mixture. <i>Journal of Molecular Modeling</i> , 2013, 19, 1273-1283.	0.8	17
85	Mechanism and Selectivity of Bioinspired Cinchona Alkaloid Derivatives Catalyzed Asymmetric Olefin Isomerization: A Computational Study. <i>Journal of the American Chemical Society</i> , 2013, 135, 7462-7473.	6.6	69
86	Intramolecular halogen-halogen bonds?. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11543.	1.3	61
87	Effect of superalkali substituents on the strengths and properties of hydrogen and halogen bonds. <i>Journal of Molecular Modeling</i> , 2013, 19, 1311-1318.	0.8	7
88	The molecular, electronic, bonding, and photophysical features of the [(c-Pt3)Ti(c-Pt3)] ⁺ inorganic metallocenes. <i>Dalton Transactions</i> , 2013, 42, 8307.	1.6	6
89	Sensitized Eu(III) luminescence through energy transfer from PtM ₂ (M = Ag or Au) alkynyl chromophores in PtM ₂ Eu ₂ heteropentanuclear complexes. <i>Journal of Materials Chemistry C</i> , 2013, 1, 3661.	2.7	25
90	Ab Initio Molecular Dynamics Study of the Reaction of U ⁺ and U ²⁺ with H ₂ O in the Gas Phase: Direct Classical Trajectory Calculations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3761-3770.	1.1	10

#	ARTICLE	IF	CITATIONS
91	Solid State Structure of Bi(N ₃) ₃ , Bi(N ₃) ₃ ·Solvates and the Structural Dynamics in the [Bi(N ₃) ₆] ³⁻ Anion. <i>Inorganic Chemistry</i> , 2013, 52, 6110-6126.	1.9	32
92	Influence of transition metal coordination on halogen bonding: CSD survey and theoretical study. <i>Chemical Physics Letters</i> , 2013, 578, 38-42.	1.2	16
93	Substituent Effects on the Cooperativity of Halogen Bonding. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5551-5557.	1.1	73
94	Hippolachnin A, a New Antifungal Polyketide from the South China Sea Sponge <i>Hippospongia lachne</i> . <i>Organic Letters</i> , 2013, 15, 3526-3529.	2.4	84
95	Click-Like Reactions with the Inert HCB ₁₁ Cl ₁₁ ⁺ Anion Lead to Carborane-Fused Heterocycles with Unusual Aromatic Character. <i>Inorganic Chemistry</i> , 2013, 52, 6223-6229.	1.9	50
96	Structure and Stability of (NG) _n CN ₃ Be ₃ ⁺ Clusters and Comparison with (NG)BeY ⁺ . <i>ChemPhysChem</i> , 2013, 14, 2511-2517.	1.0	41
97	The geometry and electronic structure of Aristolochic acid: possible implications for a frozen resonance. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 473-483.	0.9	259
98	Exploration on the structure, stability, and isomerization of planar C _n B ₅ (n = 1~7) clusters. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2514-2522.	1.0	6
99	Structure Prediction of Au ₄₄ (SR) ₂₈ : A Chiral Superatom Cluster. <i>Journal of the American Chemical Society</i> , 2013, 135, 19060-19063.	6.6	89
100	Mechanistic Studies on the Carboxylation of Hafnocene and ansa-Zirconocene Dinitrogen Complexes with CO ₂ . <i>Organometallics</i> , 2013, 32, 7077-7082.	1.1	13
101	Noble gas-coinage metal interactions of (AuRn) ⁺ (n = 1~3) series: ab initio calculations. <i>European Physical Journal D</i> , 2013, 67, 1.	0.6	6
102	Synthesis and Reactivity of the Unsaturated Trinuclear Phosphanido Complex [(C ₆ F ₅) ₂ Pt(1/4-PPh ₂) ₂] ₂ Pt(1/4-PPh ₂) ₂ . <i>Inorganic Chemistry</i> , 2013, 52, 1942-1953.		
103	Dual Bonding between H ₂ O/H ₂ S and AgCl/CuCl: Cu/Ag Bond, Sister Bond to Au Bond. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10944-10950.	1.1	14
104	High-yield Synthesis of Silver Nanoclusters Protected by DNA Monomers and DFT Prediction of their Photoluminescence Properties. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2022-2026.	7.2	50
105	Alternant conjugated oligomers with tunable and narrow HOMO-LUMO gaps as sustainable nanowires. <i>RSC Advances</i> , 2013, 3, 25881.	1.7	55
106	Phosphorescent Square-Planar Platinum(II) Complexes of 1,3-Bis(2-pyridylimino)isoindoline with a Monodentate Strong-Field Ligand. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 4789-4798.	1.0	8
107	Bonding in Diborane-Metal Complexes: A Quantum-Chemical and Experimental Study of Complexes Featuring Early and Late Transition Metals. <i>Chemistry - A European Journal</i> , 2013, 19, 7395-7409.	1.7	35
109	Molecular Insights into the pH-Dependent Adsorption and Removal of Ionizable Antibiotic Oxytetracycline by Adsorbent Cyclodextrin Polymers. <i>PLoS ONE</i> , 2014, 9, e86228.	1.1	10

#	ARTICLE	IF	CITATIONS
110	DFT Study on the Co-Xe Bond in the HCo(CO) ₃ Xe Adduct. Journal of Quantum Chemistry, 2014, 2014, 1-5.	0.6	0
111	Understanding the effects of the number of pyrazines and their positions on charge-transport properties in silylethynylated N-heteropentacenes. Journal of Molecular Modeling, 2014, 20, 2502.	0.8	4
112	Host-Guest Interactions in ExBox ⁴⁺ . ChemPhysChem, 2014, 15, 4108-4116.	1.0	19
113	Theoretical calculations of π -type pnictogen bonds in the triad intermolecular complexes. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450068.	1.8	7
114	Interplay between halogen and chalcogen bonding in the XCl ⁺ ...OCS ⁺ ...NH ₃ (X = F, OH, NC, CN, and FCC) complex. Journal of Molecular Modeling, 2014, 20, 2458.	0.8	11
115	Halogen bonds with N-heterocyclic carbenes as halogen acceptors: a partially covalent character. Molecular Physics, 2014, 112, 3024-3032.	0.8	29
116	The adsorption of water-soluble ionic liquids on graphene oxide of different oxygen content. RSC Advances, 2014, 4, 58536-58545.	1.7	11
117	Benzothienoquinolines: New one-pot synthesis and fluorescence studies of their interaction with DNA and polynucleotides. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 294, 20-30.	2.0	16
118	Ab Initio Study on the Stability of Ng _n Be ₂ N ₂ , Ng _n Be ₃ N ₂ and NgBeSiN ₂ Clusters. ChemPhysChem, 2014, 15, 2618-2625.	1.0	35
119	Dihydrogen Bonding in Compressed Ammonia Borane and Its Roles in Structural Stability. Journal of Physical Chemistry C, 2014, 118, 29591-29598.	1.5	24
120	Quantum Chemical Determination of Novel C ₈₂ Monometallofullerenes Involving a Heterogeneous Group. Inorganic Chemistry, 2014, 53, 12911-12917.	1.9	18
121	Theoretical studies on the stability of phenylpentazole and its substituted derivatives of OH , OCH_3 , OC_2H_5 and $\text{N}(\text{CH}_3)_2$. RSC Advances, 2014, 4, 56095-56101.	1.7	19
122	Photoelectron imaging and theoretical study on the structure and chemical binding of the mixed-ligand M(I) complexes, [HMSH] ⁺ (M = Cu, Ag, and Au). Journal of Chemical Physics, 2014, 140, 114307.	1.2	5
123	DFT assessment of the spectroscopic constants and absorption spectra of neutral and charged diatomic species of group 11 and 14 elements. Journal of Computational Chemistry, 2014, 35, 1762-1777.	1.5	2
124	Theoretical Insight into the Coordination of Cyclic β -D-Glucose to [Al(OH)(aq)] ²⁺ and [Al(OH) ₂ (aq)] ¹⁺ Ions. Journal of Physical Chemistry B, 2014, 118, 13890-13902.	1.2	23
125	Gas-phase water activation by Th atom: Reaction mechanisms and topological analysis. International Journal of Quantum Chemistry, 2014, 114, 760-768.	1.0	14
126	Metallophilic interaction in gold halide: Quantum chemical study of AuX (X = F, Cl, Br, I). Journal of Computational Chemistry, 2014, 35, 923-931.	1.5	19
127	Effect of Benzo-Annulation on Local Aromaticity in Heterocyclic Conjugated Compounds. Journal of Physical Chemistry A, 2014, 118, 11591-11601.	1.1	23

#	ARTICLE	IF	CITATIONS
128	Large Nonlinear Optical Responses of Dimers Bearing a Donor and Acceptor: Long, Intradimer Multicenter Bonding. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28746-28756.	1.5	37
129	Pseudo-Bonding Interaction between Boron-doped Heterofullerene and Zinc Porphine Predicted by DFT Calculation. <i>Chinese Journal of Chemical Physics</i> , 2014, 27, 285-290.	0.6	3
130	<i>Ab initio</i> investigation of the lower energy candidate structures for (H ₂ O) ₅ + water cluster. <i>Journal of Chemical Physics</i> , 2014, 141, 054309.	1.2	39
131	The effect of boron nitride nanotubes size on the HArF interaction by NBO and AIM analysis. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1692-1696.	1.0	4
132	Anthraquinone-Based Intramolecular Charge-Transfer Compounds: Computational Molecular Design, Thermally Activated Delayed Fluorescence, and Highly Efficient Red Electroluminescence. <i>Journal of the American Chemical Society</i> , 2014, 136, 18070-18081.	6.6	822
133	A designed bithiopheneimide-based conjugated polymer for organic photovoltaic with ultrafast charge transfer at donor/PC71BM interface: theoretical study and characterization. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 25799-25808.	1.3	51
134	Grid-based algorithm to search critical points, in the electron density, accelerated by graphics processing units. <i>Journal of Computational Chemistry</i> , 2014, 35, 2272-2278.	1.5	49
135	Theoretical studies on the stability of salts formed by 3-substituted 6-nitraminotetrazines with different cations. <i>Journal of Molecular Modeling</i> , 2014, 20, 2521.	0.8	0
136	Mechanism of oxygen transfer from the vanadium(V) complexes with ligands O ₂ 2 ⁻ and O ₃ 2 ⁻ . <i>Russian Chemical Bulletin</i> , 2014, 63, 1283-1288.	0.4	0
137	Structure, bonding and energetics of N-heterocyclic carbene (NHC) stabilized low oxidation state group 2 (Be, Mg, Ca, Sr and Ba) metal complexes: A theoretical study. <i>Journal of Chemical Sciences</i> , 2014, 126, 1781-1788.	0.7	10
138	Study of Chemical Modified Amphoteric Ion Exchange Membrane from Taurine. <i>ECS Electrochemistry Letters</i> , 2014, 3, A102-A104.	1.9	5
139	Geometrical and electronic structure of the Ba-doped Sin (n=1-12) cluster: A density functional study. <i>Journal of Molecular Structure</i> , 2014, 1075, 220-226.	1.8	14
140	Charge-transfer complexes of iodoform with 1,4-dioxane, -dithiane, and -diselenane: Theoretical electron density and energy decomposition analysis. <i>Computational and Theoretical Chemistry</i> , 2014, 1044, 80-86.	1.1	7
141	A Theoretical Study on the Structure, Intramolecular Interactions, and Detonation Performance of Hydrazinium Dinitramide. <i>Chemistry - an Asian Journal</i> , 2014, 9, 229-236.	1.7	14
142	Structural and spectroscopic characterization of a novel potential anti-inflammatory agent 3-(adamantan-1-yl)-4-ethyl-1H-1,2,4-triazole-5(4H)thione by first principle calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 124, 108-123.	2.0	17
143	Exploring the role of steric effect in the stability of clusters: Water hexamer as a test case. <i>Chemical Physics</i> , 2014, 434, 11-14.	0.9	17
144	Li doped effect of through novel noncovalent charge transfer on nonlinear optical properties. <i>Dyes and Pigments</i> , 2014, 106, 7-13.	2.0	31
145	Virtual screening of cocrystal formers for CL-20. <i>Journal of Molecular Structure</i> , 2014, 1072, 179-186.	1.8	7

#	ARTICLE	IF	CITATIONS
146	Electron Density Properties and Interaction: Quantum Chemical Topology Investigation on AuRn n 2+ (n=1-6). Journal of Cluster Science, 2014, 25, 1121-1135.	1.7	1
147	Dioxetanones TM peroxide bond as a charge-shifted bond: implications in the chemiluminescence process. Structural Chemistry, 2014, 25, 1075-1081.	1.0	9
148	A Time-Dependent DFT Study of the Absorption and Fluorescence Properties of Graphene Quantum Dots. ChemPhysChem, 2014, 15, 950-957.	1.0	92
149	Novel second-order nonlinear optical chromophores containing multi-heteroatoms in donor moiety: Design, synthesis, DFT studies and electro-optic activities. Dyes and Pigments, 2014, 102, 142-149.	2.0	51
150	Rational Design of Dibenzothiophene-Based Host Materials for PHOLEDs. Journal of Physical Chemistry C, 2014, 118, 2375-2384.	1.5	43
151	Dissecting molecular descriptors into atomic contributions in density functional reactivity theory. Journal of Chemical Physics, 2014, 140, 024109.	1.2	34
152	Influence of the nature of hydrogen halides and metal cations on the interaction types between borazine and hydrogen halides. Journal of Molecular Modeling, 2014, 20, 2089.	0.8	3
153	The X TM Au interactions in the CF ₃ X (X = Cl, Br) Au _n (n=2, 3, and 4) complexes. Journal of Molecular Modeling, 2014, 20, 2133.	0.8	9
154	Chemical bond between Cu(II) and Rn: ab initio study of CuRn n 2+ (n=1-6) by coupled cluster method. Structural Chemistry, 2014, 25, 259-266.	1.0	5
155	Organohelium Compounds: Structures, Stabilities and Chemical Bonding Analyses. ChemPhysChem, 2014, 15, 467-477.	1.0	2
156	Enhancement of second-order nonlinear optical response in boron nitride nanocone: Li-doped effect. Journal of Molecular Graphics and Modelling, 2014, 48, 28-35.	1.3	23
157	Spatial localization of electron pairs in molecules using the Fisher information density. Chemical Physics, 2014, 435, 49-56.	0.9	17
158	ADSORPTION OF H ₂ ON FRAGMENTS OF MOF-210: A DFT INVESTIGATION. Surface Review and Letters, 2014, 21, 1450011.	0.5	4
159	The master factors influencing the efficiency of D- TM A-configured organic sensitizers in dye-sensitized solar cell via theoretically characterization: Design and verification. Dyes and Pigments, 2014, 105, 192-201.	2.0	21
160	Substituent and transition metal effects on halogen bonding: CSD search and theoretical study. Computational and Theoretical Chemistry, 2014, 1029, 21-25.	1.1	7
161	Strong halogen bonds between halo-perfluorobenzenes (C ₆ F ₅ X) and pyridine molecules: A combined theoretical and crystallographic data study. Computational and Theoretical Chemistry, 2014, 1027, 79-83.	1.1	7
162	Design of high-performance chlorine type dyes for dye-sensitized solar cells. International Journal of Quantum Chemistry, 2014, 114, 222-232.	1.0	12
163	<i>N</i> -Diazo-Bridged Nitroazoles: Catenated Nitrogen-Atom Chains Compatible with Nitro Functionalities. Chemistry - A European Journal, 2014, 20, 6707-6712.	1.7	71

#	ARTICLE	IF	CITATIONS
164	Screening Nitrogen-Rich Bases and Oxygen-Rich Acids by Theoretical Calculations for Forming Highly Stable Salts. <i>ChemPhysChem</i> , 2014, 15, 2281-2287.	1.0	4
165	Theoretical investigations on the enhancing effect of the cation- π interaction on the halogen bond in the $M^+ \cdots HCCX \cdots NH_3$ ($M = Li^+, Na^+, Cu^+, Ag^+, Au^+$; $X = Cl, Br$) complexes. <i>Journal of Molecular</i> 2014, 20, 2235.	1.8	1
166	Vibrational (FT-IR and FT-Raman), electronic (UV-Vis), NMR (1H and ^{13}C) spectra and reactivity analyses of 4,5-dimethyl-o-phenylenediamine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 130, 516-525.	2.0	22
167	Structural and electronic characterization of a Fridericia heliotoa luciferin-related derivative, based on quantum chemistry. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2014, 288, 46-54.	2.0	0
168	Possibility of the Existence of Donor-Acceptor Interactions in Bis(azole)amines: An Electronic Structure Analysis. <i>Journal of Organic Chemistry</i> , 2014, 79, 4852-4862.	1.7	25
169	Metal- and Ligand-Supported Reduction of the $\{Fe_2S_2\}$ Cluster as a Path to Formation of Molecular Group 13 Element Complexes $\{Fe_2S_2M\}$ ($M = Al, Ga$). <i>Organometallics</i> , 2014, 33, 2713-2720.	1.1	7
170	DFT studies for the evaluation of amine functionalized polystyrene adsorbents for selective adsorption of carbon dioxide. <i>RSC Advances</i> , 2014, 4, 20323-20333.	1.7	26
171	Study of atomic and molecular oxygen chemisorption on BC ₃ nanotubes with Stone-Wales defects using density functional theory. <i>Chemical Physics</i> , 2014, 438, 16-22.	0.9	3
172	Co-crystallized fullerene and a mixed (phthalocyaninato)(porphyrinato) dysprosium double-decker SMM. <i>Chemical Science</i> , 2014, 5, 3214-3220.	3.7	40
173	Theoretical study and design of triphenylamine-malononitrile-based p-type organic dyes with different π -linkers for dyes-sensitized solar cells. <i>Dyes and Pigments</i> , 2014, 108, 106-114.	2.0	50
174	Theoretical study of the molecular properties of dimethylantracenes as properties for the prediction of their biodegradation and mutagenicity. <i>Chemosphere</i> , 2014, 111, 144-150.	4.2	7
175	Pyridyl- and pyrimidyl-phosphine-substituted [FeFe]-hydrogenase mimics: Synthesis, characterization and properties. <i>Journal of Organometallic Chemistry</i> , 2014, 767, 46-53.	0.8	19
176	A Three-Component Catalyst-Free Approach to Regioselective Synthesis of Dual Highly Functionalized Fused Pyrrole Derivatives in Water-Ethanol Media: Thermodynamics versus Kinetics. <i>ACS Sustainable Chemistry and Engineering</i> , 2014, 2, 1155-1163.	3.2	39
177	Information Conservation Principle Determines Electrophilicity, Nucleophilicity, and Regioselectivity. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3698-3704.	1.1	150
178	Exploring the mechanism of ion-pair recognition by new calix[4]pyrrole bis-phosphonate receptors: insights from quantum mechanics study. <i>RSC Advances</i> , 2014, 4, 1864-1873.	1.7	11
179	The molecular properties of nitrobenzanthrone isomers and their mutagenic activities. <i>Chemosphere</i> , 2014, 104, 228-236.	4.2	6
180	Structures and bonding characters of $(MgO)_3n$ ($n = 2-8$) clusters. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2014, 47, 025102.	0.6	19
181	Quantum-chemical (DFT, MP2) and spectroscopic studies (FT-IR and UV) of monomeric and dimeric structures of 2(3H)-Benzothiazolone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 120, 126-136.	2.0	14

#	ARTICLE	IF	CITATIONS
182	1,3-Cationic Alkylidene Migration of Nonclassical Carbocation: A Density Functional Theory Study on Gold(I)-Catalyzed Cycloisomerization of 1,5-Enynes Containing Cyclopropene Moiety. <i>Journal of the American Chemical Society</i> , 2014, 136, 1505-1513.	6.6	39
183	Insights into the adsorption of simple benzene derivatives on carbon nanotubes. <i>RSC Advances</i> , 2014, 4, 58036-58046.	1.7	19
184	Novel non-covalent interactions involved with the Al ₁₃ M cluster (M = Li, Na, K, Cu, Ag). <i>Journal of Physical Chemistry B</i> , 2014, 18, 10788-10793.	0.8	3
185	Regulatory factors and the nature of Cu-Cu interaction in copper(I) complexes with NHC and NHCP ligands: a theoretical assessment. <i>New Journal of Chemistry</i> , 2014, 38, 5786-5792.	1.4	5
186	Mechanically Triggered Fluorescence/Phosphorescence Switching in the Excimers of Planar Trinuclear Copper(I) Pyrazolate Complexes. <i>Inorganic Chemistry</i> , 2014, 53, 11604-11615.	1.9	96
187	Cy3 and Cy5 Dyes Terminally Attached to 5' End of DNA: Structure, Dynamics, and Energetics. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13564-13572.	1.2	19
188	Rational modifications on champion porphyrin dye SM315 using different electron-withdrawing moieties toward high performance dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24994-25003.	1.3	40
189	Understanding the Interactions of Neptunium and Plutonium Ions with Graphene Oxide: Scalar-Relativistic DFT Investigations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10273-10280.	1.1	57
190	Mechanistic Insights into the Pd-Catalyzed Intermolecular Asymmetric Allylic Dearomatization of Multisubstituted Pyrroles: Understanding the Remarkable Regio- and Enantioselectivity. <i>Journal of the American Chemical Society</i> , 2014, 136, 16251-16259.	6.6	64
191	Bonding analysis of the donor-acceptor sandwiches Cp ⁺ MCp ⁻ (E = B, Al, Ga; M = Li, Na, K; Cp = 1,5-C ₅ H ₅). <i>Journal of Molecular Modeling</i> , 2014, 20, 2455.	0.8	2
192	Impact of Ground- and Excited-State Aromaticity on Cyclopentadiene and Silole Excitation Energies and Excited-State Polarities. <i>Chemistry - A European Journal</i> , 2014, 20, 9295-9303.	1.7	61
193	A theoretical study on the stability and detonation performance of 2,2,3,3-tetranitroaziridine (TNAD). <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 532-539.	0.9	3
194	Theoretical studies on the stability, detonation performance and possibility of synthesis of the nitro derivatives of epoxyethane. <i>Journal of Molecular Modeling</i> , 2014, 20, 2327.	0.8	7
195	Accesses to electronic structures and the excited states of blue luminescent copper(I) complexes containing N-heterocyclic carbene ligands: a DFT/TDDFT exploitation. <i>Journal of Molecular Modeling</i> , 2014, 20, 2416.	0.8	0
196	Theoretical Study of the Intercalation Behavior of Ethylene Glycol on Kaolinite. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26017-26026.	1.5	22
197	Determination of the Mechanism of Electrocatalytic Water Oxidation by a Dimanganese Tetrakis-Schiff Base Complex: Comparison of Density Functional Theory Calculations with Experiment. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25869-25877.	1.5	6
198	Unstable, Metastable, or Stable Halogen Bonding Interaction Involving Negatively Charged Donors? A Statistical and Computational Chemistry Study. <i>Journal of Physical Chemistry B</i> , 2014, 118, 14223-14233.	1.2	9
199	Computational Study on Cycloisomerization/Oxidative Dimerization of Aryl Propargyl Ethers Catalyzed by Gold Nanoclusters: Mechanism and Selectivity. <i>Organometallics</i> , 2014, 33, 6633-6642.	1.1	14

#	ARTICLE	IF	CITATIONS
200	Molecular Design and Property Prediction of High Density Polynitro[3.3.3]-Propellane-Derivatized Frameworks as Potential High Explosives. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10857-10865.	1.1	29
201	A comparative study of the structure, energetic performance and stability of nitro-NNO-azoxy substituted explosives. <i>Journal of Materials Chemistry A</i> , 2014, 2, 20806-20813.	5.2	40
202	Confinement of (HF) ₂ in C (n= 60, 70, 80, 90) cages. <i>Chemical Physics Letters</i> , 2014, 616-617, 49-54.	1.2	12
203	Exploring photophysical properties of metal-free coumarin sensitizers: an efficient strategy to improve the performance of dye-sensitized solar cells. <i>RSC Advances</i> , 2014, 4, 53927-53938.	1.7	24
204	Solvent effect on electron and proton transfer in the excited state of a hydrogen bonded phenol-imidazole complex. <i>RSC Advances</i> , 2014, 4, 38551-38557.	1.7	4
205	Gas storage potential of ExBox ⁴⁺ and its Li-decorated derivative. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21964-21979.	1.3	11
206	Defect-induced strong localization of uranium dicarbide on the graphene surface. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22784-22790.	1.3	16
207	Probing the origin of opposite ion-pair binding behavior for two new calix[4]pyrrole bis-phosphonate receptors. <i>RSC Advances</i> , 2014, 4, 44948-44958.	1.7	5
208	Spectroscopic observation of photo-induced metastable linkage isomers of coinage metal (Cu, Ag, Au) sulfur dioxide complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 2607.	1.3	14
209	Noble gas encapsulation: clathrate hydrates and their HF doped analogues. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17943-17954.	1.3	31
210	A novel photo-responsive azobenzene-containing nanoring host for fullerene-guest facile encapsulation and release. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 27053-27064.	1.3	27
211	Novel electro-optic chromophores based on substituted benzo[1,2-b:4,5-b']dithiophene π -conjugated bridges. <i>RSC Advances</i> , 2014, 4, 25532-25539.	1.7	17
212	An environmentally benign, mild, and catalyst-free reaction of quinones with heterocyclic ketene aminals in ethanol: site-selective synthesis of rarely fused [1,2-a]indolone derivatives via an unexpected anti-Nenitzescu strategy. <i>Green Chemistry</i> , 2014, 16, 4359-4370.	4.6	50
213	Halogen bonding interaction of chloromethane with several nitrogen donating molecules: addressing the nature of the chlorine surface π -hole. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19573-19589.	1.3	38
214	Crystal Packing of Impact-Sensitive High-Energy Explosives. <i>Crystal Growth and Design</i> , 2014, 14, 6101-6114.	1.4	161
215	The enhancing effects of group V π -hole interactions on the F \cdots O halogen bond. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19282-19289.	1.3	29
216	Photoluminescence properties of a novel cyclometalated iridium(III) complex with coumarin-boronate and its recognition of hydrogen peroxide. <i>Dalton Transactions</i> , 2014, 43, 5595.	1.6	27
217	Organoselenium(^{II}) halides containing the pincer 2,6-(Me ₂ NCH ₂) ₂ C ₆ H ₃ ligand – an experimental and theoretical investigation. <i>Dalton Transactions</i> , 2014, 43, 2221-2233.	1.6	15

#	ARTICLE	IF	CITATIONS
218	Binding energies and interaction origins between nonclassical single-electron hydrogen, sodium and lithium bonds and neutral boron-containing radicals: a theoretical investigation. <i>Science Bulletin</i> , 2014, 59, 2597-2607.	1.7	1
219	Computational study on the mechanism of olefin epoxidation catalyzed by substituted binuclear peroxotungstates ([SeO ₄ WO(O ₂) ₂ MO(O ₂) ₂] ⁿ⁺) ₄ . <i>Chemical Physics Letters</i> , 2014, 567, 458-462.	1.0	4
220	Fragmentation of typical sulfonamide drugs via heterolytic bond cleavage and stepwise rearrangement. <i>RSC Advances</i> , 2014, 4, 48426-48432.	1.7	25
221	Trinuclear alkyl hydrido rare-earth complexes supported by amidopyridinato ligands: synthesis, structures, C-Si bond activation and catalytic activity in ethylene polymerization. <i>Dalton Transactions</i> , 2014, 43, 14450-14460.	1.6	12
222	A computational study on the complexation of Np(^v) with N,N,N',N'-tetramethyl-3-oxa-glutaramide (TMOGA) and its carboxylate analogs. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16536-16546.	1.3	12
223	Sc ₂ S@C ₆₈ : an obtuse di-scandium sulfide cluster trapped in a C _{2v} fullerene cage. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 15994-16002.	1.3	16
224	Theoretical challenges in understanding the inhibition mechanism of copper corrosion in acid media in the presence of three triazole derivatives. <i>RSC Advances</i> , 2014, 4, 41956-41967.	1.7	91
225	Exploring the nature of interactions among thiophene, thiophene sulfone, dibenzothiophene, dibenzothiophene sulfone and a pyridinium-based ionic liquid. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 10531.	1.3	14
226	Redox control of ferrocene-based complexes with systematically extended π -conjugated connectors: switchable and tailorable second order nonlinear optics. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4900.	1.3	69
227	Intramolecular OHO bonding in dibenzoylmethane: symmetry and spectral manifestations. <i>RSC Advances</i> , 2014, 4, 38517-38526.	1.7	15
228	Mechanistic understanding of domino cyclization between gem-dialkylthio vinylallenes and benzylamine towards economic synthesis: a computational study. <i>Green Chemistry</i> , 2014, 16, 2653.	4.6	27
229	Theoretical analysis of the intermolecular interactions in naphthalene diimide and pyrene complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24216-24222.	1.3	36
230	Theoretical and experimental studies of the interactions between Au ⁺ and nucleobases. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 2928.	1.3	15
231	An icosahedral Ta ₁₂ ²⁺ cluster with spherical aromaticity. <i>Dalton Transactions</i> , 2014, 43, 5574.	1.6	18
232	Interaction between phosphomolybdic anion and imidazolium cation in polyoxometalates-based ionic liquids: a quantum mechanics study. <i>Journal of Molecular Modeling</i> , 2014, 20, 2495.	0.8	12
233	Bent and planar structures of μ_2 -N ₂ dinuclear early transition metal complexes. <i>Dalton Transactions</i> , 2014, 43, 11658.	1.6	6
234	Theoretical insights into the absorption and emission properties of blue luminescent copper(I) complexes based on the pyrazolylpyridine ligands. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1685-1691.	1.0	4
235	Ru ^{II} -NO and Ru ^{II} -NO ₂ bonding linkage isomerism in cis-[Ru(NO)(NO)(bpy) ₂] ²⁺ complexes: a theoretical insight. <i>Dalton Transactions</i> , 2014, 43, 8792-8804.	1.6	19

#	ARTICLE	IF	CITATIONS
236	Understanding the stability, bonding nature and chemical reactivity of 3d-substituted heterofullerenes C ₅₈ TM (TM = Sc–Zn) from DFT studies. RSC Advances, 2014, 4, 44786-44794.	1.7	5
237	f-Orbital covalency in the actinocenes (An = Th–Cm): multiconfigurational studies and topological analysis. RSC Advances, 2014, 4, 12078-12086.	1.7	78
238	Molecular dynamics investigation of the effect of solvent adsorption on crystal habits of hexogen. Canadian Journal of Chemistry, 2014, 92, 849-854.	0.6	21
239	Water O–H Bond Activation by Gas-Phase Plutonium Atoms: Reaction Mechanisms and Ab Initio Molecular Dynamics Study. ChemPhysChem, 2014, 15, 3078-3088.	1.0	16
240	Density functional theory study of neutral and singly-charged (NaBH ₄) _n (n=1–6) nanoclusters. Chemical Physics, 2014, 443, 45-52.	0.9	11
241	An anatomy of intramolecular atomic interactions in halogen-substituted trinitromethanes. Physical Chemistry Chemical Physics, 2014, 16, 16780-16789.	1.3	20
242	Theoretical studies on organic D–A sensitizers with planar triphenylamine donor and different –linkers for dyes-sensitized solar cells. Journal of Molecular Modeling, 2014, 20, 2309.	0.8	17
243	Molecular Structure, Infrared Spectra, Photochemistry, and Thermal Properties of 1-Methylhydantoin. Journal of Physical Chemistry A, 2014, 118, 5994-6008.	1.1	13
244	Theoretical study of solvent effects on RDX crystal quality and sensitivity using an implicit solvation model. Journal of Molecular Modeling, 2014, 20, 2326.	0.8	7
245	Indole alkaloids from cultivated Vinca major. Tetrahedron, 2014, 70, 8723-8729.	1.0	23
246	Computational Study on the Interaction of Modified Nucleobases with Graphene and Doped Graphenes. Journal of Physical Chemistry C, 2014, 118, 16165-16174.	1.5	54
247	Li-coated B ₃₆ N ₂₄ as potential hydrogen storage material. Computational and Theoretical Chemistry, 2014, 1047, 30-37.	1.1	5
248	Theoretical Investigation on Multiple Bonds in Terminal Actinide Nitride Complexes. Inorganic Chemistry, 2014, 53, 9607-9614.	1.9	73
249	Impact of Redox Stimuli on Ferrocene–Buckybowl Complexes: Switchable Optoelectronic and Nonlinear Optical Properties. Organometallics, 2014, 33, 3341-3352.	1.1	46
250	Redox Properties of Graphenes Functionalized with Cyclopentadiene–Transition Metal Complexes: A Potential Redox-Active Material. Journal of Physical Chemistry C, 2014, 118, 24633-24640.	1.5	8
251	Dissociation of H ₂ on carbon doped aluminum cluster Al ₆ C. Journal of Chemical Physics, 2014, 141, 064302.	1.2	21
252	Multilithiation Effect on the First Hyperpolarizability of Carbon–Boron–Nitride Heteronanotubes: Activating Segment versus Connecting Pattern. Journal of Physical Chemistry C, 2014, 118, 14185-14191.	1.5	33
253	Site-Selective Dissociation Processes of Cationic Ethanol Conformers: The Role of Hyperconjugation. Journal of Physical Chemistry A, 2014, 118, 7096-7103.	1.1	0

#	ARTICLE	IF	CITATIONS
254	Experimental and computational investigation of intermolecular interactions in cyclopentanone with methanol mixture. <i>Chemical Physics Letters</i> , 2014, 612, 223-228.	1.2	5
255	Two-level hierarchical entangled framework in a novel copper(I) coordination polymer with multiform helical features and unprecedented self-penetrated subnet. <i>Inorganica Chimica Acta</i> , 2014, 423, 133-138.	1.2	6
256	Structures and Electronic Properties of Transition Metal-Containing Ionic Liquids: Insights from Ion Pairs. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2508-2518.	1.1	14
257	Highly Diastereoselective Convergent Synthesis of Polycyclic Pyrroles with Consecutive Quaternary Stereocenters: Cascade Construction of Multiple C-C and C-Hetero Bonds. <i>ACS Sustainable Chemistry and Engineering</i> , 2014, 2, 2391-2398.	3.2	25
258	Cooperativity between the halogen bonding and halogen-hydride bonding in $\text{NCX}^{\delta-}\text{NCX}^{\delta-}\text{HMgY}$ complexes (X=F, Cl, Br; Y=H, F, Cl, Br, CH ₃ , Li). <i>Computational and Theoretical Chemistry</i> , 2014, 1048, 77-83.	1.1	9
259	In Quest of Strong Be-Ng Bonds among the Neutral Ng-Be Complexes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 487-494.	1.1	68
260	Identification of the transition state for fast reactions: The trapping of hydroxyl and methyl radicals by DMPO-A DFT approach. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 52, 57-70.	1.3	8
261	Competing hydrogen bonding and halogen bonding interactions in crystal engineering: A case study of bi-functional donor molecules. <i>Chemical Physics</i> , 2014, 441, 30-37.	0.9	15
262	Influence of a Bridging Group and the Substitution Effect of Bis(1,2,4-triazine) N-Donor Extractants on Their Interactions with a Np^{IV} Cation. <i>Inorganic Chemistry</i> , 2014, 53, 7848-7860.	1.9	18
263	Stability of Noble Gas-Bound $\text{SiH}_3^+ \text{Clusters}$. <i>ChemPhysChem</i> , 2014, 15, 3554-3564.	1.0	36
264	Beyond the molecular orbital conception of electronically excited states through the quantum theory of atoms in molecules. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9249-9258.	1.3	36
265	A computational study of pyrazinamide: Tautomerism, acid-base properties, micro-solvation effects and acid hydrolysis mechanism. <i>Computational and Theoretical Chemistry</i> , 2014, 1046, 30-41.	1.1	30
266	Convergent study of Ru-ligand interactions through QTAIM, ELF, NBO molecular descriptors and TDDFT analysis of organometallic dyes. <i>Molecular Physics</i> , 2014, 112, 2063-2077.	0.8	9
267	Photoactivated cytotoxicity of ferrocenyl-terpyridine oxovanadium(IV) complexes of curcuminoids. <i>European Journal of Medicinal Chemistry</i> , 2014, 85, 458-467.	2.6	49
268	Assignment of aromaticity of the classic heterobenzenes by three aromatic criteria. <i>Computational and Theoretical Chemistry</i> , 2014, 1046, 20-24.	1.1	12
269	Low Energy Conformations and Gas-Phase Acidity and Basicity of Pyrrolysine. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7085-7095.	1.1	3
270	Confinement induced binding of noble gas atoms. <i>Journal of Chemical Physics</i> , 2014, 140, 164306.	1.2	61
271	Activation of Pt-O and Pt-H bonds: DFT studies on adsorption of $[\text{Cd}(\text{H}_2\text{O})_n]^{3+}$ ($n=8-9$) with Pt_n ($n=3-7$) cluster. <i>Computational and Theoretical Chemistry</i> , 2014, 1047, 47-54.	1.1	3

#	ARTICLE	IF	CITATIONS
272	On the opto-electronic properties of phosphine and thiolate-protected undecagold nanoclusters. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18749-18758.	1.3	19
273	Halogen bonds between I ₂ and ion pairs: Interpreting the ability of ionic liquids in efficient capture of radioactive iodine. <i>Computational and Theoretical Chemistry</i> , 2014, 1049, 97-101.	1.1	11
274	Design of D-π-A organic dyes with different acceptor and auxiliary acceptor for highly efficient dye-sensitized solar cells: a computational study. <i>RSC Advances</i> , 2014, 4, 50338-50350.	1.7	43
275	B ₃₈ : an all-boron fullerene analogue. <i>Nanoscale</i> , 2014, 6, 11692-11696.	2.8	153
276	Electronic Structure of Gold Carbonyl Compounds RAuL (R = CF ₃ , BO, Br, Cl,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 592 Td Interactions in the Clusters [RAuL] _n (n = 2-4): A Theoretical Study. <i>Organometallics</i> , 2014, 33, 5101-5110.	1.1	13
277	Coordination of Halide and Chalcogenolate Anions to Heavier 1,2,5-Chalcogenadiazoles: Experiment and Theory. <i>Organometallics</i> , 2014, 33, 4302-4314.	1.1	60
278	Obtaining highly efficient single-emissive-layer orange and two-element white organic light-emitting diodes by the solution process. <i>Journal of Materials Chemistry C</i> , 2014, 2, 5036.	2.7	21
279	Novel Recipe for Double-Hybrid Density Functional Computations of Linear and Nonlinear Polarizabilities of Molecules and Nanoclusters. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5333-5342.	1.1	20
280	Gas Phase Conformations of Selenocysteine and Related Ions: A Comprehensive Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1684-1696.	1.1	7
281	Structural, Energetic, and UV-Vis Spectral Analysis of UVA Filter 4-tert-Butyl-4-methoxydibenzoylmethane. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1511-1518.	1.1	26
282	Adsorption of HCN on reduced graphene oxides: a first-principles study. <i>Journal of Molecular Modeling</i> , 2014, 20, 2214.	0.8	25
283	Reaction of chlorine radical with tetrahydrofuran: a theoretical investigation on mechanism and reactivity in gas phase. <i>Journal of Molecular Modeling</i> , 2014, 20, 2262.	0.8	5
284	Ionothermal synthesis and crystal structure of a luminescent bipyridine bridged Zn(II) complex. <i>Journal of Molecular Structure</i> , 2014, 1060, 75-79.	1.8	3
285	Rational design and characterization of high-efficiency planar π-A type electron donors in small molecule organic solar cells: A quantum chemical approach. <i>Materials Chemistry and Physics</i> , 2014, 145, 387-396.	2.0	37
286	Electronegativity estimator built on QTAIM-based domains of the bond electron density. <i>Journal of Computational Chemistry</i> , 2014, 35, 978-985.	1.5	9
287	C- and N-Coupled Dimers of 2-Aminotetraphenylporphyrins: Regiocontrolled Synthesis, Spectroscopic Properties, and Quantum-Chemical Calculations. <i>Chemistry - A European Journal</i> , 2014, 20, 3998-4006.	1.7	26
288	Theoretical insights into the host-guest interactions between [6]cycloparaphenyleneacetylene and its anthracene-containing derivative and fullerene C ₇₀ . <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 772-782.	0.9	36
289	Photoexcitation of Light-Harvesting C ₆₀ Triads: A FLMO-TD-DFT Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2436-2448.	2.3	30

#	ARTICLE	IF	CITATIONS
308	Characterizing the multiple non-covalent interactions in N, S-heterocyclesâ€“diiodine complexes with focus on halogen bonding. <i>Computational and Theoretical Chemistry</i> , 2014, 1037, 53-62.	1.1	38
309	Investigating Dechlorane Plus (DP) distribution and isomer specific adsorption behavior in size fractionated marine sediments. <i>Science of the Total Environment</i> , 2014, 481, 114-120.	3.9	30
310	Complexes between hypohalous acids and phosphine derivatives. Pnicogen bond versus halogen bond versus hydrogen bond. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 271-277.	2.0	33
311	The comparison of cationâ€“anion interactions of phosphonium- and ammonium-based ionic liquids â€“ A theoretical investigation. <i>Chemical Physics Letters</i> , 2014, 597, 114-120.	1.2	11
312	DFT investigation of the influence of Jahnâ€“Teller distortion on the aromaticity in square-planar arsenic and antimony clusters. <i>Polyhedron</i> , 2014, 80, 69-80.	1.0	5
313	Density functional theory design and characterization of Dâ€“A type electron donors with narrow band gap for small-molecule organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2014, 1029, 68-78.	1.1	32
314	Mechanism of Mo-catalyzed Câ€“S cleavage of thiophene. <i>Journal of Organometallic Chemistry</i> , 2014, 749, 275-286.	0.8	5
315	Structures and standard molar enthalpies of formation of a series of Ln(III)â€“Cu(II) heteronuclear compounds with pyrazine-2,3-dicarboxylic acid. <i>Journal of Solid State Chemistry</i> , 2014, 215, 26-33.	1.4	15
316	The Nâ€“1 halogen bond in substituted pyridines as viewed by the source function and delocalization indices. <i>Chemical Physics Letters</i> , 2014, 601, 144-148.	1.2	29
317	Understanding Lanthanoid(III) Hydration Structure and Kinetics by Insights from Energies and Wave functions. <i>Inorganic Chemistry</i> , 2014, 53, 7700-7708.	1.9	82
318	A σ -hole interaction with radical species as electron donors: does single-electron tetrel bonding exist?. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 11617-11625.	1.3	113
319	The structure and properties of a sheathed, low reactivity silicon phthalocyanine and the potential for still more inert phthalocyanines. <i>Journal of Porphyrins and Phthalocyanines</i> , 2014, 18, 336-345.	0.4	1
320	Insight into the interaction between DNA bases and defective graphenes: Covalent or non-covalent. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 47, 8-17.	1.3	42
321	Modulation on charge recombination and light harvesting toward high-performance benzothiadiazole-based sensitizers in dye-sensitized solar cells: A theoretical investigation. <i>Journal of Power Sources</i> , 2014, 267, 300-308.	4.0	65
322	Electron density analysis of 1-butyl-3-methylimidazolium chloride ionic liquid. <i>Journal of Molecular Modeling</i> , 2014, 20, 2175.	0.8	31
323	Catalytic C6 Functionalization of 2,3-Disubstituted Indoles by Scandium Triflate. <i>Journal of Organic Chemistry</i> , 2014, 79, 1047-1054.	1.7	71
324	Is there an attractive interaction between two methyl groups?. <i>Chemical Physics Letters</i> , 2014, 608, 90-94.	1.2	7
325	Synthesis, X-ray investigation and DFT calculations of solvated barium \hat{I}^2 -diketonate complexes with 18-dibenzocrown-6: [Ba(pta) ₂ (18DBC6)](C ₆ H ₅ CH ₃) ₂ and [Ba(pta) ₂ (18DBC6)](CH ₂ Cl ₂) (pta=1,1,1-trifluoro-5,5-dimethylhexanedionato-2,4; 18DBC6=18-dibenzocrown-6). <i>Polyhedron</i> , 2014, 79, 229-238.	1.0	2

#	ARTICLE	IF	CITATIONS
326	Investigation of the reactions of U, U ⁺ and U ²⁺ with ammonia: mechanisms and topological analysis. RSC Advances, 2014, 4, 29806.	1.7	20
327	Isolation and reversible dimerization of a selenium ⁺ selenium three-electron σ -bond. Nature Communications, 2014, 5, 4127.	5.8	57
328	Planar tetracoordinate Si and Ge in π -aromatic (X=Si, Ge) cations. Computational and Theoretical Chemistry, 2014, 1032, 7-11.	1.1	17
329	Nortriterpenoids from Schisandra chinensis and their absolute configurational assignments by electronic circular dichroism study. Tetrahedron, 2014, 70, 859-868.	1.0	34
330	Dicarbazolyldicyanobenzenes as Thermally Activated Delayed Fluorescence Emitters: Effect of Substitution Position on Photoluminescent and Electroluminescent Properties. Chemistry Letters, 2014, 43, 319-321.	0.7	58
331	Chalcogen ⁺ Chalcogen Interactions in Furan-YHX and Thiophene-YHX Complexes (X = F, Cl, Br; Y = S, Se): An Ab Initio Study. Bulletin of the Chemical Society of Japan, 2015, 88, 1683-1692.	2.0	5
332	Vibronic coupling in molecular crystals: A Franck-Condon Herzberg-Teller model of H-aggregate fluorescence based on quantum chemical cluster calculations. Journal of Chemical Physics, 2015, 143, 114116.	1.2	36
333	Complexes of the Noble Gases with H ₃ O ⁺ : A Theoretical Investigation of Ng(H ₃ O ⁺) (Ng = He ⁺ –Xe).	0.5	7
334	Noncomparative scaling of aromaticity through electron itinerancy. AIP Advances, 2015, 5, 107211.	0.6	9
335	Theoretical study of hydrogen adsorption on Ca-decorated C ₄₈ B ₁₂ clusters. AIP Advances, 2015, 5, .	0.6	8
336	On the properties and atmospheric implication of amine-hydrated clusters. RSC Advances, 2015, 5, 91500-91515.	1.7	14
337	Electronic Structure Insights into the Solvation of Magnesium Ions with Cyclic and Acyclic Carbonates. ChemPhysChem, 2015, 16, 3607-3617.	1.0	15
338	Multiple weak interaction ⁺ assisted SERS detection platform for triadimefon. Journal of Raman Spectroscopy, 2015, 46, 54-58.	1.2	8
339	Quantum chemical calculation study on terphenyl arylamines hole transport materials. Journal of the Society for Information Display, 2015, 23, 182-185.	0.8	2
340	Creating σ -Holes through the Formation of Beryllium Bonds. Chemistry - A European Journal, 2015, 21, 12676-12682.	1.7	38
341	The Structure and Optical Properties of the [Au ₁₈ (SR) ₁₄] Nanocluster. Angewandte Chemie, 2015, 127, 3188-3192.	1.6	43
343	A Family of Ir ^{III} Complexes with High Nonlinear Optical Response and Their Potential Use in Light-Emitting Devices. European Journal of Inorganic Chemistry, 2015, 2015, 4946-4955.	1.0	19
344	Is Aerogen ⁺ Interaction Capable of Initiating the Noncovalent Chemistry of Group 18?. Chemistry - an Asian Journal, 2015, 10, 2615-2618.	1.7	27

#	ARTICLE	IF	CITATIONS
345	The Clar Structure in Inorganic BN Analogues of Polybenzenoid Hydrocarbons: Does it Exist or Not?. ChemPhysChem, 2015, 16, 3806-3813.	1.0	16
346	A deeper insight into strain for the sila[6]prismane () cluster with its endohedrally trapped silicon atom,. Journal of Computational Chemistry, 2015, 36, 2089-2094.	1.5	8
347	Theoretical Study of Electronic Structures and Charge Transport Properties of 9,10-Bis((<i>E</i> -2-(pyridin-2-yl) vinyl) (<i>n</i> =2,3,4) Anthracene. Chinese Journal of Chemistry, 2015, 33, 974-980.		1
348	Three-dimensional networks containing rectangular Sr ₄ and Ba ₄ units: Synthesis, structure, bonding, and potential application for Ne gas separation. International Journal of Quantum Chemistry, 2015, 115, 1501-1510.	1.0	6
349	1,3-Butadienyl Dianions as Non-Innocent Ligands: Synthesis and Characterization of Aromatic Dilithio Rhodacycles. Angewandte Chemie - International Edition, 2015, 54, 9986-9990.	7.2	49
350	Hexahalogenated and their mixed benzene derivatives as prototypes for the understanding of halogen-halogen intramolecular interactions: New insights from combined DFT, QTAIM, and RDG-based NCI analyses. Journal of Computational Chemistry, 2015, 36, 2328-2343.	1.5	20
352	Unusual H-Bond Topology and Bifurcated H-bonds in the 2-Fluoroethanol Trimer. Angewandte Chemie - International Edition, 2015, 54, 11711-11715.	7.2	37
353	Multiple Cycloaddition Reactions of Ketones with a δ -ketoiminato Al Compound. Chemistry - A European Journal, 2015, 21, 19041-19047.	1.7	7
354	Synergy between Palladium and Potassium Species for Efficient Activation of Carbon Monoxide in the Synthesis of Dimethyl Carbonate. ChemCatChem, 2015, 7, 2460-2466.	1.8	15
355	Tuning anion- π interaction via halogen substituent effects in cyanuric acids and its derivatives. International Journal of Quantum Chemistry, 2015, 115, 1147-1152.	1.0	3
356	Theoretical Study on Inverse Sandwich Complexes [E-C ₅ H ₅ N-E] ⁺ and [E-C ₅ H ₅ P-E] ⁺ (<i>n</i> =1, 2, 3; E=Al, Ga, In, Tl). Chinese Journal of Chemical Physics, 2015, 28, 703-710.	0.6	2
357	X-ray Crystallography, DFT Calculations and Molecular Docking of Indole-Arylpiperazine Derivatives as \pm 1A-Adrenoceptor Antagonists. Molecules, 2015, 20, 19674-19689.	1.7	7
358	Theoretical Investigation on the Geometrical and Electronic Structures of Gallium Aurides: Ga_0 . Journal of Nanomaterials, 2015, 2015, 1-10.		
359	Spectroscopic Aspects, Structural Elucidation, Vibrational and Electronic Investigations of 2-Methoxy-1,3-Dioxolane: An Interpretation Based on DFT and QTAIM Approach. Journal of Theoretical and Computational Science, 2015, 02, .	0.1	0
360	Adsorption, Thermodynamic and Quantum Chemical Studies of 1-hexyl-3-methylimidazolium Based Ionic Liquids as Corrosion Inhibitors for Mild Steel in HCl. Materials, 2015, 8, 3607-3632.	1.3	92
361	Strong or weak acid, which is more efficient for Beckmann rearrangement reaction over solid acid catalysts?. Catalysis Science and Technology, 2015, 5, 3675-3681.	2.1	32
362	On the properties of Au ₂ P ₃ (z = 1, 0, +1): analysis of geometry, interaction, and electron density. RSC Advances, 2015, 5, 26071-26080.	1.7	5
363	From Stiba- and Bismaheteroboroxines to N,C,N-Chelated Diorganoantimony(III) and Bismuth(III) Cations—An Unexpected Case of Aryl Group Migration. Inorganic Chemistry, 2015, 54, 6010-6019.	1.9	20

#	ARTICLE	IF	CITATIONS
364	Origin of the Regioselective Reduction of Chlorins. <i>Journal of Organic Chemistry</i> , 2015, 80, 4861-4868.	1.7	26
365	Comparative Study on the Noble-Gas Binding Ability of BeX Clusters (X = SO ₄), Tj ETQq1 1 0.784314 191 /Overlock 10 47	1.1	42
366	A Preorganized Ditopic Borane as Highly Efficient One- or Two-Electron Trap. <i>Journal of the American Chemical Society</i> , 2015, 137, 3705-3714.	6.6	90
367	Influence of borate structure on the thermal stability of boron-containing phenolic resins: A DFT study. <i>Polymer Degradation and Stability</i> , 2015, 119, 190-197.	2.7	24
368	Nitroaminofurazans with Azo and Azoxy Linkages: A Comparative Study of Structural, Electronic, Physicochemical, and Energetic Properties. <i>Journal of Physical Chemistry C</i> , 2015, 119, 12887-12895.	1.5	104
369	Bonding Motifs of Noble-Gas Compounds As Described by the Local Electron Energy Density. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6528-6541.	1.1	42
370	A combined molecular dynamic and quantum mechanic study of the solvent and guest molecule effect on the stability and length of heterocyclic peptide nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11382-11391.	1.3	29
371	A theoretical study on mitigation of CO ₂ through advanced deep eutectic solvents. <i>International Journal of Greenhouse Gas Control</i> , 2015, 39, 62-73.	2.3	55
372	Sequential metalation of benzene: electronic, bonding, magnetotropic and spectroscopic properties of coinage metalated benzenes studied by DFT. <i>Journal of Molecular Modeling</i> , 2015, 21, 153.	0.8	6
373	Azine or hydrazone? The dilemma in amidinohydrazones. <i>RSC Advances</i> , 2015, 5, 55938-55947.	1.7	27
374	Atomic Zero Steric Potential and the Regioselectivity of Reactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6468-6474.	1.1	5
375	A New Class of Nitroanilinic Dimer, the PNA "Dimer: Electronic Structure and Emission Characteristics of "Dimeric Aggregates. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8388-8399.	1.1	13
376	The interception of a copper-based carbene radical with an $\hat{\pm}$ -carbonyl diazomethane radical: C1/C1N2 copolymerization. <i>Chemical Communications</i> , 2015, 51, 11964-11967.	2.2	24
377	Acidic rearrangement of benzyl group in flavone benzyl ethers and its regioselectivity. <i>Chinese Chemical Letters</i> , 2015, 26, 793-796.	4.8	3
378	Theoretical insight into the co-crystal explosive of 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (CL-20)/1,1-diamino-2,2-dinitroethylene (FOX-7). <i>Computational Materials Science</i> , 2015, 107, 33-41.	1.4	46
379	Solubility prediction of bio-oil derived chemicals in aqueous media by Localized Molecular Orbital-Energy Decomposition Analysis (LMO-EDA) and COSMO-RS predictions. <i>Computational and Theoretical Chemistry</i> , 2015, 1067, 48-59.	1.1	3
380	Influence of F and Se substitution on the structures, stabilities and nature of the complexes between F ₂ CSe and HOX (X = F, Cl, Br, and I). <i>RSC Advances</i> , 2015, 5, 52667-52675.	1.7	7
381	A theoretical investigation on the metal-metal interaction in a series of pyrazolate bridged platinum(II) complexes. <i>Synthetic Metals</i> , 2015, 205, 222-227.	2.1	12

#	ARTICLE	IF	CITATIONS
382	A quantum mechanics-based halogen bonding scoring function for protein-ligand interactions. <i>Journal of Molecular Modeling</i> , 2015, 21, 138.	0.8	22
383	A comprehensive analysis of P ⁺ -pnictogen bonds: substitution effects and comparison with Br ⁺ -halogen bonds. <i>Journal of Molecular Modeling</i> , 2015, 21, 143.	0.8	24
384	Dual functions of Lewis acid and base of Se in F ₂ C=Se and their interplay in F ₂ CSe ⁺ ⋯NH ₃ ⁺ ⋯CHX. <i>Journal of Molecular Modeling</i> , 2015, 21, 157.	0.8	4
385	A comparison of excited state properties between two different N-heterocyclic platinum(II) complexes. <i>Journal of Molecular Structure</i> , 2015, 1097, 23-28.	1.8	3
386	Structure and dynamics of H ₂ O vis-à-vis phenylalanine recognition at a DPPC lipid membrane via interfacial H-bond types: Insights from polarized FT-IRRAS and ADMP simulations. <i>Journal of Chemical Physics</i> , 2015, 142, 024702.	1.2	7
387	The impact of molecular stacking interactions on the electronic structure and charge transport properties in distyrylbenzene (DSB-) based D ⁺ A complexes: a theoretical study. <i>RSC Advances</i> , 2015, 5, 47681-47691.	1.7	14
388	Toward the Prediction of Water Exchange Rates in Magnetic Resonance Imaging Contrast Agents: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6436-6445.	1.1	54
389	Cooperativity in bimetallic glutathione complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 62, 1-10.	1.3	5
390	Experimental and theoretical studies of highly emissive dinuclear Cu(ⁱ) halide complexes with delayed fluorescence. <i>Dalton Transactions</i> , 2015, 44, 11649-11659.	1.6	51
391	Cucurbit[6]uril: A Possible Host for Noble Gas Atoms. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10962-10974.	1.2	50
392	Theoretical studies on the stability of the salts formed by DTDO with HNO ₃ and HN(NO ₂) ₂ . <i>Journal of Chemical Sciences</i> , 2015, 127, 761-769.	0.7	1
393	Adsorption of choline benzoate ionic liquid on graphene, silicene, germanene and boron-nitride nanosheets: a DFT perspective. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16315-16326.	1.3	39
394	Theoretical study of stabilities, electronic, and catalytic performance of supported platinum on modified graphene. <i>Molecular Physics</i> , 2015, 113, 3514-3523.	0.8	3
395	Non-covalent interactions in ionic liquid ion pairs and ion pair dimers: a quantum chemical calculation analysis. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16846-16857.	1.3	59
396	Dependence of the structure of alkali metal ⁺ -trifluoride ion pairs F ₃ ⁻ M ⁺ on the counterion M ⁺ (M = Tl, Et, Cs, Rb, K, Ag, Na, Li). <i>Journal of Physical Chemistry A</i> , 2015, 119, 12706-12714.	0.6	0
398	How mutations affecting the ligand-receptor interactions: a combined MD and QM/MM calculation on CYP2E1 and its two mutants. <i>Chemical Research in Chinese Universities</i> , 2015, 31, 1029-1038.	1.3	6
399	Time-Dependent Density Functional Theory Study of Low-Lying Absorption and Fluorescence Band Shapes for Phenylene-Containing Oligoacenes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12706-12714.	1.1	8
400	Noble Gas Inserted Protonated Silicon Monoxide Cations: HNgOSi ⁺ (Ng = He, Ne, Ar, Kr.) <i>Journal of Physical Chemistry A</i> , 2015, 119, 10784-10791.	1.1	14

#	ARTICLE	IF	CITATIONS
401	Development of asymmetrical near infrared squaraines with large Stokes shift. RSC Advances, 2015, 5, 106868-106876.	1.7	15
402	The effects of extended conjugation length of purely organic phosphors on their phosphorescence emission properties. Physical Chemistry Chemical Physics, 2015, 17, 19096-19103.	1.3	17
403	Polymethylbenzene or Alkene Cycle? Theoretical Study on Their Contribution to the Process of Methanol to Olefins over H-ZSM-5 Zeolite. Journal of Physical Chemistry C, 2015, 119, 28482-28498.	1.5	105
404	Selectively Probing the Structures and Dynamics of β^2 -Peptide Aggregates Using the Amide-A Vibrational Marker. Journal of Physical Chemistry B, 2015, 119, 15451-15459.	1.2	6
405	Theoretical investigation on the nitrogen-rich energetic compound 5-nitro-2-nitratomethyl-1,2,3,4-tetrazole. Journal of Structural Chemistry, 2015, 56, 836-844.	0.3	1
406	A density functional study of small sized silver-doped silicon clusters: Ag ₂ Si _n (n = 1-13). European Physical Journal D, 2015, 69, 1.	0.6	5
407	Molecular-Level Investigation of the Adsorption Mechanisms of Toluene and Aniline on Natural and Organically Modified Montmorillonite. Journal of Physical Chemistry A, 2015, 119, 11199-11207.	1.1	20
408	Understanding the Amide-II Vibrations in β^2 -Peptides. Journal of Physical Chemistry B, 2015, 119, 14831-14839.	1.2	28
409	Exploring the Role of Substitution on the Formation of Se \cdots O/N Noncovalent Bonds. Journal of Physical Chemistry B, 2015, 119, 14857-14870.	1.2	25
410	Synthesis and Redox Properties of Thiophene Terephthalate Building Blocks for Low-Potential Conducting Redox Polymers. Journal of Physical Chemistry C, 2015, 119, 27247-27254.	1.5	11
411	Computational Study on the Intramolecular Charge Separation of D-A- π -A Organic Sensitizers with Different Linker Groups. Journal of Physical Chemistry C, 2015, 119, 26355-26361.	1.5	12
412	Theoretical Study of Xanthenone and Phenothiazine Derivatives for Blue TADF Emitter. Molecular Crystals and Liquid Crystals, 2015, 620, 166-170.	0.4	4
413	A theoretical investigation into the strength of N \cdots NO ₂ bonds, ring strain and electrostatic potential upon formation of intermolecular H-bonds between HF and the nitro group in nitrogen heterocyclic rings C _n H _{2n} N \cdots NO ₂ (n = 5), RDX and HMX. Journal of Molecular Modeling, 2015, 21, 302.	0.8	4
414	A topological assessment of the electronic structure of mesoionic compounds. Journal of Computational Chemistry, 2015, 36, 1907-1918.	1.5	4
415	Molecular design and screening of energetic nitramine derivatives. Journal of Molecular Modeling, 2015, 21, 298.	0.8	10
416	Labile Capping Bonds in Lanthanide(III) Complexes: Shorter and Weaker. Journal of Physical Chemistry A, 2015, 119, 774-780.	1.1	17
417	Chemistry of Diruthenium and Dirhodium Analogues of Pentaborane(9): Synthesis and Characterization of Metal N \cdots Heterocyclic Carbene and π -Agostic Complexes. Chemistry - A European Journal, 2015, 21, 3640-3648.	1.7	46
418	Thermally accessible triplet state of π -nucleophiles does exist. Evidence from first principles study of ethylene interaction with copper species. RSC Advances, 2015, 5, 11558-11569.	1.7	19

#	ARTICLE	IF	CITATIONS
419	Confinement induced binding in noble gas atoms within a BN-doped carbon nanotube. <i>Chemical Physics Letters</i> , 2015, 621, 29-34.	1.2	33
420	Controlling singlet-triplet splitting in carbazole-oxadiazole based bipolar phosphorescent host materials. <i>Organic Electronics</i> , 2015, 17, 216-228.	1.4	14
421	Lignans and aromatic glycosides from <i>Piper wallichii</i> and their antithrombotic activities. <i>Journal of Ethnopharmacology</i> , 2015, 162, 87-96.	2.0	36
422	Enhancing the copper(II) complexes cytotoxicity to cancer cells through bound to human serum albumin. <i>Journal of Inorganic Biochemistry</i> , 2015, 144, 47-55.	1.5	52
423	The multieffects of DMF and DBU on the [5+1] benzannulation of nitroethane and alkene ketene acetals: Hydrogen bonding and electrostatic interactions. <i>Journal of Computational Chemistry</i> , 2015, 36, 731-738.	1.5	6
424	Enthalpy of formation of CL-20. <i>Computational and Theoretical Chemistry</i> , 2015, 1057, 54-59.	1.1	22
425	The spectroscopic and quantum chemical studies of 3,4-difluoroaniline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 143, 265-280.	2.0	10
426	Photocytotoxic oxovanadium(IV) complexes of ferrocenyl-terpyridine and acetylacetonate derivatives. <i>European Journal of Medicinal Chemistry</i> , 2015, 92, 332-341.	2.6	21
427	Fluorines in tetrafluoromethane as halogen bond donors: Revisiting address the nature of the fluorine's hole. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 453-470.	1.0	44
428	Three centered hydrogen bonds of the type C=O...H(N)...C in diphenyloxamide derivatives involving halogens and a rotating CF ₃ group: NMR, QTAIM, NCI and NBO studies. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7528-7536.	1.3	16
429	A series of novel sandwich complexes: MQ(μ ₄ -E ₄) ₂ (M=Be or Mg; Q=C or Si; E=P, As, Sb or Bi) with donor-acceptor bonds. <i>Computational and Theoretical Chemistry</i> , 2015, 1058, 41-49.	1.1	1
430	Heparin makes differences: a molecular dynamics simulation study on the human ¹²⁵ I-tryptase monomer. <i>Molecular BioSystems</i> , 2015, 11, 252-261.	2.9	17
431	Computational studies on the radiative and nonradiative processes of luminescent N-heteroleptic platinum(II) complexes. <i>Organic Electronics</i> , 2015, 19, 7-14.	1.4	7
432	Influence of the metal salt on the self-assembly of isophthaloylbis- ¹² -alanine and Cu(II) ion. <i>Polyhedron</i> , 2015, 89, 313-321.	1.0	3
433	Mechanism of boron uptake by hydrocalumite calcined at different temperatures. <i>Journal of Hazardous Materials</i> , 2015, 287, 268-277.	6.5	35
434	Chemical bonding analysis in boron clusters by means of localized orbitals according to the electron localization function topology. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	15
435	Halogen Bonded Three-Dimensional Uranyl-Organic Compounds with Unprecedented Halogen-Halogen Interactions and Structure Diversity upon Variation of Halogen Substitution. <i>Crystal Growth and Design</i> , 2015, 15, 1395-1406.	1.4	36
436	Theoretical investigation on the mechanism and dynamics of oxo exchange of neptunyl(^{vi}) hydroxide in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7537-7547.	1.3	2

#	ARTICLE	IF	CITATIONS
437	Mechanism of Samarium-Catalyzed 1,5-Regioselective Azide-Alkyne [3 + 2]-Cycloaddition: A Quantum Mechanical Investigation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1359-1368.	1.1	14
438	Dispersion Makes the Difference: Bisligated Transition States Found for the Oxidative Addition of Pd(<i>P</i> t <i>Bu</i> ₃) ₂ to Ar-OSO ₂ R and Dispersion-Controlled Chemoselectivity in Reactions with Pd[P(<i>i</i> Pr)(<i>t</i> Bu) ₂] ₂ . <i>Organometallics</i> , 2015, 34, 805-812.	1.1	106
439	Nature of Noncovalent Interactions in the [n]Cycloparaphenylene- <i>f</i> C ₇₀ (n =) Tj ETQqO O rgBT /Overlock Nanotube Peapod. <i>Journal of Physical Chemistry C</i> , 2015, 119, 5168-5179.	1.5	42
440	Novel Neutral Zirconaborane [(Cp ₂ Zr)2B ₅ H ₁₁]: An arachno-B ₃ H ₉ Analogue (Cp = $\hat{1}$ -5-C ₅ H ₅). <i>Organometallics</i> , 2015, 34, 908-912.	1.1	16
441	First-Row Transition-Metal-Diborane and -Borylene Complexes. <i>Chemistry - A European Journal</i> , 2015, 21, 5074-5083.	1.7	50
442	Anisotropic charge transport in flavonoids as organic semiconductors. <i>Molecular Physics</i> , 2015, 113, 521-528.	0.8	3
443	Theoretical study of the stabilities and detonation performance of 5-nitro-3-trinitromethyl-1H-1,2,4-triazole and its derivatives. <i>Journal of Molecular Modeling</i> , 2015, 21, 26.	0.8	5
444	RAHB concept and π -skeleton in some oximes of 3-hydroxy fulvene; DFT, AIM, ELF and NBO studies. <i>Structural Chemistry</i> , 2015, 26, 1039-1048.	1.0	16
445	Synthesis, X-ray diffraction, and density functional studies of tin(IV) compounds containing a pincer-type SNS ligand. <i>Structural Chemistry</i> , 2015, 26, 189-198.	1.0	3
446	s-Block metallabenzene: aromaticity and hydrogen adsorption. <i>Journal of Molecular Modeling</i> , 2015, 21, 28.	0.8	3
447	The Structure and Optical Properties of the [Au ₁₈ (SR) ₁₄] Nanocluster. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 3145-3149.	7.2	205
448	Terminal U π E (E = N, P, As, Sb, and Bi) Bonds in Uranium Complexes: A Theoretical Perspective. <i>Journal of Physical Chemistry A</i> , 2015, 119, 922-930.	1.1	38
449	Encapsulation of an f-block metal atom/ion to enhance the stability of C ₂₀ with the <i>h</i> -symmetry. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4328-4336.	1.3	12
450	Modeling of catalytically active metal complex species and intermediates in reactions of organic halides electroreduction. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5594-5605.	1.3	2
451	Theoretical studies on the structures, intra- and inter-molecular hydrogen bonding interactions in HNF and HNF \cdot H ₂ O clusters in the gaseous, aqueous and solid phases. <i>Molecular Simulation</i> , 2015, 41, 1528-1539.	0.9	1
452	Theoretical investigation for adsorption of CO ₂ and CO on MIL-101 compounds with unsaturated metal sites. <i>Computational and Theoretical Chemistry</i> , 2015, 1055, 8-14.	1.1	15
453	Quantifying electro/nucleophilicity by partitioning the dual descriptor. <i>Journal of Computational Chemistry</i> , 2015, 36, 649-659.	1.5	39
454	New insights into the nitroaromatics-detection mechanism of the luminescent metal-organic framework sensor. <i>Dalton Transactions</i> , 2015, 44, 2897-2906.	1.6	50

#	ARTICLE	IF	CITATIONS
455	Electronic delocalization in small water rings. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2987-2990.	1.3	18
456	The origin of the absorption spectra of porphyrin N- and dithiaporphyrin S-oxides in their neutral and protonated states. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 3560-3569.	1.3	12
457	Unique bonding pattern and resulting bond stretch isomerism in Be ₃ 2 ⁺ . <i>International Journal of Quantum Chemistry</i> , 2015, 115, 426-433.	1.0	8
458	Extensive theoretical studies on two new members of the FOX-7 family: 5-(dinitromethylene)-1,4-dinitramino-tetrazole and 1,1-dinitro-4,4-diamino-5,5-bitetrazole as energetic compounds. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5840-5848.	1.3	44
459	Methanol to Olefins over H-MCM-22 Zeolite: Theoretical Study on the Catalytic Roles of Various Pores. <i>ACS Catalysis</i> , 2015, 5, 1131-1144.	5.5	72
460	Energetic Salts with π -Stacking and Hydrogen-Bonding Interactions Lead the Way to Future Energetic Materials. <i>Journal of the American Chemical Society</i> , 2015, 137, 1697-1704.	6.6	360
461	Theoretical studies on the AnO ₂ ⁿ⁺ (An = U, Np; n = 1, 2) complexes with di-(2-ethylhexyl)phosphoric acid. <i>Dalton Transactions</i> , 2015, 44, 3227-3236.	1.6	31
462	Scaling properties of information-theoretic quantities in density functional reactivity theory. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4977-4988.	1.3	65
463	Sorption of H ₃ BO ₃ /B(OH) ₄ ⁻ on calcined LDHs including different divalent metals. <i>Journal of Colloid and Interface Science</i> , 2015, 445, 183-194.	5.0	34
464	Theoretical design of triphenylamine-based derivatives with asymmetric D _{3h} configuration for dye-sensitized solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 140, 382-391.	2.0	25
465	The determination of the absolute configuration of a chiral 2,3-diindolylarylmethane by NMR spectroscopy. <i>Magnetic Resonance in Chemistry</i> , 2015, 53, 181-187.	1.1	1
466	Novel pnictogen bonding interactions with silylene as an electron donor: covalency, unusual substituent effects and new mechanisms. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9153-9160.	1.3	18
467	Theoretical prediction of the host-guest interactions between novel photoresponsive nanorings and C ₆₀ : A strategy for facile encapsulation and release of fullerene. <i>Journal of Computational Chemistry</i> , 2015, 36, 518-528.	1.5	17
468	One lithium atom binding with P-nitroaniline: lithium salts or lithium electrides?. <i>Journal of Molecular Modeling</i> , 2015, 21, 23.	0.8	11
469	Lewis-acid induced disaggregation of dimeric arylantimony oxides. <i>Chemical Communications</i> , 2015, 51, 5932-5935.	2.2	27
470	In Quest of a Superhalogen Supported Covalent Bond Involving a Noble Gas Atom. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3064-3074.	1.1	23
471	Unconventional charge distribution in the planar wheel-type M ₆ H ₆ ⁺ (M = Mn, Fe and Co): central M with negative charges and peripheral boron ring with positive charges. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9644-9650.	1.3	18
472	Density functional theory study of new azo dyes with different π -spacers for dye-sensitized solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 143, 20-34.	2.0	63

#	ARTICLE	IF	CITATIONS
473	Charge transfer or biradicaloid character: assessing TD-DFT and SAC-CI for squarylium dye derivatives. RSC Advances, 2015, 5, 18813-18821.	1.7	12
474	A simple, fast and convenient new method for predicting the stability of nitro compounds. Journal of Computer-Aided Molecular Design, 2015, 29, 471-483.	1.3	3
475	Synthesis, Characterization, and Energetic Properties of 6- <i>Amino</i> -tetrazolo[1,5- <i>b</i>]-1,2,4,5-tetrazine-7- <i>N</i> -oxide: A Nitrogen-Rich Material with High Density. Chemistry - an Asian Journal, 2015, 10, 1130-1132.		67
476	Structures and photophysical properties of copper(<i>i</i>) complexes bearing diphenylphenanthroline and bis(diphenylphosphino)alkane: the effect of phenyl groups on the phenanthroline ligand. Dalton Transactions, 2015, 44, 7554-7562.	1.6	72
477	Structure, stability and intramolecular interaction of M(N ₅) ₂ (M = Mg, Ca, Sr) Tj ETQq0 0,0rgBT /Overlock 10	1.7	21
478	Computational simulation and interpretation of the low-lying excited electronic states and electronic spectrum of thioanisole. Physical Chemistry Chemical Physics, 2015, 17, 20093-20099.	1.3	16
479	Dispersion- and Exchange-Corrected Density Functional Theory for Sodium Ion Hydration. Journal of Chemical Theory and Computation, 2015, 11, 2958-2967.	2.3	42
480	Intra-molecular magnetic exchange interaction in the tripyridinium bis[tetrachloroferrate(<i>iii</i>)] chloride molecular magnet: a broken symmetry-DFT study. Physical Chemistry Chemical Physics, 2015, 17, 19119-19125.	1.3	10
481	Interaction of BN- and BP-doped graphene nanoflakes with some representative neutral molecules and anions. Molecular Physics, 2015, 113, 2916-2929.	0.8	0
482	Understanding the Control of Singlet-Triplet Splitting for Organic Exciton Manipulating: A Combined Theoretical and Experimental Approach. Scientific Reports, 2015, 5, 10923.	1.6	151
483	Influence of position of auxiliary acceptor in <i>A</i> photosensitizes on photovoltaic performances of dye-sensitized solar cells. Journal of Materials Science, 2015, 50, 7333-7342.	1.7	12
484	Theoretical study for the interlamellar aminoalcohol functionalization of kaolinite. Applied Surface Science, 2015, 347, 439-447.	3.1	17
485	Tris-isocyanide copper(I) complexes: Synthetic, structural, and theoretical study. Inorganica Chimica Acta, 2015, 434, 31-36.	1.2	36
486	The effect of doped Pd atoms on the geometries and optical adsorption properties of Au cluster: Au ₃₂ ⁿ Pd _n (n=1, 2, 4 and 6). Materials Chemistry and Physics, 2015, 160, 105-110.	2.0	3
487	Singlet-triplet competition in the low-lying energy states of C ₄₀ ⁿ S _n (n=1-3) molecules. Structural Chemistry, 2015, 26, 1229-1240.	1.0	2
488	DFT, QTAIM, and NBO investigations of the ability of the Fe or Ni doped CNT to absorb and sense CO and NO. Journal of Molecular Modeling, 2015, 21, 225.	0.8	8
489	Electronic properties of environmental pollutants and their mutagenic activity: Nitro derivatives of azaphenanthrenes. Chemosphere, 2015, 135, 319-324.	4.2	3
490	Nonlinear optical properties of rhenium(I) complexes: Influence of the extended π -conjugated connectors and proton abstraction. Journal of Molecular Graphics and Modelling, 2015, 61, 196-203.	1.3	7

#	ARTICLE	IF	CITATIONS
491	Silicon doping on nanotubular fullerene D5hC ₉₀ from first principles. Computational and Theoretical Chemistry, 2015, 1069, 138-146.	1.1	5
492	DFT investigation and molecular dynamic simulation on the selective complexation of cis-cyclic nanopeptides with alkaline earth metal ions. Sensors and Actuators B: Chemical, 2015, 221, 1120-1129.	4.0	27
493	Effective utilization of noncovalent interaction descriptor in BX ₃ Lewis base complexes: A determination of adduct/van der Waals complexes and reassessment of the BX ₃ acid strength order. Chemical Physics Letters, 2015, 636, 117-120.	1.2	6
494	Theoretical Insight into the Ambiguous Endohedral Metallofullerene Er ₃ C ₇₄ : Covalent Interactions among Three Lanthanide Atoms. Inorganic Chemistry, 2015, 54, 8066-8076.	1.9	13
495	Neutral heterometallic cluster containing ketenylidene ligand: [Cp*Mo(CO) ₂ (η^4 -H)Ru ₂ (CO) ₆ (η^3 -É ³ 1)Tj ETQq0 0 0 rgBT /Overl	0.8	4
496	A detailed study of cholinium chloride and levulinic acid deep eutectic solvent system for CO ₂ capture via experimental and molecular simulation approaches. Physical Chemistry Chemical Physics, 2015, 17, 20941-20960.	1.3	133
497	Computational Study of Chemical Reactivity Using Information-Theoretic Quantities from Density Functional Reactivity Theory for Electrophilic Aromatic Substitution Reactions. Journal of Physical Chemistry A, 2015, 119, 8216-8224.	1.1	43
498	Influences of the substituents on the M-M bonding in Cp ₄ Al ₄ and Cp ₂ M ₂ X ₂ (M = B, Al, Ga; Cp = C ₅ H ₅ , X =) Tj ETQq1 0.784314 rgB	1.1	14
499	Molecular Dynamics Simulations of Acylpeptide Hydrolase Bound to Chlorpyrifosmethyl Oxon and Dichlorvos. International Journal of Molecular Sciences, 2015, 16, 6217-6234.	1.8	17
500	Ï-Stacking effects on the hydrogen bonding capacity of methyl 2-naphthoate. Journal of Molecular Graphics and Modelling, 2015, 61, 115-122.	1.3	12
501	Theoretical Predictions of <i>iv</i> Symmetric Three-H-Bridged Noble Gas Compounds NgBeH ₃ BeR, NgBeH ₃ BR ⁺ , and NgBH ₃ BR ⁺ . Journal of Physical Chemistry A, 2015, 119, 8400-8413.	1.1	14
502	The relationship between the strength of hydrogen bonding and spin crossover behaviour in a series of iron(ⁱⁱⁱ) Schiff base complexes. Dalton Transactions, 2015, 44, 4474-4484.	1.6	53
503	Gas-phase ammonia activation by Th, Th ⁺ , and Th ²⁺ : Reaction mechanisms, bonding analysis, and rate constant calculations. International Journal of Quantum Chemistry, 2015, 115, 6-18.	1.0	15
504	Interlayer Water Regulates the Bio-nano Interface of a β -sheet Protein stacking on Graphene. Scientific Reports, 2015, 5, 7572.	1.6	11
505	A Comparative Study on Activated Carbons Derived from a Broad Range of Agro-industrial Wastes in Removal of Large-Molecular-Size Organic Pollutants in Aqueous Phase. Water, Air, and Soil Pollution, 2015, 226, 1.	1.1	9
506	Theoretical Studies on Hexanuclear Oxometalates [M ₆ L ₁₉] ⁺ (M = Cr, Mo, W, Sg, Nd, U). Electronic Structures, Oxidation States, Aromaticity, and Stability. Inorganic Chemistry, 2015, 54, 7171-7180.	1.9	24
507	Tunable dipole induced hydrogen bonds between a hydrogen molecule and alkali halides. Physical Chemistry Chemical Physics, 2015, 17, 20361-20367.	1.3	3
508	A theoretical investigation of substituent effects on the stability and reactivity of N-heterocyclic olefin carboxylates. Organic and Biomolecular Chemistry, 2015, 13, 8533-8544.	1.5	26

#	ARTICLE	IF	CITATIONS
509	Structural evolution of (Au ₂ S) _n (n = 1–8) clusters from first principles global optimization. RSC Advances, 2015, 5, 62543-62550.	1.7	17
510	Molecular Design and Property Prediction for a Series of Novel Dicyclic Cyclotrimethylene Trinitramines (RDX) Derivatized as High Energy Density Materials. Journal of Physical Chemistry A, 2015, 119, 8250-8255.	1.1	35
511	Composition-dependent association behavior in the mixture of isopropanol and trichloromethane: a volumetric, vibration spectroscopic and quantum chemical study. RSC Advances, 2015, 5, 63719-63725.	1.7	3
512	Theoretical investigation of rare gas adsorption on and inside B-doped carbon nanotubes by DFT, QTAIM and NBO. RSC Advances, 2015, 5, 65604-65612.	1.7	4
513	Ferrocene–isocoumarin conjugated molecules: synthesis, structural characterization, electronic properties, and DFT–TDDFT computational study. Dalton Transactions, 2015, 44, 14465-14474.	1.6	8
514	Synthesis, Structure, Property of a Templated Borate [Hdmpip][B5O6(OH)4]. Journal of Cluster Science, 2015, 26, 1633-1644.	1.7	4
515	Computational study on aromaticity and resonance structures of substituted BODIPY derivatives. Computational and Theoretical Chemistry, 2015, 1068, 117-122.	1.1	10
516	Theoretical Study on the Solvation of C ₆₀ Fullerene by Ionic Liquids II: DFT Analysis of the Interaction Mechanism. Journal of Physical Chemistry B, 2015, 119, 10616-10629.	1.2	9
517	Polymeric palladium-mediated carbene polymerization. Polymer Chemistry, 2015, 6, 6163-6170.	1.9	8
518	Understanding the thermal dehydrochlorination reaction of 1-chlorohexane. Revealing the driving bonding pattern at the planar catalytic reaction center. RSC Advances, 2015, 5, 62946-62956.	1.7	9
519	Europium, uranyl, and thorium-phenanthroline amide complexes in acetonitrile solution: an ESI-MS and DFT combined investigation. Dalton Transactions, 2015, 44, 14376-14387.	1.6	63
520	Effect of “push–pull” sensitizers with modified conjugation bridges on the performance of p-type dye-sensitized solar cells. RSC Advances, 2015, 5, 64378-64386.	1.7	19
521	Exploring the halogen bond specific solvent effects in halogenated solvent systems by ESR probe. New Journal of Chemistry, 2015, 39, 5477-5483.	1.4	27
522	The discussion of descriptors for the QSAR model and molecular dynamics simulation of benzimidazole derivatives as corrosion inhibitors. Corrosion Science, 2015, 99, 76-88.	3.0	78
523	Revisiting the beryllium bonding interactions from energetic and wavefunction perspectives. Chemical Physics Letters, 2015, 633, 265-272.	1.2	17
524	An approach for the rationalization of melting temperature for deep eutectic solvents from DFT. Chemical Physics Letters, 2015, 634, 151-155.	1.2	111
525	Molecular structure, IR spectra, and chemical reactivity of cisplatin and transplatin: DFT studies, basis set effect and solvent effect. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 902-908.	2.0	26
526	Theoretical exploration of the nanoscale host–guest interactions between [n]cycloparaphenylenes (n) Tj ETQq1 1 0.784314 rgBT /Cv Chemical Physics, 2015, 17, 18802-18812.	1.3	43

#	ARTICLE	IF	CITATIONS
527	The induced current strengths and aromatic pathways of heteroporphyrins and their antiaromatic derivatives. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 983-988.	1.0	10
528	Ultraviolet Absorption Spectrum of Malonaldehyde in Water Is Dominated by Solvent-Stabilized Conformations. <i>Journal of the American Chemical Society</i> , 2015, 137, 8026-8029.	6.6	18
529	DFT calculation of the potential energy landscape topology and Raman spectra of type I CH ₄ and CO ₂ hydrates. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6963-6975.	1.3	28
530	Screening novel candidates and exploring design strategies for organic dye sensitizers with rigid π -linker: A theoretical study. <i>Materials Chemistry and Physics</i> , 2015, 162, 700-710.	2.0	12
531	Exploring the Nature of Silicon-Noble Gas Bonds in H ₃ SiNgNSi and HSiNgNSi Compounds (Ng = Xe, Rn). <i>International Journal of Molecular Sciences</i> , 2015, 16, 6402-6418.	1.8	37
532	The competition of Y ⁻ and X ⁻ halogen bonds to enhance the group V π -hole interaction in the NCY ⁻ and O ⁻ PH ₃ and O ⁻ PH ₃ NCX and O ⁻ PH ₃ NCXNCY (X, Y = F, Cl, and Br) complexes. <i>Journal of Computational Chemistry</i> , 2015, 36, 1349-1358.	1.7	27
533	Structure and Redox Properties of 5-Amino-3-nitro-1H-1,2,4-triazole (ANTA) Adsorbed on a Silica Surface: A DFT M05 Computational Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8139-8145.	1.1	14
534	Some Quinoxalin-6-yl Derivatives as Corrosion Inhibitors for Mild Steel in Hydrochloric Acid: Experimental and Theoretical Studies. <i>Journal of Physical Chemistry C</i> , 2015, 119, 16004-16019.	1.5	381
535	Electronic, bonding, and optical properties of 1d [C _n C _n] (n = 10) chains, 2d [C _n C _n] (n = 10) nanorings, and 3d [C _n C _n] (n = 10) tubes studied by DFT/TD-DFT method. <i>Journal of Computational Chemistry</i> , 2015, 36, 1334-1347.	1.5	3
536	Design and characteration of planar star-shaped oligomer electron donors for organic solar cells: a DFT study. <i>Canadian Journal of Chemistry</i> , 2015, 93, 1181-1190.	0.6	4
537	Effect of 1D twisted water chains confined in channels formed by a Gemini amphiphile on its crystal stability. <i>CrystEngComm</i> , 2015, 17, 1439-1447.	1.3	6
538	Calcium and heterometallic manganese-calcium complexes supported by tripodal pyridine-carboxylate ligands: structural, EPR and theoretical investigations. <i>Dalton Transactions</i> , 2015, 44, 12757-12770.	1.6	15
539	On the stability of noble gas bound 1-tris(pyrazolyl)borate beryllium and magnesium complexes. <i>New Journal of Chemistry</i> , 2015, 39, 6778-6786.	1.4	27
540	Towards Understanding the Decomposition/Isomerism Channels of Stratospheric Bromine Species: Ab Initio and Quantum Topology Study. <i>International Journal of Molecular Sciences</i> , 2015, 16, 6783-6800.	1.8	7
541	Hydrogen Trapping Ability of the Pyridine-Lithium ⁺ (1:1) Complex. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3056-3063.	1.1	18
542	Water Effect on Acid-Gas Capture Using Choline Lactate: A DFT Insight beyond Molecule-Molecule Pair Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5546-5557.	1.2	14
543	A DFT Study of the Extractive Desulfurization Mechanism by [BMIM] ⁺ [AlCl ₄] ⁻ Ionic Liquid. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5995-6009.	1.2	88
544	New Three-Fold Interpenetrated Uranyl Organic Framework Constructed by Terephthalic Acid and Imidazole Derivative. <i>Inorganic Chemistry</i> , 2015, 54, 3829-3834.	1.9	37

#	ARTICLE	IF	CITATIONS
563	Insight into external electric field dependent photoinduced intermolecular charge transport in BHJ solar cell materials. <i>Journal of Materials Chemistry C</i> , 2015, 3, 4810-4819.	2.7	60
564	Interactions of carbon nanotubes with the nitromethane/water mixture governing selective adsorption of energetic molecules from aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6995-7001.	1.3	11
565	One- and two-photon absorptions of the C _n and C _n -1 Si fullerenes in gas phase and solution. <i>European Physical Journal D</i> , 2015, 69, 1.	0.6	3
566	Benzimidazole-Containing Porous Organic Polymers as Highly Active Heterogeneous Solid-Base Catalysts. <i>ChemCatChem</i> , 2015, 7, 1559-1565.	1.8	29
567	Improving As(III) adsorption on graphene based surfaces: impact of chemical doping. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12056-12064.	1.3	49
568	How Does the Hemilabile Group in Ruthenium-Cp* Picolyl-NHC Complexes Affect the Mechanism of Transfer Hydrogenation Reaction? A DFT Study. <i>Catalysis Letters</i> , 2015, 145, 1331-1343.	1.4	14
569	Quantum-chemical studies of the structure and performance properties of 5-(1,2,4-triazol-5-yl)tetrazol-1-ols. <i>Chemistry of Heterocyclic Compounds</i> , 2015, 51, 153-158.	0.6	4
570	Metabolites from the mushroom <i>Ganoderma lingzhi</i> as stimulators of neural stem cell proliferation. <i>Phytochemistry</i> , 2015, 114, 155-162.	1.4	65
571	Intramolecular hydrogen bonds involving organic fluorine in the derivatives of hydrazides: an NMR investigation substantiated by DFT based theoretical calculations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15226-15235.	1.3	17
572	Is There Any Preferential Interaction of Ions of Ionic Liquids with DMSO and H ₂ O? A Comparative Study from MD Simulation. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6686-6695.	1.2	39
573	A combined experimental and density functional study of 1-(arylsulfonyl)-2-chloro-2-butenes reactivity towards the allylic chlorine. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 403-413.	0.9	0
574	The adsorption mechanism of platinum on phosphorus-doped single walled carbon nanotube. <i>Computational and Theoretical Chemistry</i> , 2015, 1059, 1-6.	1.1	18
575	An 18-Electron System Containing a Superheavy Element: Theoretical Studies of Sg@Au ₁₂ . <i>Inorganic Chemistry</i> , 2015, 54, 3695-3701.	1.9	42
576	Two novel uranyl complexes of a semi-rigid aromatic tetracarboxylic acid supported by an organic base as an auxiliary ligand or a templating agent: an experimental and theoretical exploration. <i>CrystEngComm</i> , 2015, 17, 3031-3040.	1.3	16
577	Theoretical design and characterization of pyridalithiadiazole-based chromophores with fast charge transfer at donor/acceptor interface toward small molecule organic photovoltaics. <i>RSC Advances</i> , 2015, 5, 29401-29411.	1.7	46
578	Secondary bonding networks in small (HgS) _n clusters: A theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2015, 1060, 36-42.	1.1	4
579	Theoretical Study of Acene-Bridged Dyes for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3299-3309.	1.1	48
580	Curious cases of 3,6-dinitropyrazolo[4,3-c]pyrazole-based energetic cocrystals with high nitrogen content: an alternative to salt formation. <i>Chemical Communications</i> , 2015, 51, 7337-7340.	2.2	47

#	ARTICLE	IF	CITATIONS
581	Pyridylpentazole and its derivatives: a new source of N ₅ ⁺ ?. RSC Advances, 2015, 5, 27699-27705.	1.7	7
582	Mass spectrometry and theoretical calculations about the loss of methyl radical from methoxilated coumarins. Journal of Molecular Structure, 2015, 1093, 49-58.	1.8	7
583	The origin and magnitude of intramolecular quasi-cyclic S ⁻ O and S ⁻ S interactions revisited: A computational study. Chemical Physics Letters, 2015, 631-632, 6-11.	1.2	25
584	Designation and Exploration of Halide ⁻ Anion Recognition Based on Cooperative Noncovalent Interactions Including Hydrogen Bonds and Anion ⁻ . Journal of Physical Chemistry A, 2015, 119, 5842-5852.	1.1	25
585	Divalent metals can reside on bonds in fullerenes. Dalton Transactions, 2015, 44, 9561-9568.	1.6	9
586	First-principle study of silicon cluster doped with rhodium: Rh ₂ Si _n (n=11) clusters. Materials Chemistry and Physics, 2015, 160, 227-236.	2.0	11
587	How the cation ⁻ cation ⁻ stacking occurs: A theoretical investigation into ionic clusters of imidazolium. Journal of Molecular Graphics and Modelling, 2015, 60, 118-123.	1.3	20
588	Theoretical Investigations on 4, 10-dinitro-2, 6, 8, 12-tetraoxa-4, 10-diazatetracyclo[5.5.0.0 ^{3,9} .0 ^{3,11}]dodecane. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2015, 641, 1238-1242.	0.6	2
589	Combination Multinitrogen with Good Oxygen Balance: Molecule and Synthesis Design of Polynitro-Substituted Tetrazolotriazine-Based Energetic Compounds. Journal of Organic Chemistry, 2015, 80, 5643-5651.	1.7	36
590	Binding Modes and Interaction Mechanism Between Different Base Pairs and Methylene Blue Trihydrate: A Quantum Mechanics Study. Advances in Experimental Medicine and Biology, 2015, 827, 187-203.	0.8	8
591	Influence of Silver Doping on the Photoluminescence of Protected Ag _n Au ₂₅ Nanoclusters: A Time-Dependent Density Functional Theory Investigation. Journal of Physical Chemistry C, 2015, 119, 10766-10775.	1.5	40
592	Structural, Magnetic, and Redox Diversity of First-Row Transition Metal Complexes of a Pyridine-Based Macrocyclic: Well-Marked Trends Supported by Theoretical DFT Calculations. Inorganic Chemistry, 2015, 54, 3352-3369.	1.9	39
593	Density Functional Theory Calculations for the Structural, Electronic, and Magnetic Properties of (Gd ₂ O ₃) _n ^{0,±1} Clusters with n = 1-10. Journal of Physical Chemistry C, 2015, 119, 8349-8356.	1.5	18
594	Homolytic or Heterolytic Dihydrogen Splitting with Ditantalum/Dizirconium Dinitrogen Complexes? A Computational Study. Organometallics, 2015, 34, 1255-1263.	1.1	8
595	The effect of ring sizes and alkali metal cations on interaction energy, charge transfer and nonlinear optical properties of crown ether derivatives. RSC Advances, 2015, 5, 30107-30119.	1.7	13
596	The driving forces for twisted or planar intramolecular charge transfer. Physical Chemistry Chemical Physics, 2015, 17, 9248-9257.	1.3	92
597	The nature of the bonding in symmetrical pincer palladacycles. Dalton Transactions, 2015, 44, 7570-7577.	1.6	15
598	The important role of the location of the alkoxy group on the thiophene ring in designing efficient organic nonlinear optical materials based on double-donor chromophores. Journal of Materials Chemistry C, 2015, 3, 3913-3921.	2.7	24

#	ARTICLE	IF	CITATIONS
599	Double Holeâ€“Lump Interaction between Halogen Atoms. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3746-3752.	1.1	29
600	Density Functional Theory Study on the Cholinium Dihydrogenphosphate Ionic Liquid for Acid Gas Removal. <i>Journal of Solution Chemistry</i> , 2015, 44, 890-899.	0.6	3
601	Theoretical studies on the absorption spectra and intramolecular charge transfer of push-pull zinc porphyrin dyes for dye-sensitized solar cells. <i>Chemical Research in Chinese Universities</i> , 2015, 31, 276-280.	1.3	6
602	The DFT local reactivity descriptors of Î±-tocopherol. <i>Journal of Molecular Modeling</i> , 2015, 21, 99.	0.8	16
603	Investigation of Properties of Mg _n Clusters and Their Hydrogen Storage Mechanism: A Study Based on DFT and a Global Minimum Optimization Method. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3636-3643.	1.1	40
604	Slight channel difference influences the reaction pathway of methanol-to-olefins conversion over acidic H-ZSM-22 and H-ZSM-12 zeolites. <i>Catalysis Science and Technology</i> , 2015, 5, 3507-3517.	2.1	51
605	Theoretical Study on the Rational Design of Cyano-Substituted P3HT Materials for OSCs: Substitution Effect on the Improvement of Photovoltaic Performance. <i>Journal of Physical Chemistry C</i> , 2015, 119, 8501-8511.	1.5	39
606	A New Graphdiyne Nanosheet/Pt Nanoparticleâ€“Based Counter Electrode Material with Enhanced Catalytic Activity for Dyeâ€“Sensitized Solar Cells. <i>Advanced Energy Materials</i> , 2015, 5, 1500296.	10.2	180
607	Activation of Methane and Carbon Dioxide Mediated by Transitionâ€“Metal Doped Magnesium Oxide Clusters [MMgO] ^{+0/âˆ’} (M=Scâ€“Zn). <i>Chemistry - A European Journal</i> , 2015, 21, 7780-7789.	1.7	28
608	An insight into hydration structure of sodium glycinate from ab initio quantum chemical study. <i>Journal of Molecular Modeling</i> , 2015, 21, 234.	0.8	4
609	Density functional reactivity theory study of S _N 2 reactions from the information-theoretic perspective. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27052-27061.	1.3	34
610	Theoretical Insight into Sc ₂ O@C ₈₄ : Interplay between Small Cluster and Large Carbon Cage. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10428-10439.	1.1	12
611	Third order NLO properties of corannulene and its Li-doped dimers: effect of concaveâ€“convex and convexâ€“convex structures. <i>RSC Advances</i> , 2015, 5, 79783-79791.	1.7	24
612	Theoretical evidence of charge transfer interaction between SO ₂ and deep eutectic solvents formed by choline chloride and glycerol. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28729-28742.	1.3	80
613	Charging-induced asymmetric spin distribution in an asymmetric (9,0) carbon nanotube. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28860-28865.	1.3	6
614	Theoretical insight into the interplay between lithium and halogenâ€“hydride bonds: An <i>ab initio</i> study. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550046.	1.8	7
615	Experimental and theoretical studies on the influence of ionic liquids as additives on ammonia-based CO ₂ capture. <i>International Journal of Greenhouse Gas Control</i> , 2015, 42, 454-460.	2.3	7
616	Stereoselective synthesis of highly branched chiral cyclobutane-cored triamines and their conjugation to Gd-DOTA. <i>Tetrahedron</i> , 2015, 71, 8085-8095.	1.0	0

#	ARTICLE	IF	CITATIONS
617	Electron Dynamics and IR Peak Coalescence in Bridged Mixed Valence Dimers Studied by Ultrafast 2D-IR Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10738-10749.	1.2	6
618	Specific Reagent for Cr(III): Imaging Cellular Uptake of Cr(III) in Hct116 Cells and Theoretical Rationalization. <i>Journal of Physical Chemistry B</i> , 2015, 119, 13018-13026.	1.2	24
619	Copper(I) complexes of phenanthrolineimidazole ligands: structures, photophysical properties, and quantum chemical studies. <i>Transition Metal Chemistry</i> , 2015, 40, 723-732.	0.7	10
620	A new C=C embedded porphyrin sheet with superior oxygen reduction performance. <i>Nano Research</i> , 2015, 8, 2901-2912.	5.8	35
621	Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4992-5001.	2.3	42
622	[XeOXeOXe] ₂ ⁺ , the Missing Oxide of Xenon(II); Synthesis, Raman Spectrum, and X-ray Crystal Structure of [XeOXeOXe][^{1/4} -F(ReO ₂ F ₃) ₂] ₂ . <i>Journal of the American Chemical Society</i> , 2015, 137, 13398-13413.	6.6	17
623	A novel class of compounds—superalkalides: M ⁺ (en) ₃ M ²⁺ O ⁻ (M, M ²⁺ = Li, Na, and K; en = Tj ETQqO ₀ 0 ₀ rgBT / Overlock 10). <i>Chemical Physics</i> , 2015, 17, 28754-28764.	1.3	35
624	2D quasi-planar or 3D structures? A comparison between CrBn (n = 2 ~ 10) wheel-like clusters and their corresponding 3D pyramidal clusters, and their hydrogen storage capability. <i>International Journal of Modern Physics B</i> , 2015, 29, 1550172.	1.0	4
625	Intramolecularly Group 15 Stabilized Aryltellurenyl Halides and Triflates. <i>Organometallics</i> , 2015, 34, 5341-5360.	1.1	24
626	Tuning of chalcogen bonds by cation-π interactions: cooperative and diminutive effects. <i>Journal of Molecular Modeling</i> , 2015, 21, 300.	0.8	8
627	Encapsulation of sulfur, oxygen, and nitrogen mustards by cucurbiturils: a DFT study. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2015, 83, 387-400.	0.9	29
628	A coupled-cluster study on the noble gas binding ability of metal cyanides versus metal halides (metal = Cu, Ag, Au). <i>Journal of Computational Chemistry</i> , 2015, 36, 2168-2176.	1.5	41
629	Structures and Electronic Properties of (KI) _n (n = 1, 2, 3, 4) and K(KI) _n (n = 1, 2, 3) Clusters: Photoelectron Spectroscopy, Isomer-Depletion, and ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11154-11161.	1.1	3
630	Cell membrane causes the lipid bilayers to behave as variable capacitors: A resonance with self-induction of helical proteins. <i>Biophysical Chemistry</i> , 2015, 207, 114-127.	1.5	19
631	Application-oriented computational studies on a series of D ⁺ -A structured porphyrin sensitizers with different electron-donor groups. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30624-30631.	1.3	8
632	Structural isomerism in gold nanoparticles revealed by X-ray crystallography. <i>Nature Communications</i> , 2015, 6, 8667.	5.8	258
633	Spectroscopic analysis of diphosphatriazolite anion (P ₂ N ₃ ⁻) by coupled-cluster methods as a step toward N ₅ ⁻ . <i>Chemical Physics Letters</i> , 2015, 640, 68-71.	1.2	8
634	Density Functional Theory and Electrochemical Studies: Structure-Efficiency Relationship on Corrosion Inhibition. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2391-2402.	2.5	53

#	ARTICLE	IF	CITATIONS
635	Selective Extraction of Americium(III) over Europium(III) with the Pyridylpyrazole Based Tetradentate Ligands: Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2015, 54, 10648-10655.	1.9	30
636	Sulfur Dioxide–Pyridine Dimer. FTIR and Theoretical Evidence for a Low-Symmetry Structure. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10390-10398.	1.1	23
637	The influence of L ligands on the $\{RuNO\}_{6/7}$ bonding situation in $cis-[Ru(NO)(NO)_2L_4]$ complexes: a theoretical insight. <i>RSC Advances</i> , 2015, 5, 69057-69066.	1.7	9
638	The impact of charges in force field parameterization for molecular dynamics simulations of deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2015, 211, 506-514.	2.3	69
639	Rotational spectroscopy of methyl benzoylformate and methyl mandelate: structure and internal dynamics of a model reactant and product of enantioselective reduction. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 21942-21949.	1.3	5
640	Hydrogen trapping potential of $(HF)_m$ ($m=1-8$) and $(H_2O)_n$ ($n=1-10$) clusters. <i>Computational and Theoretical Chemistry</i> , 2015, 1071, 18-26.	1.1	8
641	The C N coupling reaction of bimetallic cations $[MAu(CH)] + (M = Pt, Ir, Os)$ with NH_3 . <i>Computational and Theoretical Chemistry</i> , 2015, 1072, 52-57.	1.1	0
642	Understanding the Boron–Nitrogen Interaction and Its Possible Implications in Drug Design. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14393-14401.	1.2	5
643	High-temperature molecular dynamics simulation of cellobiose and maltose. <i>AIChE Journal</i> , 2015, 61, 2562-2570.	1.8	12
644	Synthesis and optical nonlinear properties of novel Y-shaped chromophores with excellent electro-optic activity. <i>Journal of Materials Chemistry C</i> , 2015, 3, 11423-11431.	2.7	14
645	Oxocomplexes of Mo(vi) and W(vi) with 8-hydroxyquinoline-5-sulfonate in solution: structural studies and the effect of the metal ion on the photophysical behaviour. <i>Dalton Transactions</i> , 2015, 44, 19076-19089.	1.6	10
646	Theoretical study on the structure and cation–anion interaction of triethylammonium chloroaluminate ionic liquid. <i>Computational and Theoretical Chemistry</i> , 2015, 1073, 67-74.	1.1	13
647	A theoretical study on single-electron reduction of a thiolate-bridged diiron diazene complex. <i>Chemical Physics Letters</i> , 2015, 639, 300-303.	1.2	1
648	Polymerized cellulose building blocks: relative energy, electronic property, and reactivity from quantum chemical approach. <i>Polymers for Advanced Technologies</i> , 2015, 26, 1336-1339.	1.6	2
649	Structures and bonding of auropolyborenes $[Au_2(B_4)_x B_3]^+$, $[Au_2(B_4)_x B_2]^+$ and $[Au_2(B_4)_x B]^+$ ($x = 2, 3$): comparison with dihydride polyborenes. <i>RSC Advances</i> , 2015, 5, 87855-87863.	1.7	3
650	Structural and electronic properties of covalently functionalized 2-aminoethoxy-metallophthalocyanine–graphene hybrid materials: a computational study. <i>RSC Advances</i> , 2015, 5, 85730-85740.	1.7	7
651	Organic fluorine involved intramolecular hydrogen bonds in the derivatives of imides: NMR evidence corroborated by DFT based theoretical calculations. <i>RSC Advances</i> , 2015, 5, 86013-86022.	1.7	21
652	Alkali and alkaline-earth atom-decorated B38 fullerenes and their potential for hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 13022-13028.	3.8	38

#	ARTICLE	IF	CITATIONS
653	Second-Order Nonlinear Optical Response of Electron Donor–Acceptor Hybrids Formed between Corannulene and Metallofullerenes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24965-24975.	1.5	60
654	Lithium Di- and Trimethyl Dimolybdenum(II) Complexes with Mo–Mo Quadruple Bonds and Bridging Methyl Groups. <i>Journal of the American Chemical Society</i> , 2015, 137, 12378-12387.	6.6	16
655	Enthalpy of formation of guanidine and its amino and nitro derivatives. <i>Structural Chemistry</i> , 2015, 26, 1629-1640.	1.0	13
656	X–H···C hydrogen bonds in n-alkane-HX (X = F, OH) complexes are stronger than C–H···X hydrogen bonds. <i>Journal of Chemical Sciences</i> , 2015, 127, 1035-1045.	0.7	10
657	Unwilling U–U bonding in U ₂ @C ₈₀ : cage-driven metal–metal bonds in di-uranium fullerenes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24182-24192.	1.3	47
658	Pnicogen–pnicogen interactions in O ₂ XP:PH ₂ Y complexes (X=H, F, CN; Y=H, OH, OCH ₃ , CH ₃ , NH ₂). <i>Chemical Physics Letters</i> , 2015, 638, 122-127.	1.2	22
659	A Quasi-relativistic Density Functional Theory Study of the Actinyl(VI, V) (An = U, Np, Pu) Complexes with a Six-Membered Macrocyclic Containing Pyrrole, Pyridine, and Furan Subunits. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9178-9188.	1.1	35
660	Microwave spectroscopic and theoretical investigations of the strongly hydrogen bonded hexafluoroisopropanol–water complex. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24774-24782.	1.3	20
661	Halogen bonding interactions in ion pairs versus conventional charge-assisted and neutral halogen bonds: a theoretical study based on imidazolium species. <i>RSC Advances</i> , 2015, 5, 74284-74294.	1.7	20
662	Rotational Spectra of Two Hydrogen-Bonded Methyl Salicylate Monohydrates: Relative Stability and Tunneling Motions. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3126-3131.	2.1	30
663	The Effect of Doping and Confinement on the Adsorption of Pt on CNTs upon Be, B, N and O Doping: A Theoretical Study. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2015, 25, 1502-1510.	1.9	7
664	In silico studies on the origin of selective uptake of carbon dioxide with cucurbit[7]uril amorphous material. <i>RSC Advances</i> , 2015, 5, 72469-72475.	1.7	6
665	Investigation into the metallophilic interaction in coinage-metal halides: an ab initio study of CMX (CM = Cu and Ag, X = F–I). <i>Journal of Molecular Modeling</i> , 2015, 21, 205.	0.8	5
666	Noncovalent Binding of Polycyclic Aromatic Hydrocarbons with Genetic Bases Reducing the <i>in Vitro</i> Lateral Transfer of Antibiotic Resistant Genes. <i>Environmental Science & Technology</i> , 2015, 49, 10340-10348.	4.6	38
667	A Simple ab Initio Model for the Hydrated Electron That Matches Experiment. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9148-9159.	1.1	88
668	Theoretical Study of Renewable Ionic Liquids in the Pure State and with Graphene and Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12224-12237.	1.2	15
669	Paddlewheel 1,2,4-diazaphospholide dibismuthanes with very short bismuth–bismuth single bonds. <i>Chemical Communications</i> , 2015, 51, 16184-16187.	2.2	23
670	Excluding hyperconjugation from the Z conformational preference and investigating its origin: formic acid and beyond. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26946-26954.	1.3	5

#	ARTICLE	IF	CITATIONS
671	Theoretical insights into the structures and mechanical properties of HMX/NQ cocrystal explosives and their complexes, and the influence of molecular ratios on their bonding energies. <i>Journal of Molecular Modeling</i> , 2015, 21, 245.	0.8	27
672	Intermolecular forces in acetonitrile + ethanol binary liquid mixtures. <i>Chemical Physics Letters</i> , 2015, 639, 161-165.	1.2	29
673	Trends in Na-Ion Solvation with Alkyl-Carbonate Electrolytes for Sodium-Ion Batteries: Insights from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 22747-22759.	1.5	84
674	Radical Mechanism of Isocyanide-Alkyne Cycloaddition by Multicatalysis of Ag ₂ CO ₃ , Solvent, and Substrate. <i>ACS Catalysis</i> , 2015, 5, 6177-6184.	5.5	54
675	The nature of Pd ^{II} -carbene and Pd ^{II} -halogen bonds in (bisNHC)PdX ₂ type catalysts: insights from density functional theory. <i>RSC Advances</i> , 2015, 5, 80661-80667.	1.7	15
676	Theoretical design of the cyclic lipopeptide nanotube as a molecular channel in the lipid bilayer, molecular dynamics and quantum mechanics approach. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25536-25549.	1.3	17
677	Unusual bonding modes of perfluorobenzene in its polymeric (dimeric, trimeric and tetrameric) forms: entirely negative fluorine interacting cooperatively with entirely negative fluorine. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 31624-31645.	1.3	34
678	Intriguing properties of unusual silicon nanocrystals. <i>RSC Advances</i> , 2015, 5, 78192-78208.	1.7	37
679	Actinide (An = Th ^{IV} -Pu) dimetalloenes: promising candidates for metal-metal multiple bonds. <i>Dalton Transactions</i> , 2015, 44, 17045-17053.	1.6	41
680	Interaction Mechanism Insights on the Solvation of Fullerene C ₈₀ with Choline-based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12455-12463.	1.2	3
681	Theoretical Studies on the Energetic Salts of Substituted 3,3'-Amino- <i>N,N'</i> -azo-1,2,4-triazoles: The Role of Functional Groups. <i>Journal of Chemical & Engineering Data</i> , 2015, 60, 2869-2878.	1.0	8
682	Theoretical insights into the separation of Am(III) over Eu(III) with PhenBHPPA. <i>Dalton Transactions</i> , 2015, 44, 16737-16745.	1.6	34
683	Systematic analysis of structural and spectroscopic properties of neptunimine (HN=NpH ₂) and plutonimine (HN=PuH ₂). <i>Journal of Molecular Modeling</i> , 2015, 21, 316.	0.8	4
684	Probing molecular interactions underlying imidazolium and pyridinium based ionic liquids. <i>Journal of Molecular Liquids</i> , 2015, 212, 885-899.	2.3	11
685	Multistate and Multicolor Photochromism through Selective Cycloreversion in Asymmetric Platinum(II) Complexes with Two Different Dithienylethene ²⁻ Acetylides. <i>Inorganic Chemistry</i> , 2015, 54, 11511-11519.	1.9	24
686	In silico design of adamantane derived organic superbases with an extended hydrogen bond network and their use as molecular containers for the storage of H ₂ and CO ₂ . <i>RSC Advances</i> , 2015, 5, 102247-102255.	1.7	7
687	Theoretical studies of traditional and halogen-shared halogen bonds: the doped all-metal aromatic clusters MA ₃ ⁺ (M=As, Ge, Sn, Pb) as halogen bond acceptors. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	3
688	Photophysical properties of copper(I) complexes containing pyrazine-fused phenanthroline ligands: a joint experimental and theoretical investigation. <i>Journal of Molecular Modeling</i> , 2015, 21, 313.	0.8	10

#	ARTICLE	IF	CITATIONS
689	Comparative study on the methods for predicting the reactive site of nucleophilic reaction. <i>Science China Chemistry</i> , 2015, 58, 1845-1852.	4.2	105
691	Monomeric Chiral and Achiral Basket-Handle Porphyrins: Synthesis, Structural Features, and Arrested Tautomerism. <i>Journal of Organic Chemistry</i> , 2015, 80, 12359-12378.	1.7	14
692	Molecular insight into the interaction mechanisms of amino-2-imidazole derivatives with BACE1 protease: A QM/MM and QTAIM study. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 389-397.	1.0	20
693	Access to Novel Graphene-Like Sheet of Hydroboron: First-Principles Investigation. <i>Chemistry - an Asian Journal</i> , 2015, 10, 362-369.	1.7	2
694	Mechanistic aspects of the reaction of uranium atom with H ₂ O in the gas phase. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2015, 304, 489-499.	0.7	9
695	Mechanism of the Gaseous Hydrolysis Reaction of SO ₂ : Effects of NH ₃ versus H ₂ O. <i>Journal of Physical Chemistry A</i> , 2015, 119, 102-111.	1.1	61
696	A metal-metal bond passing through the arene ligand: a theoretical study on inverse sandwiches X[Sc ₈ H ₈] ⁿ X (X = F, Cl, Br; n = 1, 2). <i>New Journal of Chemistry</i> , 2015, 39, 1558-1562.	1.4	4
697	Solvent Effects on the Optical Spectra and Excited-State Decay of Triphenylamine-thiadiazole with Hybridized Local Excitation and Intramolecular Charge Transfer. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5233-5240.	1.1	73
698	Competition between halogen bond and hydrogen bond in complexes of superalkali Li ₃ S and halogenated acetylene XCCH (X = F, Cl, Br, and I). <i>International Journal of Quantum Chemistry</i> , 2015, 115, 99-105.	1.0	9
699	Infrared spectra of HMSH and HMMSH (M = Zn, Cd, Hg) in solid argon. <i>Journal of Molecular Spectroscopy</i> , 2015, 310, 16-22.	0.4	3
700	Using beryllium bonds to change halogen bonds from traditional to chlorine-shared to ion-pair bonds. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2259-2267.	1.3	49
701	Metastable behavior of noble gas inserted tin and lead fluorides. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 972-982.	1.3	49
702	A theoretical study of the UV absorption of 4-methylbenzylidene camphor: from the UVB to the UVA region. <i>Photochemical and Photobiological Sciences</i> , 2015, 14, 465-472.	1.6	9
703	Revealing the interactions between pentagon-octagon-pentagon defect graphene and organic donor/acceptor molecules: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4919-4925.	1.3	22
704	Roles of hydrogen bonds and π-π stacking in the optical detection of nitro-explosives with a luminescent metal-organic framework as the sensor. <i>RSC Advances</i> , 2015, 5, 3045-3053.	1.7	62
705	Synthesis and Solid State Structures of Schiff Base Copper (II) and Nickel(II) Complexes Derived From cis-1,2-diaminocyclohexane. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 2015, 45, 327-332.	0.6	7
706	A DFT Study on the Stability and Aromaticity of Heterobenzenes Containing Group 15 Elements. <i>Heteroatom Chemistry</i> , 2015, 26, 206-214.	0.4	24
707	NCI analysis of the interaction cation-π in complexes with molecular bowls derived from fullerene. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 123-129.	1.1	8

#	ARTICLE	IF	CITATIONS
708	Experimental and theoretical studies of C-H...M interactions in palladium and platinum complexes derived from 1,2-bis-(2-hydroxymethylphenylthio)ethane. <i>Polyhedron</i> , 2015, 87, 181-193.	1.0	10
709	Two nitro derivatives of azabenz[a]pyrene N-oxide: Electronic properties and their relation to mutagenic activity. <i>Journal of Hazardous Materials</i> , 2015, 285, 94-102.	6.5	4
710	Photoinduced Proton Transfer Promoted by Peripheral Subunits for Some Hantzsch Esters. <i>Journal of Physical Chemistry A</i> , 2015, 119, 39-49.	1.1	9
711	Theoretical investigation of the N...Sn coordination in (Me ₃ SnCN) ₂ . <i>Structural Chemistry</i> , 2015, 26, 301-318.	1.0	22
712	Deprotonation-Triggered Stokes Shift Fluorescence of an Unexpected Basic-Stable Metal-Organic Framework. <i>Inorganic Chemistry</i> , 2015, 54, 65-68.	1.9	19
713	Conformational analysis, spectroscopic study (FT-IR, FT-Raman, UV, ¹ H and ¹³ C NMR), molecular orbital energy and NLO properties of 5-iodosalicylic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 295-305.	2.0	21
714	A DFT investigation on the electronic properties of octahaloditechnetate anions: Correlation between charge and bond strength. <i>Inorganica Chimica Acta</i> , 2015, 424, 308-315.	1.2	4
715	Enhancing π - π -type copper...thiophene interactions by metal doping (metal = Li, Na, K, Ca, Sc). <i>Dalton Transactions</i> , 2015, 44, 1283-1291.	1.6	12
716	Ca...Ca interaction in inverse sandwich Ca...C ₈ H ₈ ...Ca. <i>Dalton Transactions</i> , 2015, 44, 345-350.	1.6	8
717	Synthesis of four-armed triphenylamine-based molecules and their applications in organic solar cells. <i>New Journal of Chemistry</i> , 2015, 39, 994-1000.	1.4	9
718	Interlayer charge-transfer in impacting the second hyperpolarizabilities: Radical and cation species of hexathiophenalenylium and its nitro dimers. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 55, 33-40.	1.3	11
719	The acidity/basicity of metal-containing ionic liquids: insights from surface analysis and the Fukui function. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 1339-1346.	1.3	10
720	A study of two thermostable NLO chromophores with different π -electron bridges using fluorene as the donor. <i>New Journal of Chemistry</i> , 2015, 39, 1038-1044.	1.4	10
721	The importance of molecular conformation to the properties: a DFT study of the polynitro heterocyclic compounds based on dodecahydrodiimidazo [4,5-b:4',5'-e]pyrazine structure. <i>Structural Chemistry</i> , 2015, 26, 667-674.	1.0	3
722	Conformational, electronic and antioxidant properties of lucidone, linderone and methylinderone: DFT, QTAIM and NBO studies. <i>Molecular Physics</i> , 2015, 113, 683-697.	0.8	39
723	Theoretical Study of the Nontraditional Enol-Based Photoacidity of Firefly Oxyluciferin. <i>ChemPhysChem</i> , 2015, 16, 455-464.	1.0	18
724	Design, synthesis, biological evaluation and toxicity studies of N,N-disubstituted biguanides as quorum sensing inhibitors. <i>Medicinal Chemistry Research</i> , 2015, 24, 1974-1987.	1.1	17
725	On the properties of S...O and S...F noncovalent interactions: the analysis of geometry, interaction energy and electron density. <i>New Journal of Chemistry</i> , 2015, 39, 1611-1618.	1.4	36

#	ARTICLE	IF	CITATIONS
726	DFT and TD-DFT Assessment of the Structural and Optoelectronic Properties of an Organic Ag ₁₄ Nanocluster. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5088-5098.	1.1	31
727	Understanding the bifurcated halogen bonding N-Hal-N in bidentate diazaheterocyclic compounds. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 229-237.	1.1	29
728	Decomposition of Intermolecular Interactions in the Crystal Structure of Some Diacetyl Platinum(II) Complexes: Combined Hirshfeld, AIM, and NBO Analyses. <i>Molecules</i> , 2016, 21, 1669.	1.7	13
729	Concomitant Effects of Transition Metal Chelation and Solvent Polarity on the First Molecular Hyperpolarizability of 4-Methoxyacetophenone Thiosemicarbazone: A DFT Study. <i>Journal of Theoretical Chemistry</i> , 2016, 2016, 1-19.	1.5	18
730	A DFT Study of Some Structural and Spectral Properties of 4-Methoxyacetophenone Thiosemicarbazone and Its Complexes with Some Transition Metal Chlorides: Potent Antimicrobial Agents. <i>Advances in Chemistry</i> , 2016, 2016, 1-15.	1.1	8
731	An Experimental and Theoretical Investigation of the Electronic Structures and Photoelectrical Properties of Ethyl Red and Carmine Acid for DSSC Application. <i>Materials</i> , 2016, 9, 813.	1.3	54
732	Exploring the Interaction Natures in Plutonyl (VI) Complexes with Topological Analyses of Electron Density. <i>International Journal of Molecular Sciences</i> , 2016, 17, 414.	1.8	10
733	The Trans Influence in Unsymmetrical Pincer Palladacycles: An Experimental and Computational Study. <i>Inorganics</i> , 2016, 4, 25.	1.2	8
734	Charge Transfer Enhancement in the D- π -A Type Porphyrin Dyes: A Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT) Study. <i>Molecules</i> , 2016, 21, 1618.	1.7	9
735	First-Principles Investigation on Triazine Based Thermally Activated Delayed Fluorescence Emitters. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 291-296.	0.6	25
736	Structural and Infrared Spectroscopic Study on Solvation of Acetylene by Protonated Water Molecules. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 31-37.	0.6	0
737	From Corannulene to Indacenopirone: Effect of Carbon Framework Topology on Aromaticity and Reduction Limits. <i>Organometallics</i> , 2016, 35, 3105-3111.	1.1	24
738	C ₂ H ₅ OH-HX (X=OH, SH, F) interactions: Is there a carbon bond?. <i>Journal of Chemical Sciences</i> , 2016, 128, 1191-1198.	0.7	1
739	The Effect of Donor Group Rigidification on the Electronic and Optical Properties of Arylamine-Based Metal-Free Dyes for Dye-Sensitized Solar Cells: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5917-5927.	1.1	69
740	Evaluating the Free Energies of Solvation and Electronic Structures of Lithium-Ion Battery Electrolytes. <i>ChemPhysChem</i> , 2016, 17, 2916-2930.	1.0	36
741	Density functional theory study on the possibility of Si, Ge, and Sn doped carbon nanotubes as efficient support materials for platinum. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 515-523.	1.0	4
742	A noble interaction: An assessment of noble gas binding ability of metal oxides (metal = Cu, Ag, Au). <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1016-1024.	1.0	26
743	Theoretical studies on structures and nonlinear optical properties of alkali doped electrides B ₁₂ N ₁₂ -M (M = Li, Na, K). <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1296-1302.	1.0	29

#	ARTICLE	IF	CITATIONS
744	Structure and stability of noble gas bound compounds (Ea€%o=â€%oC, Ge, Sn, Pb; Xâ€%o=â€%oH, F, Cl, Br). Journal of Computational Chemistry, 2016, 37, 226-236.	1.5	28
745	How the substituents in corannulene and sumanene derivatives alter their molecular assemblings and charge transport properties?-A theoretical study with a dimer model. Journal of Computational Chemistry, 2016, 37, 813-824.	1.5	20
746	ORBKIT: A modular python toolbox for crossâ€platform postprocessing of quantum chemical wavefunction data. Journal of Computational Chemistry, 2016, 37, 1511-1520.	1.5	88
747	Crystal Structure and Properties of 7â€minoâ€3â€Nitroiminoâ€2,4,6,8â€Tetraazabicyclo[3.3.0]Octane Hydrochloride. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2016, 642, 635-642.	0.6	5
748	Modulating excited state properties of thermally activated delayed fluorescence molecules by tuning the connecting pattern. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
749	Structures and enhanced third-order nonlinear optical performance of four complexes investigated by thin film Z-scan technique. Transition Metal Chemistry, 2016, 41, 721-730.	0.7	2
750	Aromatic nucleophilic substitution in aprotic solvents using hydrogenâ€bonded biological amines. Kinetic studies and quantum chemical calculations. Journal of Physical Organic Chemistry, 2016, 29, 565-573.	0.9	3
751	Investigation of substituent effects in aerogenâ€bonding interaction between ZO₃ (Z=Kr, Tj ETQq1 1,0,784314 rgBT /O	1.0	39
752	Halogen bonding in biological context: a computational study of D2 dopamine receptor. Journal of Physical Organic Chemistry, 2016, 29, 645-655.	0.9	21
753	Chemical mechanism of surface-enhanced Raman scattering via charge transfer in fluorenoneâ€Ag complex. Journal of Physics Condensed Matter, 2016, 28, 214002.	0.7	6
754	Syntheses and Promising Properties of Dense Energetic 5,5â€2â€Dinitraminoâ€3,3â€2â€azoâ€1,2,4â€oxadiazole and Its Salts. Angewandte Chemie, 2016, 128, 3252-3255.	1.6	22
755	Syntheses and Promising Properties of Dense Energetic 5,5â€2â€Dinitraminoâ€3,3â€2â€azoâ€1,2,4â€oxadiazole and Its Salts. Angewandte Chemie - International Edition, 2016, 55, 3200-3203.	7.2	75
756	Theoretical Study on the Reaction Mechanism of Ti with CH₃CN in the Gas Phase. Journal of Physical Chemistry A, 2016, 120, 5457-5463.	1.1	7
757	Computational studies of stable hexanuclear Cu₂Ag₂Au₂ (<i> </i>â€%o+â€%o<i> </i>â€%o+â€%o<i> </i>â€%o+â€%o<i> </i>â€%o+â€%o<i> </i>â€%o+â€%o) clusters. International Journal of Quantum Chemistry, 2016, 116, 1006-1015.	1.0	6
758	The hydrogen storage on heptacoordinate carbon motif CTi72+. International Journal of Hydrogen Energy, 2016, 41, 11301-11307.	3.8	24
759	Unsaturation in binuclear heterometallic carbonyls: the cyclopentadienyliron manganese carbonyl CpFeMn(CO)_n system as a hybrid of the Cp₂Fe₂(CO)_n and Mn₂(CO)_n systems. New Journal of Chemistry, 2016, 40, 7482-7492.	1.4	4
760	Baeckeins J and K, Two Novel <i>C</i>â€Methylated Biflavonoids from the Roots of <i>Baeckeaâ€frutescens</i> and Their Cytoprotective Activities. Helvetica Chimica Acta, 2016, 99, 499-505.	1.0	3
761	Electron density properties and metallophilic interactions of gold halides AuX₂ and Au₂X (Xâ€%o=â€%oFâ€I): <i>Ab Initio</i> calculations. International Journal of Quantum Chemistry, 2016, 116, 1350-1357.	1.0	8

#	ARTICLE	IF	CITATIONS
762	Radical attached aluminum nanoclusters: an alternative way of cluster stabilization. Physical Chemistry Chemical Physics, 2016, 18, 21746-21759.	1.3	2
763	Structures and electronic properties of B ₂ Si ₆ ^{+/0} : anion photoelectron spectroscopy and theoretical calculations. RSC Advances, 2016, 6, 62165-62171.	1.7	11
764	C ₂ in a Box: Determining Its Intrinsic Bond Strength for the X ₁ g ⁺ Ground State. Chemistry - A European Journal, 2016, 22, 4087-4099.	1.7	120
765	In Situ Synthesis and Characterization of Poly(aryleneethynylene)-Grafted Reduced Graphene Oxide. Chemistry - A European Journal, 2016, 22, 2247-2252.	1.7	14
766	Nature of the Xe ^{VI} N Bonds in F ₆ XeNCCH ₃ and F ₆ Xe(NCCH ₃) ₂ and the Stereochemical Activity of Their Xenon Valence Electron Lone Pairs. Chemistry - A European Journal, 2016, 22, 4833-4842.	1.7	16
767	Adjacent Lone Pair (ALP) Effect: A Computational Approach for Its Origin. Chemistry - A European Journal, 2016, 22, 7415-7421.	1.7	10
768	A DFT Insight on L _n Pu ⁺ (L = C ₄ H ₄), Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 51 Interactions and Electronic Spectroscopy. European Journal of Inorganic Chemistry, 2016, 2016, 1589-1595.	1.0	6
769	Preferred Binding of Carboxylates by Chiral Urea Derivatives Containing <i>trans</i> -Phenylethyl Group. Helvetica Chimica Acta, 2016, 99, 416-424.	1.0	2
770	Trifunctional Squaramide Catalyst for Efficient Enantioselective Henry Reaction Activation. Advanced Synthesis and Catalysis, 2016, 358, 1801-1809.	2.1	41
771	Effect of conformation on UV-Vis absorption spectra of disazo reactive red dyes. Wuhan University Journal of Natural Sciences, 2016, 21, 512-518.	0.2	2
772	Theoretical Insights into Halogenated Uranium Cyanide/Iso cyanide Compounds. Inorganic Chemistry, 2016, 55, 12559-12567.	1.9	4
773	Insights into the geometries, electronic and magnetic properties of neutral and charged palladium clusters. Scientific Reports, 2016, 6, 19656.	1.6	73
774	The redox mechanism of Np ^{VI} with hydrazine: a DFT study. RSC Advances, 2016, 6, 109045-109053.	1.7	10
775	Assessing covalency in equatorial U ^{IV} N bonds: density based measures of bonding in BTP and isoamethyrin complexes of uranyl. Physical Chemistry Chemical Physics, 2016, 18, 16830-16839.	1.3	24
776	Vibrational smearing of the electron density as function of the strength and directionality of interatomic interactions: nonvalent interactions of a nitro group within an island-type crystal [Fe(NO)2(SC6H4NO2)]2. Russian Chemical Bulletin, 2016, 65, 1473-1487.	0.4	8
777	The significant role of covalency in determining the ground state of cobalt phthalocyanines molecule. AIP Advances, 2016, 6, .	0.6	8
778	Molecular adsorbates as probes of the local properties of doped graphene. Scientific Reports, 2016, 6, 24796.	1.6	13
779	Photoelectron spectroscopy and density functional theory studies of N-rich energetic materials. Journal of Chemical Physics, 2016, 145, 164302.	1.2	7

#	ARTICLE	IF	CITATIONS
780	<i>Ab initio</i> investigation of structure, stability, thermal behavior, bonding, and infrared spectra of ionized water cluster $(\text{H}_2\text{O})_6^+$. <i>Journal of Chemical Physics</i> , 2016, 145, 154307.	1.2	12
781	Trifluoromethyl Derivatives of a Monometallic Cyanide Cluster Fullerene, $\text{YCN@C}_{82}(\text{C}_3)_{16/18}$. <i>Inorganic Chemistry</i> , 2016, 55, 12523-12526.	1.9	11
782	Theoretical studies of hydrogen bonding interactions between novolac resin and DMP-30. <i>RSC Advances</i> , 2016, 6, 114560-114565.	1.7	4
783	Computational Modeling of the Catalytic Cycle of Glutathione Peroxidase Nanomimic. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10108-10115.	1.1	8
784	Metal-Diazo Radicals of $\hat{\text{I}}^{\pm}$ -Carbonyl Diazomethanes. <i>Scientific Reports</i> , 2016, 6, 22876.	1.6	10
785	Ionic adsorption on the brucite (0001) surface: A periodic electrostatic embedded cluster method study. <i>Journal of Chemical Physics</i> , 2016, 145, 204708.	1.2	7
786	Enhanced hydrogen adsorption on Li-coated B12C6N6. <i>Journal of Chemical Physics</i> , 2016, 145, 164301.	1.2	25
787	Unconventional $\text{O}^{\delta-}\cdots\text{H}^{\delta+}\cdots\text{C}$ Hydrogen Bonding and Effects of Conformational Changes on Infrared Spectroscopy of <i>o</i> -Cresol in Solutions. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10196-10206.	1.1	3
788	Symmetric bifurcated halogen bonds: substituent and cooperative effects. <i>Molecular Physics</i> , 2016, 114, 3610-3619.	0.8	4
789	Z-scan measurements and TDDFT study of the two-photon absorption properties of diaqua-bis(4-hydroxy-3-methoxybenzaldehyde)-cobalt(II). <i>Molecular Crystals and Liquid Crystals</i> , 2016, 641, 71-77.	0.4	1
790	Terminal Modulation of $\text{D}^{\delta+}\cdots\text{I}^{\delta-}$ A Small Molecule for Organic Photovoltaic Materials: A Theoretical Molecular Design. <i>Journal of Physical Chemistry C</i> , 2016, 120, 28939-28950.	1.5	41
791	Structural and theoretical characterization of a new twisted 4 -^2 -substituted terpyridine compound: 4 -^2 -(isoquinolin-4-yl)-2,2 -^2 :6 -^2 ,2 -^2 -terpyridine. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 932-938.		2
792	DFT calculations in the assignment of solid-state NMR and crystal structure elucidation of a lanthanum(III) complex with dithiocarbamate and phenanthroline. <i>Dalton Transactions</i> , 2016, 45, 19473-19484.	1.6	15
793	Theoretical study on the charge transfer mechanism at donor/acceptor interface: Why TTF/TCNQ is inadaptable to photovoltaics?. <i>Journal of Chemical Physics</i> , 2016, 145, 244705.	1.2	13
794	Possible sequestration of polar gas molecules by superhalogen supported aluminum nitride nanoflakes. <i>Journal of Molecular Modeling</i> , 2016, 22, 271.	0.8	3
795	Hydration of potassium iodide dimer studied by photoelectron spectroscopy and <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2016, 145, 184307.	1.2	7
796	Theoretical study of the gaseous hydrolysis of NO_2 in the presence of NH_3 as a source of atmospheric HONO. <i>Environmental Chemistry</i> , 2016, 13, 611.	0.7	21
797	The role of TM TM s (M^{TM}) <i>d</i> valence electrons in TM@X_{12} and M@X_{12} clusters. <i>AIP Advances</i> , 2016, 6, 06		7

#	ARTICLE	IF	CITATIONS
798	Exploring the Photodeactivation Pathways of Pt[O ^N C ^N] Complexes: A Theoretical Perspective. ChemPhysChem, 2016, 17, 69-77.	1.0	18
799	A theoretical prediction of the relationships between the impact sensitivity and electrostatic potential in strained cyclic explosive and application to H-bonded complex of nitrocyclohydrocarbon. Journal of Molecular Modeling, 2016, 22, 97.	0.8	9
800	A theoretical study on the hydrogen-bonding interactions between flavonoids and ethanol/water. Journal of Molecular Modeling, 2016, 22, 95.	0.8	17
801	Theoretical investigation on activation of CH and CC bonds of 2-butyne by gas-phase Nb atom. Computational and Theoretical Chemistry, 2016, 1085, 23-30.	1.1	7
802	New insights into the selectivity of four 1,10-phenanthroline-derived ligands toward the separation of trivalent actinides and lanthanides: a DFT based comparison study. Dalton Transactions, 2016, 45, 8107-8117.	1.6	46
803	Synthesis and Characterization of Phenothiazine-Based Platinum(II)-Acetylide Photosensitizers for Efficient Dye-Sensitized Solar Cells. Chemistry - A European Journal, 2016, 22, 3750-3757.	1.7	27
804	T-shaped phenol-benzene complexation driven by π -involved noncovalent interactions. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	8
805	The impact of increasing number of nitrogens and their sequences on the aromaticity of azacarbazole derivatives: A theoretical study. Computational and Theoretical Chemistry, 2016, 1084, 119-125.	1.1	0
806	The Effect of Water and Bases on the Clustering of a Cyclohexene Autoxidation Product C ₆ H ₈ O ₇ with Sulfuric Acid. Journal of Physical Chemistry A, 2016, 120, 2240-2249.	1.1	30
807	Conformational, electronic, and spectroscopic characterization of isophthalic acid (monomer and) Tj ETQq1 1 0.784314 rgBT /Overlook Biomolecular Spectroscopy, 2016, 165, 33-46.	2.0	32
808	Influence of original and simulated microscopic units on SHG response in semiorganic NLO materials. RSC Advances, 2016, 6, 39534-39540.	1.7	9
809	A theoretical design and investigation on Zn-porphyrin-polyoxometalate hybrids with different π -linkers for searching high performance sensitizers of p-type dye-sensitized solar cells. Dyes and Pigments, 2016, 130, 168-175.	2.0	27
810	Recognition of S-Cl Chalcogen Bonding in Metal-Bound Alkylthiocyanates. Crystal Growth and Design, 2016, 16, 2979-2987.	1.4	22
811	Blue-shifted emission and enhanced quantum efficiency via π -bridge elongation in carbazole-carborane dyads. Physical Chemistry Chemical Physics, 2016, 18, 15719-15726.	1.3	41
812	Magnetic exchange coupling of chalcogen-centered radicals mediated via the 2D curved π -network: A broken-symmetry approach. Computational Materials Science, 2016, 120, 53-59.	1.4	4
813	Structure, Bonding, and Electronic Properties of Four Rare Earth Complexes with a Phenoxyacetic Acid Ligand: X-ray Diffraction and DFT Studies. Industrial & Engineering Chemistry Research, 2016, 55, 6716-6722.	1.8	13
814	Theoretical study of the structures and first hyperpolarizabilities of C ₆ OCl _n and Li@C ₆ OCl _n (n=4, 6) Tj ETQq0 0 0 rgBT /Overlook	0.8	3
815	Zero Steric Potential and bond order. Chemical Physics Letters, 2016, 652, 106-111.	1.2	5

#	ARTICLE	IF	CITATIONS
816	Hybridization and de-hybridization between the locally-excited (LE) state and the charge-transfer (CT) state: a combined experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24176-24184.	1.3	117
817	Syntheses, characterization and electrochemical and spectroscopic properties of ruthenium-iron complexes of 2,3,5,6-tetrakis(2-pyridyl)pyrazine and ferrocene-acetylide ligands. <i>Dalton Transactions</i> , 2016, 45, 10620-10629.	1.6	12
818	Thermal stability of phenolic resin: new insights based on bond dissociation energy and reactivity of functional groups. <i>RSC Advances</i> , 2016, 6, 55007-55016.	1.7	22
819	Spectral investigations of 2,5-difluoroaniline by using mass, electronic absorption, NMR, and vibrational spectra. <i>Journal of Molecular Structure</i> , 2016, 1123, 284-299.	1.8	12
820	Tailoring Surface Adsorption and Reactivity of Fullerene-Based Compounds: A Theoretical Probe into C ₂ -Gas Fullerene Surface Interactions. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12654-12665.	1.5	5
821	Electronic structure, hydrogen bonding and spectroscopic profile of a new 1,2,4-triazole-5(4H)-thione derivative: A combined experimental and theoretical (DFT) analysis. <i>Journal of Molecular Structure</i> , 2016, 1120, 215-227.	1.8	7
822	First-principle investigation on growth patterns and properties of cobalt-doped lithium nanoclusters. <i>Journal of Molecular Modeling</i> , 2016, 22, 133.	0.8	3
823	NCI concept as a powerful tool to investigate the origin of Diels-Alder reaction accelerating inside the self-assembled softball nanoreactor. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2016, 85, 237-246.	0.9	2
824	A novel dehydrogenation style of NH ₃ BH ₃ by catalyst of transition metal clusters. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 11746-11760.	3.8	13
825	Molecular structure, hydrogen-bonding patterns and topological analysis (QTAIM and NCI) of 5-methoxy-2-nitroaniline and 5-methoxy-2-nitroaniline with 2-amino-5-nitropyridine (1:1) co-crystal. <i>Journal of Molecular Structure</i> , 2016, 1119, 505-516.	1.8	18
826	Impact of heterogeneous passivation of trimethylphosphine oxide and di-methylphosphine oxide surface ligands on the electronic structure of Cd _n Se _n (n = 6, 15) quantum dots: A DFT study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2016, 83, 284-296.	1.3	6
827	Synthesis and Simple Immobilization of Palladium(II) Acyclic Diaminocarbene Complexes on Polystyrene Support as Efficient Catalysts for Sonogashira and Suzuki-Miyaura Cross-Coupling. <i>Organometallics</i> , 2016, 35, 1684-1697.	1.1	79
828	Controlling charge separation and recombination by chemical design in donor-acceptor dyads. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18536-18548.	1.3	16
829	The mutual influence between σ -hole pnictogen bonds and σ -hole halogen bonds in complexes of PO ₂ Cl and XCN/C ₆ H ₆ (X = F, Cl, Br). <i>Structural Chemistry</i> , 2016, 27, 1427-1437.	1.0	18
830	Germynes and stannynes stabilized within N ₂ PE rings (E = Ge or Sn): combined experimental and theoretical study. <i>Dalton Transactions</i> , 2016, 45, 10343-10354.	1.6	10
831	Simulations of iron K pre-edge X-ray absorption spectra using the restricted active space method. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3250-3259.	1.3	67
832	The nature of excited states in dipolar donor/fullerene complexes for organic solar cells: evolution with the donor stack size. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15955-15963.	1.3	25
833	An <i>ab initio</i> study on the nature of σ -hole interactions in pnictogen-bonded complexes with carbene as an electron donor. <i>Molecular Physics</i> , 2016, 114, 2115-2122.	0.8	18

#	ARTICLE	IF	CITATIONS
834	The stabilities and electronic structures of $\text{AlnSi}_{12}\text{N}_{12}$ ($n = 0, 1, 2,$ and 4). <i>Journal of Materials Research</i> , 2016, 31, 241-249.	1.2	1
835	Theoretical Study of Tetrahydrofuran-Stabilized Al_{13} Superatom Cluster. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3950-3957.	1.1	20
836	Density functional theory calculations on S-S bond dissociation energies of disulfides. <i>Journal of Physical Organic Chemistry</i> , 2016, 29, 6-13.	0.9	22
837	Ab initio investigation of structure, stability, polarizability, and electronic structure of Ga_4As_4 cluster. <i>Computational and Theoretical Chemistry</i> , 2016, 1084, 109-118.	1.1	1
838	Removal of oxygen functional groups in lignite by hydrothermal dewatering: An experimental and DFT study. <i>Fuel</i> , 2016, 178, 85-92.	3.4	77
839	Improving approximate determination of the noninteracting electronic kinetic energy density from electron density. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 237-246.	1.0	29
840	Theoretically predicted Fox-7 based new high energy density molecules. <i>Journal of Molecular Structure</i> , 2016, 1118, 28-33.	1.8	9
841	Prediction of neutral noble gas insertion compounds with heavier pnictides: FNgY ($\text{Ng} = \text{Kr}$ and Xe ; $\text{Y} = \text{Tl}, \text{Pb}, \text{Bi}, \text{Po}, \text{At}, \text{Rn}$). <i>Journal of Physical Chemistry A</i> , 2016, 120, 7843-7852.	1.3	21
842	Three-dimensional hydrogen bonding network in the structures of (dimethylcyanamide)cobalt(II) complexes. <i>Inorganica Chimica Acta</i> , 2016, 447, 142-149.	1.2	16
843	Intramolecular photo-induced electron transfer in nonlinear optical chromophores: Fullerene (C_{60}) derivatives. <i>Organic Electronics</i> , 2016, 33, 290-299.	1.4	27
844	On the Potential of Using the Al_7 Superatom as an Excess Electron Acceptor To Construct Materials with Excellent Nonlinear Optical Properties. <i>Inorganic Chemistry</i> , 2016, 55, 4421-4427.	1.9	18
845	Structurally Well-Defined Sigmoidal Gold Clusters: Probing the Correlation between Metal Atom Arrangement and Chiroptical Response. <i>Journal of the American Chemical Society</i> , 2016, 138, 5634-5643.	6.6	48
846	Size evolution and ligand effects on the structures and stability of $(\text{AuL})_n$ ($\text{L} = \text{Cl}, \text{SH}$). <i>Journal of Physical Chemistry A</i> , 2016, 120, 4705-4712.	1.7	27
847	Theoretical investigations on the stability of alkali metal substituted phenylpentazole. <i>Journal of Molecular Modeling</i> , 2016, 22, 106.	0.8	7
848	Decreasing the singlet-triplet gap for thermally activated delayed fluorescence molecules by structural modification on the donor fragment: First-principles study. <i>Chemical Physics Letters</i> , 2016, 652, 16-21.	1.2	43
849	Contrasting Effects of Water on the Barriers to Decarboxylation of Two Oxalic Acid Monohydrates: A Combined Rotational Spectroscopic and Ab Initio Study. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1143-1147.	2.1	15
850	Theoretical investigation of carboranylpyrrole structures and the thermal resistance and conducting properties of carboranylpyrrole polymers. <i>Structural Chemistry</i> , 2016, 27, 1061-1069.	1.0	1
851	The effects of exact exchange of density functionals on the evaluation of second hyperpolarizabilities of streptocyanines using sum-over-states method. <i>Computational and Theoretical Chemistry</i> , 2016, 1085, 40-45.	1.1	6

#	ARTICLE	IF	CITATIONS
852	Can Fluorinated Molecular Cages Be Utilized as Building Blocks of Hyperhalogens?. <i>ChemPhysChem</i> , 2016, 17, 1468-1474.	1.0	12
853	Topological Analysis of the Fukui Function. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2016, , 227-241.	0.6	19
854	Alkaloids from <i>Hippeastrum argentinum</i> and Their Cholinesterase-Inhibitory Activities: An in Vitro and in Silico Study. <i>Journal of Natural Products</i> , 2016, 79, 1241-1248.	1.5	32
855	Nickel(0)-Catalyzed Denitrogenative Transannulation of Benzotriazinones with Alkynes: Mechanistic Insights of Chemical Reactivity and Regio- and Enantioselectivity from Density Functional Theory and Experiment. <i>ACS Catalysis</i> , 2016, 6, 3496-3505.	5.5	33
856	pnictogen bonds or chalcogen bonds exploiting the effect of substitution on the formation of P π -Se noncovalent bonds. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 13820-13829.	1.3	56
857	The influence of different donor/acceptor matches on chromophore's nonlinear optical activity. <i>Dyes and Pigments</i> , 2016, 131, 215-223.	2.0	9
858	Aromatic-like behavior of germanium nanocrystals. <i>RSC Advances</i> , 2016, 6, 47434-47442.	1.7	4
859	Assessment of the basis set effect on the structural and electronic properties of organic-protected gold nanoclusters. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	6
860	Identification and H(D)-bond energies of C \cdots H(D) \cdots Cl interactions in chloride-haloalkane clusters: a combined X-ray crystallographic, spectroscopic, and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14104-14112.	1.3	54
861	Diversity of monomeric dioxo chromium species in Cr/silicalite-2 catalysts: A hybrid density functional study. <i>Computational Materials Science</i> , 2016, 118, 147-154.	1.4	25
862	Synthesis, properties, and some rhodium, iridium, and platinum complexes of a series of bulky m-terphenylphosphine ligands. <i>Polyhedron</i> , 2016, 116, 170-181.	1.0	28
863	The Optical Signature of Charges in Conjugated Polymers. <i>ACS Central Science</i> , 2016, 2, 309-315.	5.3	77
864	Loading of a Phenanthroline-Based Platinum(II) Complex onto the Surface of a Carbon Nanotube via π - π Stacking. <i>Australian Journal of Chemistry</i> , 2016, 69, 1124.	0.5	10
865	Theoretical investigation of structure diversity and electronic properties in the series isomeric [26]hexaphyrin (1.1.1.1.1.1) and [28]hexaphyrin (1.1.1.1.1.1). <i>Computational and Theoretical Chemistry</i> , 2016, 1087, 18-25.	1.1	11
866	Exploring noble gas-hydride interactions between ZOF ₂ (Z = Kr, Xe) and metal hydrides: An ab initio study. <i>Chemical Physics Letters</i> , 2016, 654, 23-28.	1.2	23
867	New cyclometalated Ir(III) complexes with bulky ligands with potential applications in LEC devices: experimental and theoretical studies of their photophysical properties. <i>New Journal of Chemistry</i> , 2016, 40, 6253-6263.	1.4	13
868	Molecular partitioning based on the kinetic energy density. <i>Chemical Physics Letters</i> , 2016, 652, 40-45.	1.2	2
869	Luminescent monometallic Cu(I) triphenylphosphine complexes based on methylated 5-trifluoromethyl-3-(2-pyridyl)-1,2,4-triazole ligands. <i>New Journal of Chemistry</i> , 2016, 40, 5325-5332.	1.4	20

#	ARTICLE	IF	CITATIONS
870	Functionalization of fullerene via the Bingel reaction with $\hat{I}\pm$ -chlorocarbanions: an ONIOM approach. <i>Journal of Molecular Modeling</i> , 2016, 22, 113.	0.8	7
871	Tuning of tetrel bonds interactions by substitution and cooperative effects in $XH_3Si\hat{A}\hat{A}NCH\hat{A}\hat{A}HM$ ($X = H, F, Cl, Br; M = Li, Na, BeH$ and MgH) complexes. <i>Molecular Physics</i> , 2016, 114, 1974-1982.	0.8	9
872	Benzimidazole ligands in the corrosion inhibition for carbon steel in acid medium: DFT study of its interaction on Fe30 surface. <i>Journal of Molecular Structure</i> , 2016, 1119, 314-324.	1.8	53
873	A comparative study of 1,3,5-Trinitroperhydro-1,3,5-triazine (RDX) and Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) under high pressures using Raman spectroscopy and DFT calculations. <i>Journal of Molecular Structure</i> , 2016, 1119, 240-249.	1.8	17
874	Information Functional Theory: Electronic Properties as Functionals of Information for Atoms and Molecules. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3634-3642.	1.1	59
875	Topological analysis of metal-ligand and hydrogen bonds in transition metal hybrid structures – A computational study. <i>Polyhedron</i> , 2016, 115, 193-203.	1.0	4
876	A synthetic, catalytic and theoretical investigation of an unsymmetrical SCN pincer palladacycle. <i>Royal Society Open Science</i> , 2016, 3, 150656.	1.1	13
877	Experimental and theoretical studies on some selected ionic liquids with different cations/anions as corrosion inhibitors for mild steel in acidic medium. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2016, 64, 252-268.	2.7	145
878	Theoretical insight into the sensitive mechanism of multilayer-shaped cocrystal explosives: compression and slide. <i>Journal of Molecular Modeling</i> , 2016, 22, 108.	0.8	2
879	Cellobiose as a model system to reveal cellulose dissolution mechanism in acetate-based ionic liquids: Density functional theory study substantiated by NMR spectra. <i>Carbohydrate Polymers</i> , 2016, 149, 348-356.	5.1	42
880	Enzyme Catalysis that Paves the Way for S-Sulfhydration via Sulfur Atom Transfer. <i>Journal of Physical Chemistry B</i> , 2016, 120, 4608-4615.	1.2	13
881	Three cation-templated Cu self-assemblies: synthesis, structures, and photocatalytic properties. <i>New Journal of Chemistry</i> , 2016, 40, 6086-6092.	1.4	25
882	Mechanisms of CO_2 capture in ionic liquids: a computational perspective. <i>Faraday Discussions</i> , 2016, 192, 479-492.	1.6	26
883	Theoretical insight into the binding energy and detonation performance of $\hat{I}\mu$ -, \hat{I}^3 -, \hat{I}^2 -CL-20 cocrystals with \hat{I}^2 -HMX, FOX-7, and DMF in different molar ratios, as well as electrostatic potential. <i>Journal of Molecular Modeling</i> , 2016, 22, 123.	0.8	35
884	Adsorption Behavior of Glucosamine-Based, Pyrimidine-Fused Heterocycles as Green Corrosion Inhibitors for Mild Steel: Experimental and Theoretical Studies. <i>Journal of Physical Chemistry C</i> , 2016, 120, 11598-11611.	1.5	401
885	Theoretical study on complexation of U with ODA, IDA and TDA based on density functional theory. <i>RSC Advances</i> , 2016, 6, 46467-46474.	1.7	6
886	Interaction of CO_2 with metal cluster-functionalized ionic liquids. <i>Journal of CO_2 Utilization</i> , 2016, 16, 257-263.	3.3	10
887	Computational evidence that hyperconjugative orbital interactions are responsible for the stability of intramolecular $Te\hat{O}/Te\hat{S}$ non-covalent interactions and comparable to hydrogen bonds in quasi-cyclic systems. <i>New Journal of Chemistry</i> , 2016, 40, 9132-9138.	1.4	10

#	ARTICLE	IF	CITATIONS
888	Nanoreactor Based on Macroporous Single Crystals of Metal-Organic Framework. <i>Small</i> , 2016, 12, 5702-5709.	5.2	74
889	DFT investigation on the selective complexation of ionic liquids based on α -amino acid anion and N7,N9-dimethyladeninium cation with CO ₂ . <i>RSC Advances</i> , 2016, 6, 85924-85932.	1.7	9
890	Metallophilic interactions in polymeric group 11 thiols. <i>Solid State Sciences</i> , 2016, 60, 92-98.	1.5	48
891	Theoretical investigation of the singlet-triplet splittings for carbazole-based thermally activated delayed fluorescence emitters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26623-26629.	1.3	47
892	Rapid Hydrogen and Oxygen Atom Transfer by a High-Valent Nickel-Oxygen Species. <i>Journal of the American Chemical Society</i> , 2016, 138, 12987-12996.	6.6	66
893	Reactivity of electrophilic chlorine atoms due to σ^* -holes: a mechanistic assessment of the chemical reduction of a trichloromethyl group by sulfur nucleophiles. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27300-27307.	1.3	9
894	Understanding the sorption mechanisms of aflatoxin B1 to kaolinite, illite, and smectite clays via a comparative computational study. <i>Journal of Hazardous Materials</i> , 2016, 320, 80-87.	6.5	58
895	Exploring the Intricacies of Weak Interactions in Metal-Metal Bonds Using an Unsymmetrical Carbonyl Precursor and a Triple-Bonded W ₂ W ₆ . <i>Paddlewheel. Inorganic Chemistry</i> , 2016, 55, 9471-9481.	1.9	3
896	DFT Studies on Styrene Polymerization Catalyzed by Cationic Rare-Earth-Metal Complexes: Origin of Ligand-Dependent Activities. <i>Organometallics</i> , 2016, 35, 3205-3214.	1.1	28
897	Exploring molecular flexibility and the interactions of Quercetin derivatives in the active site of α -glucosidase using molecular docking and charge density analysis. <i>Computational and Theoretical Chemistry</i> , 2016, 1094, 55-68.	1.1	9
898	Efficient Reductive Decomposition of Perfluorooctanesulfonate in a High Photon Flux UV/Sulfite System. <i>Environmental Science & Technology</i> , 2016, 50, 10554-10561.	4.6	161
899	Catalytic decomposition of hydrazine borane over pristine and Al-embedded boron nitride nanotubes: A DFT study. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 20172-20184.	3.8	7
900	Combinatorial Vibration-Mode Assignment for the FTIR Spectrum of Crystalline Melamine: A Strategic Approach toward Theoretical IR Vibrational Calculations of Triazine-Based Compounds. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7427-7433.	1.1	96
901	H-bond and dipole-dipole interactions between water and COO functional group in methyl benzoate derivatives: Substituent and heteroatom effects. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 70, 7-13.	1.3	2
902	Deciphering the Structural Evolution and Electronic Properties of Magnesium Clusters: An Aromatic Homonuclear Metal Mg ₁₇ Cluster. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7947-7954.	1.1	68
903	Theoretical insight into the temperature-dependent acetonitrile (ACN) solvent effect on the diacetone diperoxide (DADP)/1,3,5-tribromo-2,4,6-trinitrobenzene (TBTNB) cocrystallization. <i>Computational Materials Science</i> , 2016, 121, 232-239.	1.4	8
904	Theoretical study of cooperativity between hydrogen bond-hydrogen bond, halogen bond-halogen bond and hydrogen bond-halogen bond in ternary FX-diazine-XF (X = H and Cl) complexes. <i>Molecular Physics</i> , 2016, 114, 3464-3474.	0.8	10
905	Theoretical study on the mechanism of palladium-catalyzed sp ² CH bond activation using cyano as a directing group. <i>Journal of Organometallic Chemistry</i> , 2016, 824, 88-98.	0.8	6

#	ARTICLE	IF	CITATIONS
906	Computational insight into the cooperative role of non-covalent interactions in the aza-Henry reaction catalyzed by quinine derivatives: mechanism and enantioselectivity. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 9588-9597.	1.5	11
907	Spectroscopic and electrochemical properties of ruthenium complexes with photochromic triarylamine-dithienylethene-acetylide ligands. <i>Inorganic Chemistry Frontiers</i> , 2016, 3, 1432-1443.	3.0	11
908	A theoretical study of weak interactions in phenylenediamine homodimer clusters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29249-29257.	1.3	23
909	Invariom approach to electron density studies of open-shell compounds: the case of an organic nitroxide radical. <i>RSC Advances</i> , 2016, 6, 91694-91710.	1.7	7
910	Singlet-Triplet Splitting Energy Management via Acceptor Substitution: Complanation Molecular Design for Deep-Blue Thermally Activated Delayed Fluorescence Emitters and Organic Light-Emitting Diodes Application. <i>Advanced Functional Materials</i> , 2016, 26, 8042-8052.	7.8	141
911	Probing the potential of halogen-free superhalogen anions as effective electrolytes of Li-ion batteries: a theoretical prospect from combined ab initio and DFT studies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28576-28584.	1.3	25
912	Towards <i>N</i> -Alkylimidazole Borane-based Hypergolic Fuels. <i>Chemistry - an Asian Journal</i> , 2016, 11, 3528-3533.	1.7	21
913	Ab-initio modeling of an anion C-60 pseudopotential for fullerene-based compounds. <i>European Physical Journal D</i> , 2016, 70, 1.	0.6	5
914	Interstate Crossing-Induced Chemiexcitation Mechanism as the Basis for Imidazopyrazinone Bioluminescence. <i>ChemistrySelect</i> , 2016, 1, 3343-3356.	0.7	21
915	Carbene π -N ⁺ Coordination Bonds in Drugs: A Quantum Chemical Study. <i>Journal of Chemical Sciences</i> , 2016, 128, 1607-1614.	0.7	22
916	The influence of an inner electric field on the performance of three types of Zn-porphyrin sensitizers in dye sensitized solar cells: a theoretical study. <i>Journal of Materials Chemistry C</i> , 2016, 4, 10130-10145.	2.7	31
917	Theoretical studies on the hydrogen-bonding interactions between luteolin and water: a DFT approach. <i>Journal of Molecular Modeling</i> , 2016, 22, 257.	0.8	10
918	Structure, temperature effect and bonding order analysis of hydrated bromide clusters. <i>Chemical Physics</i> , 2016, 479, 129-142.	0.9	4
919	Acyclic π -Phosphinoamido-Germylene: Synthesis and Characterization. <i>Organometallics</i> , 2016, 35, 3635-3640.	1.1	15
920	Theoretical investigation on activation of ethene by the HNbN ⁻ anion in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2016, 1096, 74-79.	1.1	1
921	Characterization of the nucleation precursor (H ₂ SO ₄) ₃ (CH ₃) ₂ NH complex: intra-cluster interactions and atmospheric relevance. <i>RSC Advances</i> , 2016, 6, 5824-5836.	1.7	9
922	Theoretical insights into the stabilities, detonation performance, and electrostatic potentials of cocrystals containing \hat{I}^{\pm} - or \hat{I}^2 -HMX and TATB, FOX-7, NTO, or DMF in various molar ratios. <i>Journal of Molecular Modeling</i> , 2016, 22, 249.	0.8	10
923	Influence of oligothiophene-functionalized co-sensitizer on the electron injection efficiency for multiple dye-TiO ₂ interface. <i>Organic Electronics</i> , 2016, 38, 384-395.	1.4	6

#	ARTICLE	IF	CITATIONS
924	Difference in Energy between Two Distinct Types of Chalcogen Bonds Drives Regioisomerization of Binuclear (Diaminocarbene)Pd ^{II} Complexes. <i>Journal of the American Chemical Society</i> , 2016, 138, 14129-14137.	6.6	114
925	Theoretical characterization of the conformational features of unnatural oligonucleotides containing a six nucleotide genetic alphabet. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28492-28501.	1.3	9
926	Nucleophilicity of Oximes Based upon Addition to a Nitriliumcloso-Decaborate Cluster. <i>Organometallics</i> , 2016, 35, 3612-3623.	1.1	52
927	Bader's Theory of Atoms in Molecules (AIM) and its Applications to Chemical Bonding. <i>Journal of Chemical Sciences</i> , 2016, 128, 1527-1536.	0.7	389
928	Synthesis and characterization of two novel second-order nonlinear optical chromophores based on julolidine donors with excellent electro-optic activity. <i>RSC Advances</i> , 2016, 6, 99743-99751.	1.7	11
929	Highly Efficient Thermally Activated Delayed Fluorescence in Dinuclear Ag(I) Complexes with a Bis-Bidentate Tetraphosphane Bridging Ligand. <i>Inorganic Chemistry</i> , 2016, 55, 9528-9536.	1.9	71
930	Origin of the Different Reactivity of the Triatomic Anions HMoN ^{â€} and ZrNH ^{â€} toward Alkane: Compositions of the Active Orbitals. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7786-7791.	1.1	4
931	Density Functional Theory Analysis of Anthraquinone Derivative Hydrogenation over Palladium Catalyst. <i>ChemPhysChem</i> , 2016, 17, 3974-3984.	1.0	9
932	Methanol-mediated excited-state double proton transfer in 1 H-pyrrolo[3,2-h]quinoline: Concerted or Sequential Mechanism?. <i>Computational and Theoretical Chemistry</i> , 2016, 1095, 65-70.	1.1	3
933	Silicon Tetrahydroborate and Silylene Dihydroborate with Interelement Bâ€Hâ€Si and Bâ•Si Bonds. <i>Organometallics</i> , 2016, 35, 3272-3280.	1.1	13
934	Comparison of p-type sensitizers with different electron-induced effects in dye-sensitized solar cells: A theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2016, 1095, 118-124.	1.1	11
935	A mechanistic study on guanidine-catalyzed chemical fixation of CO ₂ with 2-aminobenzonitrile to quinazoline-2,4(1H,3H)-dione. <i>Organic Chemistry Frontiers</i> , 2016, 3, 823-835.	2.3	29
936	Direct siliconâ€nitrogen bonded host materials with enhanced ĩfâ€ĳ conjugation for blue phosphorescent organic light-emitting diodes. <i>Journal of Materials Chemistry C</i> , 2016, 4, 10047-10052.	2.7	18
937	Arene C(sp ²)-H Metalation at Ni ^{II} Modeled with a Reactive PONC _{Ph} Ligand. <i>Inorganic Chemistry</i> , 2016, 55, 8041-8047.	1.9	32
938	Hydrogen bonds in methaneâ€water clusters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23508-23515.	1.3	16
939	Sc ₃ N@C _s (39715)â€C ₈₂ : a missing isomer linked to Sc ₃ N@C _{2v} (39718)â€C ₈₂ by a single step Stoneâ€Wales transformation. <i>RSC Advances</i> , 2016, 6, 75588-75593.	1.7	4
940	Fluorinated antimony(â€v) derivatives: strong Lewis acidic properties and application to the complexation of formaldehyde in aqueous solutions. <i>Chemical Science</i> , 2016, 7, 6768-6778.	3.7	65
941	Topological Study of Bonding in Aquo and Bis(triazinyl)pyridine Complexes of Trivalent Lanthanides and Actinides: Does Covalency Imply Stability?. <i>Inorganic Chemistry</i> , 2016, 55, 10034-10042.	1.9	41

#	ARTICLE	IF	CITATIONS
942	Controllable Orientation of Ester-Group-Induced Intermolecular Halogen Bonding in a 2D Self-Assembly. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3164-3170.	2.1	41
943	Structure, stability, and nature of bonding in carbon monoxide bound complexes (Ea%o=â€%ogroup 14 element); J1,ETQq1 1,5 1,3 0.7843		
944	Insights on the structural and electronic properties of ScC n + , YC n + , LaC n + (n=3-6) systems. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	2
945	Two-Dimensional Inorganic Cationic Network of Thorium Iodate Chloride with Unique Halogen-Halogen Bonds. <i>Inorganic Chemistry</i> , 2016, 55, 8570-8575.	1.9	8
946	In Silico Design of Halogen-Bonding-Based Organocatalyst for Diels-Alder Reaction, Claisen Rearrangement, and Cope-Type Hydroamination. <i>Journal of Organic Chemistry</i> , 2016, 81, 7459-7470.	1.7	43
947	Organic heterocyclic molecules become superalkalis. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24356-24360.	1.3	17
948	Bis(4-nitraminofurazanyl-3-oxo)azofurazan and Derivatives: 1,2,5-Oxadiazole Structures and High-Performance Energetic Materials. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 11548-11551.	7.2	62
949	Prolonging the Emissive Lifetimes of Copper(I) Complexes with 3MLCT and 3(ï€-ï€*) State Equilibria - A Fluorene Moiety as an Energy Reservoir. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 4885-4890.	1.0	13
950	An emission-tunable fluorescent organic molecule for specific cellular imaging. <i>RSC Advances</i> , 2016, 6, 77745-77751.	1.7	4
951	How Do Distance and Solvent Affect Halogen Bonding Involving Negatively Charged Donors?. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8784-8793.	1.2	19
952	Noble gas supported B₃⁺ cluster: formation of strong covalent noble gas-boron bonds. <i>RSC Advances</i> , 2016, 6, 78611-78620.	1.7	40
953	Molecular dynamics simulations of simple aromatic compounds adsorption on single-walled carbon nanotubes. <i>RSC Advances</i> , 2016, 6, 80972-80980.	1.7	8
954	Prefunctionalized Porous Organic Polymers: Effective Supports of Surface Palladium Nanoparticles for the Enhancement of Catalytic Performances in Dehalogenation. <i>Chemistry - A European Journal</i> , 2016, 22, 12533-12541.	1.7	28
955	Novel Uranyl Coordination Polymers Based on Quinoline-Containing Dicarboxylate by Altering Auxiliary Ligands: From 1D Chain to 3D Framework. <i>Crystal Growth and Design</i> , 2016, 16, 4886-4896.	1.4	27
956	A comparative study of a fluorene-based non-fullerene electron acceptor and PC61BM in an organic solar cell at a quantum chemical level. <i>RSC Advances</i> , 2016, 6, 81164-81173.	1.7	45
957	Theoretical insight into the binding affinity enhancement of serine with the uranyl ion through phosphorylation. <i>RSC Advances</i> , 2016, 6, 69773-69781.	1.7	15
958	Unraveling weak interactions in aniline-pyrrole dimer clusters. <i>Science China Chemistry</i> , 2016, 59, 1270-1276.	4.2	6
959	The Case of Two Compounds with Similar Configuration but Nearly Mirror Image CD Spectra Refuted. Reassignment of the Absolute Configuration of (1 <i>S</i>)-Formyl-3,4-dihydrospiro[indan-1,2-ï€(1 <i>S</i>)-pyridine]. <i>Journal of Organic Chemistry</i> , 2016, 81, 7725-7732.	1.7	8

#	ARTICLE	IF	CITATIONS
960	Theoretical study on the application of double-donor branched organic dyes in dye-sensitized solar cells. <i>Materials Chemistry and Physics</i> , 2016, 181, 284-294.	2.0	7
961	Metallic-like bonding in plasma-born silicon nanocrystals for nanoscale bandgap engineering. <i>Nanoscale</i> , 2016, 8, 18062-18069.	2.8	4
962	Adsorption and corrosion inhibition properties of N-{n-[1-R-5-(quinoxalin-6-yl)-4,5-dihydropyrazol-3-yl]phenyl}methanesulfonamides on mild steel in 1 M HCl: experimental and theoretical studies. <i>RSC Advances</i> , 2016, 6, 86782-86797.	1.7	141
963	Computational Discovery of Hydrogen Bond Design Rules for Electrochemical Ion Separation. <i>Chemistry of Materials</i> , 2016, 28, 6207-6218.	3.2	17
964	Computational insights into CH ₃ MX (M = Cu, Ag and Au; X = H, F, Cl, Br and I). <i>RSC Advances</i> , 2016, 6, 84016-84024.	1.7	4
965	Anion-Controlled Positional Switching of a Phenyl Group about the Dinuclear Core of a AuSb Complex. <i>Inorganic Chemistry</i> , 2016, 55, 9162-9172.	1.9	34
966	Melokhanines Aâ€“, Bioactive Monoterpenoid Indole Alkaloids with Diverse Skeletons from <i>Melodinus khasianus</i> . <i>Journal of Natural Products</i> , 2016, 79, 2158-2166.	1.5	92
967	Probing the low-energy structures of aluminumâ€“magnesium alloy clusters: a detailed study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26177-26183.	1.3	41
968	Insight into the pseudo σ -hole interactions in the M ₃ H ₆ ⁺ (NCF) _n (M) Tj ETQg0 0 0 rgBT /Overlo	1.3	36
969	Variational first hyperpolarizabilities of 2,3-naphtho-15-crown-5 ether derivatives with cation-complexing: a potential and selective cation detector. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26487-26494.	1.3	15
970	The reactivity of tungsten hexachloride with tetrahydrofuran and 2-methoxyethanol. <i>Polyhedron</i> , 2016, 117, 769-776.	1.0	10
971	Role of Nonbond Interactions in the Glass Transition of Novolac-Type Phenolic Resin: A Molecular Dynamics Study. <i>Industrial & Engineering Chemistry Research</i> , 2016, 55, 9440-9451.	1.8	20
972	Theoretical Investigation of Noncovalent Interactions between Low-Rank Coal and Water. <i>Energy & Fuels</i> , 2016, 30, 7118-7124.	2.5	35
973	Theoretical insight into the interaction between SnX ₂ (X = H, F, Cl, Br, I) and benzene. <i>Journal of Molecular Modeling</i> , 2016, 22, 208.	0.8	6
974	Investigation of structure-directing interactions within copper(i) thiocyanate complexes through X-ray analyses and non-covalent interaction (NCI) theoretical approach. <i>CrystEngComm</i> , 2016, 18, 7104-7115.	1.3	19
975	(BB)-Carboryne Complex of Ruthenium: Synthesis by Double Bâ€“H Activation at a Single Metal Center. <i>Journal of the American Chemical Society</i> , 2016, 138, 10531-10538.	6.6	102
976	Bis(4-nitraminofurazanylâ€“azoxy)azofurazan and Derivatives: 1,2,5-Oxadiazole Structures and High-Performance Energetic Materials. <i>Angewandte Chemie</i> , 2016, 128, 11720-11723.	1.6	21
977	Unraveling the Amine-Induced Disproportionation Reaction of Perchlorinated Silanesâ€“A DFT Study. <i>Chemistry - A European Journal</i> , 2016, 22, 14328-14335.	1.7	16

#	ARTICLE	IF	CITATIONS
978	Benchmark calculations of excess electrons in water cluster cavities: balancing the addition of atom-centered diffuse functions versus floating diffuse functions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23812-23821.	1.3	5
979	DFT/TDDFT investigation on the chemical reactivities, aromatic properties, and UV-Vis absorption spectra of 1-butoxy-4-methoxybenzenepillar[5]arene constitutional isomers. <i>Journal of Molecular Modeling</i> , 2016, 22, 209.	0.8	1
980	A new insight into π - π stacking involving remarkable orbital interactions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25452-25457.	1.3	48
981	Endohedral metalloborofullerenes M@B44 (M = Ca, Sr, Ba): a computational investigation. <i>Journal of Molecular Modeling</i> , 2016, 22, 297.	0.8	8
982	Evolution of Aromatic Species in Supercages and Its Effect on the Conversion of Methanol to Olefins over H-MCM-22 Zeolite: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27964-27979.	1.5	24
983	Nucleophilic T-Shaped (LXL)Au(I)-Pincer Complexes: Protonation and Alkylation. <i>Journal of the American Chemical Society</i> , 2016, 138, 15873-15876.	6.6	56
984	Fine regulation of cellulose dissolution and regeneration by low pressure CO ₂ in DMSO/organic base: dissolution behavior and mechanism. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32772-32779.	1.3	28
985	Understanding the role of hydrogen bonding in Brønsted acidic ionic liquid-catalyzed transesterification: a combined theoretical and experimental investigation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32723-32734.	1.3	14
986	Charge Distribution Dependent Spectral Analysis of the Oxidized Diferrocenyl-Oligothiophene-Vinylene Molecular Wires. <i>Scientific Reports</i> , 2016, 6, 35726.	1.6	2
987	Unprecedented Enhancement of Noble Gas Noble Metal Bonding in NgAu ₃ ⁺ (Ng = Ar, Kr, and Xe) Ion through Hydrogen Doping. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9998-10006.	1.1	18
988	Efficient SO ₂ Capture through Multiple Chalcogen Bonds, Sulfur-Centered Hydrogen Bonds and S \cdots C \cdots C Interactions: A Computational Study. <i>ChemistrySelect</i> , 2016, 1, 1688-1694.	0.7	13
989	A computational study on structure, stability and bonding in Noble Gas bound metal Nitrates, Sulfates and Carbonates (Metal = Cu, Ag, Au). <i>Journal of Chemical Sciences</i> , 2016, 128, 1537-1548.	0.7	27
990	Cation-anion radical interactions between halopyridinium cations and metal dithiolene complexes [M(C ₂ S ₂) ₂ CN] ⁺ : A theoretical study of halogen bonds in conducting or magnetic molecular materials. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1872-1881.	1.0	5
991	A theoretical evidence for cooperative enhancement in aerogen-bonding interactions: Open-chain clusters of KrOF ₂ and XeOF ₂ . <i>Chemical Physics Letters</i> , 2016, 662, 80-85.	1.2	36
992	The strengthening effect of a hydrogen or lithium bond on the Z \cdots N aerogen bond (Z = Ar, Kr and Xe): a comparative study. <i>Molecular Physics</i> , 2016, 114, 3265-3276.	0.8	16
993	Comparing Nucleophilicity of Heavier Heteroleptic Amidinato-Amido Tetrellylenes: An Experimental and Theoretical Study. <i>ChemistrySelect</i> , 2016, 1, 1991-1995.	0.7	9
994	Probing Molecular Interactions in Functionalized Asymmetric Quaternary Ammonium-Based Dicationic Ionic Liquids. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7732-7744.	1.1	18
995	Theoretical design and characterization of high-efficiency organic dyes with different electron-withdrawing groups based on C275 toward dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2016, 40, 9320-9328.	1.4	18

#	ARTICLE	IF	CITATIONS
996	Comparative analysis of interactions between the hydropyridine dicarboxylate derivatives and different proteins by molecular docking and charge density analysis. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650050.	1.8	1
997	Theoretical study of the non linear optical properties of alkali metal (Li, Na, K) doped aluminum nitride nanocages. RSC Advances, 2016, 6, 94228-94235.	1.7	62
998	Oâ€“Hâˆ•C hydrogen bond in the methaneâ€“water complex. Russian Journal of Physical Chemistry A, 2016, 90, 1978-1985.	0.1	8
999	Theoretical investigation on exciton-dissociation and charge-recombination processes of PC61BM-PTDPPSe interface. Journal of Molecular Modeling, 2016, 22, 241.	0.8	2
1000	Noble gas bound beryllium chromate and beryllium hydrogen phosphate: a comparison with noble gas bound beryllium oxide. RSC Advances, 2016, 6, 92786-92794.	1.7	20
1001	Two rhodamine 6G derivative compounds: a structural and fluorescence single-crystal study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 684-692.	0.5	9
1002	Br...Br and van der Waals interactions along a homologous series: crystal packing of 1,2-dibromo-4,5-dialkoxybenzenes. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 693-701.	0.5	2
1003	Structure and internal rotation dynamics of the acetone-neon complex studied by microwave spectroscopy. Journal of Molecular Spectroscopy, 2016, 330, 228-235.	0.4	3
1004	Reactivity of CS ₂ â€“ Syntheses and Structures of Transitionâ€“Metal Species with Dithioformate and Methanedithiolate Ligands. European Journal of Inorganic Chemistry, 2016, 2016, 4913-4920.	1.0	18
1005	Role of functionalized acceptors in heteroleptic bipyridyl Cu(I) complexes for dye-sensitized solar cells. Electronic Materials Letters, 2016, 12, 589-595.	1.0	1
1006	Understanding the kinetics of thermal decomposition of 2,3-epoxy-2,3-dimethylbutane using RRKM theory. RSC Advances, 2016, 6, 91882-91892.	1.7	8
1007	Energetic dinitromethyl group functionalized azofurazan and its azofurazanates. RSC Advances, 2016, 6, 91477-91482.	1.7	32
1008	On describing the optoelectronic characteristics of poly(benzodithiophene-co-quinoxaline)â€“fullerene complexes: the influence of optimally tuned density functionals. Physical Chemistry Chemical Physics, 2016, 18, 27654-27670.	1.3	7
1009	MP2 study on the selectivity of gold catalysis with alkene and furan activation. Computational and Theoretical Chemistry, 2016, 1090, 245-252.	1.1	2
1010	Two- and Three-Centered Hydrogen Bonds Involving Organic Fluorine Stabilize Conformations of Hydrazide Halo Derivatives: NMR, IR, QTAIM, NCI, and Theoretical Evidence. Journal of Physical Chemistry A, 2016, 120, 7810-7816.	1.1	13
1011	Efficient modulation of optical and electrical properties of X-shaped thermally activated delayed fluorescence emitters by substitution. Journal of Molecular Modeling, 2016, 22, 173.	0.8	2
1012	Computational Design of New Heterofullereneâ€“Based Biomimetic Î±â€“Carbonic Anhydrase Analogues. ChemPhysChem, 2016, 17, 3120-3128.	1.0	5
1013	Stabilization of a Chlorinated C ₆₆ :C ₂ v Cage by Encapsulating Monometal Species: Coordination between Metal and Double Hexagon-Condensed Pentalenes. Inorganic Chemistry, 2016, 55, 7667-7675.	1.9	3

#	ARTICLE	IF	CITATIONS
1014	Capacitance, the Next of Kin to Chemical Softness and Density of States, an Unexpected Perk of Being the "Middle Child". Journal of Physical Chemistry C, 2016, 120, 17175-17183.	1.5	5
1015	Interaction of Boron-Nitrogen Doped Benzene Isomers with Water. Journal of Physical Chemistry A, 2016, 120, 6287-6302.	1.1	15
1016	molSimplify: A toolkit for automating discovery in inorganic chemistry. Journal of Computational Chemistry, 2016, 37, 2106-2117.	1.5	127
1017	The Interactions between Imidazolium-Based Ionic Liquids and Stable Nitroxide Radical Species: A Theoretical Study. Journal of Physical Chemistry A, 2016, 120, 6089-6102.	1.1	19
1018	Dielectric properties of pyridine-ethanol mixtures: density functional theory and experiments. RSC Advances, 2016, 6, 66007-66010.	1.7	8
1019	Stability of functionalized corannulene cations [$R_{20}H_{10}^{+}$]: An influence of the nature of R-Group. Journal of Computational Chemistry, 2016, 37, 2266-2278.	1.5	8
1020	Theoretical investigations toward TMEDA-catalyzed [2 + 4] annulation of allenolate with 1-aza-1,3-diene: mechanism, regioselectivity, and role of the catalyst. RSC Advances, 2016, 6, 70723-70731.	1.7	20
1021	Surface Charge-Transfer Doping of Graphene Nanoflakes Containing Double-Vacancy (5 \times 5) and Stone-Wales (5 \times 7) Defects through Molecular Adsorption. ChemPhysChem, 2016, 17, 3289-3299.	1.0	10
1022	Z-Isomers of (4 \pm 6 ϵ^3 , 2 \pm 1 ϵ^3)-phenylflavan substituted with $R^2=R=OH$. Conformational properties, electronic structure and aqueous solvent effects. Journal of Molecular Modeling, 2016, 22, 187.	0.8	3
1023	In silico study to evaluate the governing criteria in the BF ₃ catalyzed Diels-Alder reaction. Computational and Theoretical Chemistry, 2016, 1091, 176-185.	1.1	1
1024	Achieving Optimal Self-Adaptivity for Dynamic Tuning of Organic Semiconductors through Resonance Engineering. Journal of the American Chemical Society, 2016, 138, 9655-9662.	6.6	71
1025	Single-electron aerogen bonds: Do they exist?. Chemical Physics Letters, 2016, 659, 196-202.	1.2	24
1026	Small Cation-Based High-Performance Energetic Nitraminofurazanates. Chemistry - A European Journal, 2016, 22, 11846-11853.	1.7	33
1027	GenLocDip: A Generalized Program to Calculate and Visualize Local Electric Dipole Moments. Journal of Computational Chemistry, 2016, 37, 2324-2334.	1.5	6
1028	Influence of the chelator structures on the stability of Re and Tc tricarbonyl complexes with iminodiacetic acid tridentate ligands: a computational study. Journal of Molecular Modeling, 2016, 22, 179.	0.8	5
1029	Effect of Peptide Sequences on Supramolecular Interactions of Naphthaleneimide/Tripeptide Conjugates. Langmuir, 2016, 32, 7630-7638.	1.6	31
1030	Computational investigation on MB n (M = Li-Cs, Be-Ba, Sc-La and Ti; n = 28 and 38). Journal of Molecular Modeling, 2016, 22, 184.	0.8	12
1031	Infrared Spectra of Novel NgBeSO ₂ Complexes (Ng = Ne, Ar, Kr, Xe) in Low Temperature Matrixes. Journal of Physical Chemistry A, 2016, 120, 8590-8598.	1.1	22

#	ARTICLE	IF	CITATIONS
1032	Preparation of diazoalkane complexes of iron(Fe^{II}). RSC Advances, 2016, 6, 97650-97658.	1.7	9
1033	Where Does the Density Localize? Convergent Behavior for Global Hybrids, Range Separation, and DFT+U. Journal of Chemical Theory and Computation, 2016, 12, 5931-5945.	2.3	65
1034	Influence of N-Oxide Introduction on the Stability of Nitrogen-Rich Heteroaromatic Rings: A Quantum Chemical Study. Journal of Physical Chemistry A, 2016, 120, 9446-9457.	1.1	38
1035	Ab Initio Study of Ionized Water Radical Cation (H_2O^+) in Combination with the Particle Swarm Optimization Method. Journal of Physical Chemistry A, 2016, 120, 9489-9499.	1.1	11
1036	The intrinsic strength of the halogen bond: electrostatic and covalent contributions described by coupled cluster theory. Physical Chemistry Chemical Physics, 2016, 18, 33031-33046.	1.3	128
1037	Mechanistic study of allopurinol oxidation using aldehyde oxidase, xanthine oxidase and cytochrome P450 enzymes. RSC Advances, 2016, 6, 109672-109680.	1.7	8
1038	DFT studies on structural properties and electron density topologies of the iron selenides Fe_mSe_n (1) Fe_2Se_3 and Fe_3Se_4 .	0.15	2
1039	Sequestration and Activation of Small Gas Molecules on BN-Flakes and the Effect of Various Metal Oxide Molecules therein. Journal of Physical Chemistry C, 2016, 120, 27782-27799.	1.5	9
1040	Tuning of carbon bonds by substituent effects: an <i>ab initio</i> study. Molecular Physics, 2016, 114, 3658-3668.	0.8	9
1041	Theoretical Prediction on Photovoltaic Properties of $\text{4Cl-BPPQ/PC}_{61}\text{BM}$ System via Density Functional Theory Calculations. Chinese Journal of Chemistry, 2016, 34, 1143-1150.	2.6	8
1042	Second-Order Nonlinear Optical Properties of Carboranylated Square-Planar Pt(II) Zwitterionic Complexes: One-/Two-Dimensional Difference and Substituent Effect. Journal of Physical Chemistry A, 2016, 120, 9330-9340.	1.1	11
1043	Origin of Zeolite Confinement Revisited by Energy Decomposition Analysis. Journal of Physical Chemistry C, 2016, 120, 27349-27363.	1.5	12
1044	Mechanistic aspects of the activation of C-H bond in C_2H_6 by Th atom: bonding analysis and reaction coefficients. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	1
1045	Reactivity of $[\text{M}_2(\text{Cl})_2(\text{cod})_2]$ ($\text{M}=\text{Ir}, \text{Rh}$) and $[\text{Ru}(\text{Cl})_2(\text{cod})(\text{CH}_3\text{CN})_2]$ with $\text{Na}[\text{H}_2\text{B}(\text{bt})_2]$: Formation of Agostic versus Borate Complexes. Chemistry - A European Journal, 2016, 22, 17291-17297.	1.7	11
1046	The simulation of UV spectroscopy and electronic analysis of temozolomide and dacarbazine chemical decomposition to their metabolites. Journal of Molecular Modeling, 2016, 22, 270.	0.8	12
1047	Effect of Anion and Alkyl Side Chain on Structural and Dynamic Features of Ester Functionalized Ionic Liquids: Confirming Nanoscale Organization. Journal of Physical Chemistry B, 2016, 120, 11539-11555.	1.2	9
1048	Control of Radiative Exciton Recombination by Charge Transfer Induced Surface Dipoles in MoS_2 and WS_2 Monolayers. Scientific Reports, 2016, 6, 24105.	1.6	32
1049	DFT/TD-DFT calculations on the sensing mechanism of a dual response near-infrared fluorescent chemosensor for superoxide anion and hydrogen polysulfides: photoinduced electron transfer. RSC Advances, 2016, 6, 104735-104741.	1.7	23

#	ARTICLE	IF	CITATIONS
1050	Ultrasensitive molecular sensor using N-doped graphene through enhanced Raman scattering. <i>Science Advances</i> , 2016, 2, e1600322.	4.7	174
1051	GPView: A program for wave function analysis and visualization. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 70, 305-314.	1.3	7
1052	Plasiatine, an Unprecedented Indole-Phenylpropanoid Hybrid from <i>Plantago asiatica</i> as a Potent Activator of the Nonreceptor Protein Tyrosine Phosphatase Shp2. <i>Scientific Reports</i> , 2016, 6, 24945.	1.6	8
1053	Giant spin-orbit effects on ¹ H and ¹³ C NMR shifts for uranium(<i>vi</i>) complexes revisited: role of the exchange-correlation response kernel, bonding analyses, and new predictions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30462-30474.	1.3	42
1054	1-Nitro-2-trinitromethyl substituted imidazoles: a new family of high performance energetic materials. <i>Journal of Materials Chemistry A</i> , 2016, 4, 17791-17800.	5.2	38
1055	The catassembled generation of naphthalene diimide coordination networks with lone pair-π interactions. <i>Science China Chemistry</i> , 2016, 59, 1492-1497.	4.2	7
1056	Theoretical identification of structural heterogeneities of divalent nickel active sites in NiMCM-41 nanoporous catalysts. <i>Journal of Nanostructure in Chemistry</i> , 2016, 6, 365-372.	5.3	21
1057	Computational modelling of panchromatic porphyrins with strong NIR absorptions for solar energy capture. <i>Chemical Physics Letters</i> , 2016, 665, 40-46.	1.2	4
1058	Halogen transfer through halogen bonds in halogen-bound ammonia homodimers. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30961-30971.	1.3	8
1059	Photoionization of multishell fullerenes studied by ab initio and model approaches*. <i>European Physical Journal D</i> , 2016, 70, 1.	0.6	11
1060	Expanding the environmental applications of metal (Al, Ti, Mn, Fe) doped graphene: adsorption and removal of 1,4-dioxane. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32281-32292.	1.3	23
1061	Computational study of the interaction between NO, NO ⁺ , and NO ⁺ with H ₂ O. <i>Journal of Molecular Modeling</i> , 2016, 22, 276.	0.8	8
1062	Investigation of allosteric modulation mechanism of metabotropic glutamate receptor 1 by molecular dynamics simulations, free energy and weak interaction analysis. <i>Scientific Reports</i> , 2016, 6, 21763.	1.6	23
1063	DFT studies on the heterogeneous oxidation of SO ₂ by oxygen functional groups on graphene. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31691-31697.	1.3	39
1064	Cooperative halogen bonds in V-shaped H ₃ N·X ₁ X ₂ ·X ₃ Y (X ₁ , X ₂ , X ₃ = Cl and Br; Y = F, Cl and) <i>Tj ETQgO O 0 rgBT /Overlo</i>	1.7	8
1065	Role of Noncovalent Sulfur-Oxygen Interactions in Phenoxyl Radical Stabilization: Synthesis of Super Tocopherol-like Antioxidants. <i>Organic Letters</i> , 2016, 18, 5464-5467.	2.4	33
1066	Integration of inherent and induced chirality into subphthalocyanine analogue. <i>Scientific Reports</i> , 2016, 6, 28026.	1.6	10
1067	Exploring short intramolecular interactions in alkylaromatic substrates. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29616-29628.	1.3	11

#	ARTICLE	IF	CITATIONS
1068	Switching of Adsorption Properties in a Zwitterionic Metal-Organic Framework Triggered by Photogenerated Radical Triplets. <i>Chemistry of Materials</i> , 2016, 28, 7825-7832.	3.2	65
1069	The Nitrite Scavenging Properties of Catechol, Resorcinol, and Hydroquinone: A Comparative Study on Their Nitration and Nitrosation Reactions. <i>Journal of Food Science</i> , 2016, 81, C2692-C2696.	1.5	12
1070	Effect of NO ₂ substitution and solvent on UV-visible spectra, redox potentials and electron transfer mechanisms of copper 12-nitrotriarylcorroles. Proposed electrogeneration of a Cu(I) oxidation state. <i>Journal of Porphyrins and Phthalocyanines</i> , 2016, 20, 753-765.	0.4	8
1071	The structures and properties of $\text{AgCl} \cdot \text{Tj ETQq1 1 0.784314rgBT / Overlock 10}$ ($n = 20(13)$). <i>Computational and Theoretical Chemistry</i> , 2016, 1007, 70-78.		
1072	Electrophilic phenoxy-substituted phosphonium cations. <i>Dalton Transactions</i> , 2016, 45, 18156-18162.	1.6	31
1073	Theoretical Study on the Mechanism of the Thermal Retro-Cycloaddition of Isoxazolinofullerenes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8830-8842.	1.1	6
1074	Hydrogen-bonding Interactions between Apigenin and Ethanol/Water: A Theoretical Study. <i>Scientific Reports</i> , 2016, 6, 34647.	1.6	21
1075	Crystallographic and Theoretical Investigation on the Nature and Characteristics of Type I C-H...S=C Interactions. <i>Crystal Growth and Design</i> , 2016, 16, 6734-6742.	1.4	22
1076	Theoretical Study of the ESIPT Process for a New Natural Product Quercetin. <i>Scientific Reports</i> , 2016, 6, 32152.	1.6	84
1077	Demulsification of heavy oil-in-water emulsions by reduced graphene oxide nanosheets. <i>RSC Advances</i> , 2016, 6, 106297-106307.	1.7	55
1078	Flexible and highly fluorescent aromatic polyimide: design, synthesis, properties, and mechanism. <i>Journal of Materials Chemistry C</i> , 2016, 4, 10509-10517.	2.7	51
1079	Electron density properties and metallophilic interactions of coinage metal halides M_2X_2 ($M = \text{Cu, Ag and Au, X = F, I}$): <i>Ab initio</i> calculation. <i>Materials Research Express</i> , 2016, 3, 115702.	0.8	1
1080	The Pt (II) ... Cl Interactions: Nature and Strength. <i>ChemistrySelect</i> , 2016, 1, 5698-5705.	0.7	5
1081	Homocyclic chalcogen-chalcogen bond interactions in complexes pairing YO_3 and YHX molecules ($Y = \text{S, Se; X = H, Cl, Br, C, N, OH}$). <i>Quantum Chemistry</i> , 2016, 116, 529-536.	1.0	13
1082	Photoinduced Electron Transfer in Organic Solar Cells. <i>Chemical Record</i> , 2016, 16, 734-753.	2.9	66
1083	Design, Synthesis, and Structural Analysis of Divalent N ^I Compounds and Identification of a New Electron-Donating Ligand. <i>Chemistry - A European Journal</i> , 2016, 22, 1088-1096.	1.7	33
1084	Enhanced Aerogen Interaction by a Cationic Force. <i>Chemistry - A European Journal</i> , 2016, 22, 2586-2589.	1.7	21
1085	Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic [10]Annulenylic Dicationic Rings. <i>Chemistry - A European Journal</i> , 2016, 22, 2793-2800.	1.7	30

#	ARTICLE	IF	CITATIONS
1086	Comparative studies on group III σ -hole and π -hole interactions. <i>Journal of Computational Chemistry</i> , 2016, 37, 1321-1327.	1.5	49
1087	Competition between chalcogen bond and halogen bond interactions in $YOX_4:NH_3$ ($Y = S, Se$; $X = F, Cl, Br$) complexes: An ab initio investigation. <i>Structural Chemistry</i> , 2016, 27, 1439-1447.	1.0	12
1088	Theoretical study of optical activity of 1:1 hydrogen bond complexes of water with S-warfarin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 168, 180-189.	2.0	4
1089	Strengthening of the halogen-bonding by an aerogen bond interaction: substitution and cooperative effects in $O_3 \cdot Z \cdot NCX \cdot Y$ ($Z = Ar, Kr, Xe$; $X = Cl, Br, I$; $Y = H, F, OH$) complexes. <i>Molecular Physics</i> , 2016, 114, 2177-2186.	0.8	22
1090	Theoretical insight into the influence of molecular ratio on the binding energy and mechanical property of $HMX/2$ -picoline- N -oxide cocrystal, cooperativity effect and surface electrostatic potential. <i>Molecular Physics</i> , 2016, 114, 2164-2176.	0.8	27
1091	Insights into Stereoselective Aminomethylation Reaction of α, β -Unsaturated Aldehyde with N,O-Acetal via N-Heterocyclic Carbene and Brønsted Acid/Base Cooperative Organocatalysis. <i>Journal of Organic Chemistry</i> , 2016, 81, 5370-5380.	1.7	59
1092	BNg_3F_3 : the first three noble gas atoms inserted into mono-centric neutral compounds – a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17534-17545.	1.3	16
1093	Halogen and hydrogen bonding in <i>cis</i> -dichlorobis(propionitrile)platinum(II) chloroform monosolvate. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2016, 231, 435-440.	0.4	13
1094	Intermolecular charge transfer as evidence for unusual $O \cdots H \cdots C(sp^3)$ hydrogen bond. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 180-192.	1.1	16
1095	Spectroscopy (FT-IR, FT-Raman), hydrogen bonding, electrostatic potential and HOMO-LUMO analysis of tioxelone based on DFT calculations. <i>Journal of Molecular Structure</i> , 2016, 1121, 188-195.	1.8	49
1096	From information theory to quantitative description of steric effects. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17917-17929.	1.3	16
1097	Pentamidium-Catalyzed Asymmetric Phase-Transfer Conjugate Addition: Prediction of Stereoselectivity via DFT Calculations and Docking Sampling of Transition States, and Origin of Stereoselectivity. <i>Australian Journal of Chemistry</i> , 2016, 69, 983.	0.5	10
1098	A DFT study on the kinetics and mechanism of cyclodiglycine thermal decomposition in the gas phase. <i>Progress in Reaction Kinetics and Mechanism</i> , 2016, 41, 205-213.	1.1	4
1099	$NX \cdots Y$ halogen bonds. Comparison with $NH \cdots Y$ H-bonds and $CX \cdots Y$ halogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18015-18023.	1.3	17
1100	Vibrational analysis and formation mechanism of typical deep eutectic solvents: An experimental and theoretical study. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 68, 158-175.	1.3	105
1101	Dopaminergic isoquinolines with hexahydrocyclopenta[<i>ij</i>]-isoquinolines as D ₂ -like selective ligands. <i>European Journal of Medicinal Chemistry</i> , 2016, 122, 27-42.	2.6	17
1102	Correlating the Structure and Optical Absorption Properties of $Au_{76}(SR)_{44}$ Cluster. <i>Journal of Physical Chemistry C</i> , 2016, 120, 13739-13748.	1.5	30
1103	First principles optimally tuned range-separated density functional theory for prediction of phosphorus σ -hydrogen spin σ -spin coupling constants. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18431-18440.	1.3	29

#	ARTICLE	IF	CITATIONS
1104	Optical response and gas sequestration properties of metal cluster supported graphene nanoflakes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18811-18827.	1.3	26
1105	Tautomerism in substituted pyridofuroxans: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 105-111.	1.1	7
1106	Probing chemical bonding and optoelectronic properties of Square-Planar Aluminum, Gallium, and Nickel complexes. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 129-133.	1.1	4
1107	Porous organic polymer bifunctionalized with triazine and thiophene groups as a novel adsorbent for removing Cu (II). <i>Microporous and Mesoporous Materials</i> , 2016, 233, 10-15.	2.2	33
1108	DFT Study of Acceptorless Alcohol Dehydrogenation Mediated by Ruthenium Pincer Complexes: Ligand Tautomerization Governing Metal Ligand Cooperation. <i>Inorganic Chemistry</i> , 2016, 55, 6539-6551.	1.9	62
1109	A study of solvent selectivity on the crystal morphology of FOX-7 via a modified attachment energy model. <i>RSC Advances</i> , 2016, 6, 59784-59793.	1.7	32
1110	Detailed theoretical investigation on ESIPT process of pigment yellow 101. <i>RSC Advances</i> , 2016, 6, 59389-59394.	1.7	37
1111	Why HS ⁺ and CN ⁺ can be detected by different chemosensors with similar structures: a quantum mechanics and molecular dynamics study. <i>RSC Advances</i> , 2016, 6, 63548-63558.	1.7	2
1112	Theoretical study on the structure–property relationship of D–A–A–A-type dye-sensitized solar cells: –bridge and the side alkyl chain. <i>Canadian Journal of Chemistry</i> , 2016, 94, 794-801.	0.6	0
1113	Energetic aminated-azole assemblies from intramolecular and intermolecular N–H–O and N–H–N hydrogen bonds. <i>Chemical Communications</i> , 2016, 52, 8123-8126.	2.2	60
1114	2,4-Diamino-5-(phenylthio)-5H-chromeno [2,3-b] pyridine-3-carbonitriles as green and effective corrosion inhibitors: gravimetric, electrochemical, surface morphology and theoretical studies. <i>RSC Advances</i> , 2016, 6, 53933-53948.	1.7	155
1115	Adsorption of carbon monoxide on boroxol-ring-doped zigzag boron nitride nanotube: Electronic study via DFT. <i>European Physical Journal Plus</i> , 2016, 131, 1.	1.2	6
1116	From isosuperatoms to isosupermolecules: new concepts in cluster science. <i>Nanoscale</i> , 2016, 8, 12787-12792.	2.8	42
1117	Theoretical prediction on a special bridging metal–Xe–metal bond with remarkable stability in Re ₂ Cp ₂ (PF ₃) ₄ Xe. <i>Science China Chemistry</i> , 2016, 59, 760-764.	4.2	0
1118	12-vertex ruthenacarborane half-sandwich complexes: Redox properties and second-order nonlinear optical responses. <i>Journal of Organometallic Chemistry</i> , 2016, 801, 54-59.	0.8	4
1119	Synthesis, Structure, and Photophysical Properties of Mo ₂ (NN) ₂ and Mo ₂ (NN) ₂ (T ^{sup} PB) ₂ , Where NN = <i>N,N</i> -Diphenylphenylpropiolamidinate and T ^{sup} PB = 2,4,6-Triisopropylbenzoate. <i>Inorganic Chemistry</i> , 2016, 55, 5836-5844.	1.9	5
1120	Hypo-electronic triple-decker sandwich complexes: synthesis and structural characterization of [(Cp*Mo) ₂ {(E)–B ₄ H ₄ –E–Ru(CO) ₃ }] (E = S, Se, Te or Ru(CO) ₃ and Cp* = <i>η</i> -C ₅ Me ₅). <i>Dalton Transactions</i> , 2016, 45, 10999-11007.	1.6	19
1121	Theoretical studies on oxidation-switchable second-order nonlinear optical responses of Metallosalen-Keggin polyoxometalate derivatives. <i>RSC Advances</i> , 2016, 6, 53438-53443.	1.7	3

#	ARTICLE	IF	CITATIONS
1122	Solution-processed OLEDs based on phosphorescent PtAu ₂ complexes with phenothiazine-functionalized acetylides. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6096-6103.	2.7	39
1123	Insights into the reaction mechanism of propene H/D exchange over acidic zeolite catalysts from theoretical calculations. <i>Catalysis Science and Technology</i> , 2016, 6, 6328-6338.	2.1	9
1124	Synthesis and reactivity of a terminal uranium(IV) sulfide supported by siloxide ligands. <i>Chemical Science</i> , 2016, 7, 5846-5856.	3.7	23
1125	Schiff pentadentate ligands based on an [ON ₂ O ₂] core displaying structural isomerism and their coordination to dibutyltin moieties. <i>Inorganic Chemistry Communication</i> , 2016, 70, 75-78.	1.8	3
1126	A theoretical study of π -stacking interactions in C-substituted tetrazoles. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 67, 85-93.	1.3	6
1127	Adsorption properties of boroxol ring doped zigzag boron nitride nanotube toward NO molecule using DFT. <i>International Journal of Modern Physics B</i> , 2016, 30, 1650101.	1.0	1
1128	Computational Studies on the Mo-Doped Gold Nanoclusters Au _n Mo(n=1-10): Structures, Stabilities and Magnetic Properties. <i>Journal of Cluster Science</i> , 2016, 27, 993-1004.	1.7	5
1129	Theoretical investigation on correlation between steric effects and selectivity in gas-solid chlorination of polyvinyl chloride. <i>Chemical Engineering Science</i> , 2016, 151, 64-78.	1.9	6
1130	Theoretical characterization on photovoltaic properties of PC61BM-PTDPPPTFT4 system with a molecular model. <i>Computational and Theoretical Chemistry</i> , 2016, 1089, 6-12.	1.1	0
1131	Characterization of Cu-ligand bonds in tris-pyrazolylmethane isocyanide copper(I) complexes based upon combined X-ray diffraction and theoretical study. <i>Inorganica Chimica Acta</i> , 2016, 450, 140-145.	1.2	10
1132	Influences of the confinement effect and acid strength of zeolite on the mechanisms of Methanol-to-Olefins conversion over H-ZSM-5: A theoretical study of alkenes-based cycle. <i>Microporous and Mesoporous Materials</i> , 2016, 231, 216-229.	2.2	30
1133	Complexation of [Gd(DTTA-Me)(H ₂ O) ₂] ⁺ by Fluoride and Its Consequences to Water Exchange. <i>Inorganic Chemistry</i> , 2016, 55, 6231-6239.	1.9	9
1134	The photoluminescence mechanism of ultra-small gold clusters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17320-17325.	1.3	13
1135	Excited-state dynamics and electron transfer process of 1,3,5-triamino-2,4,6-trinitrobenzene. <i>RSC Advances</i> , 2016, 6, 55560-55567.	1.7	8
1136	Spirooxazine-Fulgide Biphotochromic Molecular Switches with Nonlinear Optical Responses across Four States. <i>Journal of Physical Chemistry C</i> , 2016, 120, 14840-14853.	1.5	37
1137	A family of heterotetrameric clusters of chloride species and halomethanes held by two halogen and two hydrogen bonds. <i>CrystEngComm</i> , 2016, 18, 5278-5286.	1.3	55
1138	Methane adsorption on the surface of a model of shale: A density functional theory study. <i>Applied Surface Science</i> , 2016, 387, 379-384.	3.1	25
1139	Paddlewheel 1,2,4-diazaphospholide distibines with the shortest antimony-antimony single bonds. <i>Dalton Transactions</i> , 2016, 45, 10505-10509.	1.6	7

#	ARTICLE	IF	CITATIONS
1158	Flavonolâ€“carbon nanostructure hybrid systems: a DFT study on the interaction mechanism and UV/Vis features. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4760-4771.	1.3	7
1159	Ionic Liquids as Electrolytes for Electrochemical Double-Layer Capacitors: Structures that Optimize Specific Energy. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 3396-3406.	4.0	175
1160	Theoretical insights into nature of ĩ€-hole interactions between triel centers (B and Al) and radical methyl as a potential electron donor: Do single-electron triel bonds exist?. <i>Structural Chemistry</i> , 2016, 27, 1157-1164.	1.0	28
1161	Surface study and sensing activity of nanotubular indium trioxide to NH ₃ , H ₂ S, NO ₂ and CO environmental pollutants. <i>Applied Surface Science</i> , 2016, 363, 421-431.	3.1	5
1162	Theoretical insight into electronic structure and optoelectronic properties of heteroleptic Cu(I)-based complexes for dye-sensitized solar cells. <i>Materials Chemistry and Physics</i> , 2016, 173, 139-145.	2.0	19
1163	Axial, Helical, and Planar Chirality in Directly Linked Basket-Handle Porphyrin Arrays. <i>Journal of Organic Chemistry</i> , 2016, 81, 1075-1088.	1.7	17
1164	Synthesis, Bonding, and Reactivity of Vanadium(IV) Oxidoâ€“Fluorido Compounds with Neutral Chelate Ligands of the General Formula $[V^{IV}(O)(F)(L)_{2}]^{+}$. <i>Inorganic Chemistry</i> , 2016, 55, 1364-1366.	1.9	7
1165	Aromatic stabilization of functionalized corannulene cations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11781-11791.	1.3	19
1166	Synthesis, structural study and biological activity of new derivatives of chrysin containing a 2-mercaptopyridyl or 5-(trifluoromethyl)-2-mercaptopyridyl fragments. <i>Journal of Molecular Structure</i> , 2016, 1110, 196-207.	1.8	12
1167	Can an entirely negative fluorine in a molecule, viz. perfluorobenzene, interact attractively with the entirely negative site(s) on another molecule(s)? Like liking like!. <i>RSC Advances</i> , 2016, 6, 19098-19110.	1.7	42
1168	Stability and Characteristics of the Halogen Bonding Interaction in an Anionâ€“Anion Complex: A Computational Chemistry Study. <i>Journal of Physical Chemistry B</i> , 2016, 120, 610-620.	1.2	44
1169	Dicarboxylate ligand-modulated assembly of new luminescent zinc(ii) coordination polymers with in situ formed tetrazole ligands: an experimental and theoretical study. <i>RSC Advances</i> , 2016, 6, 3341-3349.	1.7	15
1170	Theoretical investigation of the backboneâ€“ and ĩ€-stacking interactions in substituted-benzene 3-methyl-2â€“deoxyadenosine: a perspective to the DNA repair. <i>Molecular Physics</i> , 2016, 114, 774-783.	0.8	3
1171	Quantum chemical insight into the reactivity of 1,3-dipoles on coronene as model for nanographenes. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 173-182.	0.1	1
1172	Molecular structure, spectroscopy (FT-IR, FT-Raman), thermodynamic parameters, molecular electrostatic potential and HOMO-LUMO analysis of 2, 6-dichlorobenzamide. <i>Journal of Molecular Structure</i> , 2016, 1108, 307-314.	1.8	26
1173	Vibrational Spectra and Theoretical Calculations of <i>cis</i> - and <i>trans</i> -3-Fluoro-N-methylaniline in the Neutral (S_0) and Cationic (D_0) Ground States. <i>Journal of Physical Chemistry A</i> , 2016, 120, 81-94.	1.1	9
1174	Computational assessment of several hydrogen-free high energy compounds. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 63, 85-90.	1.3	5
1175	Exploring the interaction between human focal adhesion kinase and inhibitors: a molecular dynamic simulation and free energy calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 2351-2366.	2.0	11

#	ARTICLE	IF	CITATIONS
1176	Simultaneous interactions of amphoteric halogen in XY (X = Cl, Br and Y = F, Cl, Br) with C and O atoms of CO ₂ in ring-shaped CO ₂ -X(Y)-CO ₂ complexes. Computational and Theoretical Chemistry, 2016, 1076, 32-41.	1.1	11
1177	Computational and spectroscopic studies of the imidazole-fused phenanthroline derivatives containing phenyl, naphthyl, and anthryl groups. Journal of Molecular Structure, 2016, 1108, 46-53.	1.8	11
1178	Effects of Cl ⁻ 3-doping on electronic and structural properties of Stone-Wales defective boron nitride nanotubes as well as their NO gas sensitivity. RSC Advances, 2016, 6, 11353-11369.	1.7	6
1179	Use of ⁷⁷ Se and ¹²⁵ Te NMR Spectroscopy to Probe Covalency of the Actinide-Chalcogen Bonding in [Th(E) _n]{N(SiMe ₃) ₂] ₃ (E = Se, Te) Tj ETQq 1 1 0.784314 138, 814-825.	1.0	1
1180	Effect of Î€-conjugate units on the ferrocene-based complexes: Switchable second order nonlinear optics controlled by redox stimuli. Dyes and Pigments, 2016, 126, 29-37.	2.0	11
1181	DFT perspective toward [3 + 2] annulation reaction of enals with Î±-ketoamides through NHC and Brønsted acid cooperative catalysis: mechanism, stereoselectivity, and role of NHC. Organic Chemistry Frontiers, 2016, 3, 190-203.	2.3	74
1182	A DFT Study on Rh-Catalyzed Asymmetric Dearomatization of 2-Naphthols Initiated with Câ€“H Activation: A Refined Reaction Mechanism and Origins of Multiple Selectivity. ACS Catalysis, 2016, 6, 262-271.	5.5	63
1183	In silico studies with substituted adenines to achieve a remarkable stability of mispairs with thymine nucleobase. New Journal of Chemistry, 2016, 40, 1807-1816.	1.4	8
1184	N-Heterocyclic Carbene (NHC)-Catalyzed sp ³ Î²-Câ€“H Activation of Saturated Carbonyl Compounds: Mechanism, Role of NHC, and Origin of Stereoselectivity. ACS Catalysis, 2016, 6, 279-289.	5.5	99
1185	DFT investigations of uranium complexation with amidoxime-, carboxyl- and mixed amidoxime/carboxyl-based host architectures for sequestering uranium from seawater. Inorganica Chimica Acta, 2016, 441, 117-125.	1.2	24
1186	Density functional theory study of Mo-doped M@(BN) ₄₈ (M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu) clusters. Journal of Molecular Structure, 2016, 1108, 92-95.	1.8	2
1187	Direct transition mechanism for molecular diffusion in gas hydrates. RSC Advances, 2016, 6, 1966-1972.	1.7	25
1188	Enhanced third-order nonlinear optical properties of three 2D coordination polymers based on bis(imidazole) ligands and dicarboxylic ligands. Polyhedron, 2016, 111, 16-25.	1.0	12
1189	Theoretical and Experimental Study of Inclusion Complexes of Î²-Cyclodextrins with Chalcone and 2â€²,4â€²-Dihydroxychalcone. Journal of Physical Chemistry B, 2016, 120, 3000-3011.	1.2	46
1190	Rate-limited effect of reverse intersystem crossing process: the key for tuning thermally activated delayed fluorescence lifetime and efficiency roll-off of organic light emitting diodes. Chemical Science, 2016, 7, 4264-4275.	3.7	212
1191	High stability of the He atom confined in a U@C ₆₀ fullerene. RSC Advances, 2016, 6, 29288-29293.	1.7	3
1192	First principles study on the structural evolution and properties of (MCl) _n (n = 1-12, M =) Tj ETQq 0,0 rgBT /Overlock 10	1.7	10
1193	Solvent effect on molecular structure, IR spectra, thermodynamic properties and chemical stability of zoledronic acid: DFT study. Journal of Molecular Modeling, 2016, 22, 84.	0.8	15

#	ARTICLE	IF	CITATIONS
1194	The effect of heteroatoms and end groups of polymethines on the all-optical switching processing application: a CC2 calculation. <i>Structural Chemistry</i> , 2016, 27, 1211-1220.	1.0	5
1195	Ion-π interaction in impacting the nonlinear optical properties of ion-buckybowl complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 64, 139-146.	1.3	5
1196	Probing the effects of the ester functional group, alkyl side chain length and anions on the bulk nanostructure of ionic liquids: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 9734-9751.	1.3	7
1197	Solid state and dynamic solution structures of O-carbamidine amidoximes gives further insight into the mechanism of zinc(II)-mediated generation of 1,2,4-oxadiazoles. <i>Journal of Molecular Structure</i> , 2016, 1111, 142-150.	1.8	44
1198	Insights into the use of Au ₁₉ Cu and Au ₁₉ Pd clusters for adsorption of trivalent arsenic. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	11
1199	Probing solvent-solvent and solute-solvent interactions in surfactant binary mixtures: solvatochromic parameters, preferential solvation, and quantum theory of atoms in molecules analysis. <i>RSC Advances</i> , 2016, 6, 18515-18524.	1.7	10
1200	Understanding the [2n+2n] reaction mechanism between a carbenoid intermediate and CO ₂ . <i>Molecular Physics</i> , 2016, 114, 1374-1391.	0.8	20
1201	Conformational transition of Aβ ₄₂ inhibited by a mimetic peptide. A molecular modeling study using QM/MM calculations and QTAIM analysis. <i>Computational and Theoretical Chemistry</i> , 2016, 1080, 56-65.	1.1	23
1202	Understanding the anion-π interactions with tetraoxacalix[2]arene[2]triazine. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6913-6924.	1.3	35
1203	Impact of persulfate and ultraviolet light activated persulfate pre-oxidation on the formation of trihalomethanes, haloacetonitriles and halonitromethanes from the chlor(am)ination of three antibiotic chloramphenicols. <i>Water Research</i> , 2016, 93, 48-55.	5.3	97
1204	Investigation of the adsorption characteristics of some selected sulphonamide derivatives as corrosion inhibitors at mild steel/hydrochloric acid interface: Experimental, quantum chemical and QSAR studies. <i>Journal of Molecular Liquids</i> , 2016, 215, 763-779.	2.3	73
1205	DFT studies on the mechanism of palladium catalyzed arylthiolation of unactive arene to diaryl sulfide. <i>RSC Advances</i> , 2016, 6, 18300-18307.	1.7	7
1206	Synthesis of π-extended N-fused heteroacenes via regioselective Cadogan reaction. <i>Tetrahedron Letters</i> , 2016, 57, 1468-1472.	0.7	8
1207	A DFT study on PBu ₃ -catalyzed intramolecular cyclizations of N-allylic substituted β-amino nitriles for the formation of functionalized pyrrolidines: mechanisms, selectivities, and the role of catalysts. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 3130-3141.	1.5	32
1208	Hydrogen bonded D ₃ h-HA...Y (Y = O, S, Hal) molecular complexes: A natural bond orbital analysis. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 601-609.	0.1	5
1209	OH-initiated oxidation mechanism and kinetics of organic sunscreen benzophenone-3: A theoretical study. <i>Chemical Papers</i> , 2016, 70, .	1.0	6
1210	A new perspective on quantifying electron localization and delocalization in molecular systems. <i>Computational and Theoretical Chemistry</i> , 2016, 1080, 33-37.	1.1	40
1211	Electron conjugation versus π-π repulsion in substituted benzenes: why the carbon-nitrogen bond in nitrobenzene is longer than in aniline. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11821-11828.	1.3	33

#	ARTICLE	IF	CITATIONS
1212	Penetrating the Elusive Mechanism of Copper-Mediated Fluoromethylation in the Presence of Oxygen through the Gas-Phase Reactivity of Well-Defined [LCuO] ⁺ Complexes with Fluoromethanes (CH ₃ F _n , n = 1–3). <i>Journal of the American Chemical Society</i> , 2016, 138, 3125-3135.	6.6	32
1213	Theoretical study of the effect of ligand topology on Fe(IV)O and Ru(IV)O complex reactivities. <i>Inorganica Chimica Acta</i> , 2016, 443, 235-242.	1.2	2
1214	Electron density topography based model to explore N-methyl-d-aspartate receptor channel blockers. <i>Chemical Physics Letters</i> , 2016, 648, 53-59.	1.2	1
1215	Cationic P←N interaction in XH ₃ P + a ⁻ NCY complexes (X = H, F, CN, NH ₂ , OH; Y = H, Li, F, Cl) and its cooperativity with hydrogen/lithium/halogen bond. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 64, 131-138.	1.3	5
1216	Intrinsic Properties of Two Benzodithiophene-Based Donor–Acceptor Copolymers Used in Organic Solar Cells: A Quantum-Chemical Approach. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1051-1064.	1.1	8
1217	Synthesis and electronic properties of polycyclic aromatic hydrocarbons doped with phosphorus and sulfur. <i>Dalton Transactions</i> , 2016, 45, 1896-1903.	1.6	24
1218	Comparison of the directionality of the halogen, hydrogen, and lithium bonds between HOOH and XF (X = Cl, Br, H, Li). <i>Journal of Molecular Modeling</i> , 2016, 22, 52.	0.8	4
1219	Systematic theoretical investigation of structure and electronic properties of pure copper and lithium doped copper clusters. <i>Molecular Physics</i> , 2016, 114, 1644-1656.	0.8	5
1220	Adsorption of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) on a soil organic matter. A DFT M05 computational study. <i>Chemosphere</i> , 2016, 148, 294-299.	4.2	6
1221	Cooperativity of tetrel bonds tuned by substituent effects. <i>Molecular Physics</i> , 2016, 114, 1528-1538.	0.8	34
1222	Charge-transfer interactions between TCNQ and silver clusters Ag ₂₀ and Ag ₁₃ . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7190-7196.	1.3	22
1223	Fluorine substitution effects of halide anion receptors based on the combination of a distinct hydrogen bond and anion–π noncovalent interactions: a theoretical investigation. <i>RSC Advances</i> , 2016, 6, 14666-14677.	1.7	10
1224	5-Arylpyrimido-[4,5-b]quinoline-diones as new and sustainable corrosion inhibitors for mild steel in 1 M HCl: a combined experimental and theoretical approach. <i>RSC Advances</i> , 2016, 6, 15639-15654.	1.7	133
1225	Understanding the Mechanism of the Lewis Acid Promoted [3 + 2] Cycloaddition of Propargylic Alcohol and 1±-Oxo Ketene Dithioacetals. <i>Journal of Organic Chemistry</i> , 2016, 81, 1989-1997.	1.7	13
1226	Theoretical design and selectivity researches on the enrofloxacin imprinted polymer. <i>Structural Chemistry</i> , 2016, 27, 1135-1142.	1.0	6
1227	Synthesis, Structure, and Photophysical Properties of Two Four-Coordinate Cu ^I –NHC Complexes with Efficient Delayed Fluorescence. <i>Inorganic Chemistry</i> , 2016, 55, 2157-2164.	1.9	70
1228	Exploring the electrochemical properties of hole transport materials with spiro-cores for efficient perovskite solar cells from first-principles. <i>Nanoscale</i> , 2016, 8, 6146-6154.	2.8	124
1229	Development of a predictive model for corrosion inhibition of carbon steel by imidazole and benzimidazole derivatives. <i>Corrosion Science</i> , 2016, 108, 23-35.	3.0	177

#	ARTICLE	IF	CITATIONS
1230	Intermolecular perturbation in the self-assembly of melamine. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	7
1231	Theoretical and infrared investigation of 2-acetylpyridine isolated in solid nitrogen and in neat condensed phases. <i>Journal of Molecular Structure</i> , 2016, 1115, 214-219.	1.8	0
1232	Experimental and theoretical investigations on spectroscopic properties of the imidazole-fused phenanthroline and its derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 161, 27-32.	2.0	13
1233	Single Step Stone-Ångström Transformation Linking Two Thermodynamically Stable Sc ₂ O@C ₇₈ Isomers. <i>Inorganic Chemistry</i> , 2016, 55, 2220-2226.	1.9	19
1234	The effect of functional groups on the SO ₂ adsorption on carbon surface I: A new insight into noncovalent interaction between SO ₂ molecule and acidic oxygen-containing groups. <i>Applied Surface Science</i> , 2016, 369, 552-557.	3.1	45
1235	Fine structural tuning of diketopyrrolopyrrole-cored donor materials for small molecule-fullerene organic solar cells: A theoretical study. <i>Organic Electronics</i> , 2016, 32, 134-144.	1.4	88
1236	Structure, stability and reactivity of neutral and charged monomeric chromium oxide clusters. <i>Computational and Theoretical Chemistry</i> , 2016, 1082, 58-66.	1.1	6
1237	Rationalization of the selectivity between 1,3- and 1,2-migration: a DFT study on gold(<i>i</i> -scp)-catalyzed propargylic ester rearrangement. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 3558-3563.	1.5	22
1238	New iridium(III) cyclometalates with extended absorption features for bulk heterojunction solar cells. <i>Journal of Organometallic Chemistry</i> , 2016, 812, 280-286.	0.8	11
1239	Insights into the hydrogen dissociation mechanism on lithium edge-decorated carbon rings and graphene nanoribbon. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 5709-5715.	3.8	14
1240	An <i>ab initio</i> study on competition between pnictogen and chalcogen bond interactions in binary XHS:PH ₂ X complexes (X = F, Cl, CCH, COH, CH ₃ , OH, OCH ₃ and Tj ETQq0 0.3 rgBT / Overlock 10	0.8	11
1241	Theoretical studies on the bonding and electron structures of a [Au ₃ Sb ₆] ³⁺ complex and its oligomers. <i>Dalton Transactions</i> , 2016, 45, 11657-11667.	1.6	8
1242	A theoretical investigation of the removal of methylated arsenic pollutants with silicon doped graphene. <i>RSC Advances</i> , 2016, 6, 28500-28511.	1.7	19
1243	Theoretical assessment of the electro-optical features of the group III nitrides (B ₁₂ N ₁₂ , Al ₁₂ N ₁₂ and Tj ETQq1 1 0.784314 rgBT / Overlock 83	3.1	83
1244	Aromatic Dicypra[10]annulenes. <i>Journal of the American Chemical Society</i> , 2016, 138, 60-63.	6.6	74
1245	Electronic and optical properties of the Au ₂₂ [1,8-bis(diphenylphosphino) octane] ₆ nanoclusters disclosed by DFT and TD-DFT calculations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	12
1246	A Computational Study of the Interaction and Polarization Effects of Complexes Involving Molecular Graphene and C ₆₀ or a Nucleobases. <i>Journal of Physical Chemistry A</i> , 2016, 120, 284-298.	1.1	20
1247	Viability of aromatic all-pnictogen anions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11738-11745.	1.3	9

#	ARTICLE	IF	CITATIONS
1248	Anions of uracils: N1 or N3? That is the question. Computational and Theoretical Chemistry, 2016, 1078, 81-87.	1.1	12
1249	Quasi-Chalcogen Characteristics of Al ₁₂ Be: A New Member of the Three-Dimensional Periodic Table. Journal of Physical Chemistry C, 2016, 120, 2464-2471.	1.5	25
1250	High-efficiency solution-processed OLEDs based on cationic Ag ₆ Cu heteroheptanuclear cluster complexes with aromatic acetylides. Journal of Materials Chemistry C, 2016, 4, 1787-1794.	2.7	46
1251	Cooperative effects between halogen bonds and pnictogen bonds in XBr TM â TM â TM OFH2Pâ TM â TM â TM NH3 (X = F, Cl, CN, NC ₅) Tj ETC	0.8	5
1252	Synthesis of new phosphorescent imidoyl-indazol and phosphine mixed ligand Cu(<i>scpi</i>) complexes â€“ structural characterization and photophysical properties. RSC Advances, 2016, 6, 5141-5153.	1.7	24
1253	The origin of the stereoselective alkylation of 3-substituted-2-oxopiperazines: A computational investigation. Computational and Theoretical Chemistry, 2016, 1078, 1-8.	1.1	0
1254	Uâ€“O _{yl} Stretching Vibrations as a Quantitative Measure of the Equatorial Bond Covalency in Uranyl Complexes: A Quantum-Chemical Investigation. Inorganic Chemistry, 2016, 55, 573-583.	1.9	53
1255	Urea hydration from dielectric relaxation spectroscopy: old findings confirmed, new insights gained. Physical Chemistry Chemical Physics, 2016, 18, 2597-2607.	1.3	30
1256	Recognition of halides and Y-shaped oxoanions by carbonylchromium-based urea-like molecules: A theoretical analysis of hydrogen bonding modes. Journal of Molecular Graphics and Modelling, 2016, 64, 1-10.	1.3	3
1257	A DFT study on the formaldehyde (H ₂ CO and (H ₂ CO) ₂) monitoring using pristine B ₁₂ N ₁₂ nanocluster. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 78, 1-9.	1.3	25
1258	Molecular engineering of starburst triarylamine donor with selenophene containing Î€-linker for dye-sensitized solar cells. Journal of Materials Chemistry C, 2016, 4, 713-726.	2.7	23
1259	Enhanced optical nonlinearity based on silicon ring. Molecular Physics, 2016, 114, 835-844.	0.8	0
1260	Warning to Theoretical Structure Elucidation of Endohedral Metallofullerenes. Journal of Physical Chemistry C, 2016, 120, 1275-1283.	1.5	29
1261	Theoretical study on fluorescent probes for cyanide based on the indolium functional group. Organic Electronics, 2016, 30, 1-11.	1.4	8
1262	Sm@C1(153491)-C94: A missing isomer from Sm@C94 mono-metallofullerenes. Chemical Physics Letters, 2016, 644, 35-40.	1.2	4
1263	Intensified effects of multi-Cu modification on the electronic properties of the modified base pairs containing hetero-ring-expanded pyrimidine bases. Physical Chemistry Chemical Physics, 2016, 18, 2913-2923.	1.3	8
1264	Calculation on frequency and temperature properties of birefringence of nematic liquid crystal 5CB in terahertz band. Chemical Physics Letters, 2016, 645, 205-209.	1.2	17
1265	Theoretical study of the catalytic oxidation mechanism of 5-hydroxymethylfurfural to 2,5-diformylfuran by PMo-containing Keggin heteropolyacid. Catalysis Science and Technology, 2016, 6, 3776-3787.	2.1	29

#	ARTICLE	IF	CITATIONS
1266	Theoretical studies on the derivatives of tris([1,2,4]triazolo)[4,3-a:4a',3a'-c:4a''2a''2,3a''2a''2-e][1,3,5]triazine as high energetic compounds. RSC Advances, 2016, 6, 5419-5427.	1.7	4
1267	A theoretical analysis of the effects of electron-withdrawing substitutions on electronic structures and phosphorescent efficiency of a series of Ir(III) complexes with 2-phenylpyridine ligands. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	2
1268	The electric field effect on the hydrogen storage properties of (MgO) ₉ . Computational and Theoretical Chemistry, 2016, 1081, 1-8.	1.1	8
1269	Hydrolysis mechanisms of BNPP mediated by facial copper(II) complexes bearing single alkyl guanidine pendants: cooperation between the metal centers and the guanidine pendants. Dalton Transactions, 2016, 45, 1593-1603.	1.6	10
1270	Theoretical Study of Geometries, Stabilities, and Electronic Properties of Cationic (FeS) _n + (n = 1-5) Clusters. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2016, 71, 45-51.	0.7	3
1271	Extended X-ray Absorption Fine Structure and Density Functional Theory Studies on the Complexation Mechanism of Amidoximate Ligand to Uranyl Carbonate. Industrial & Engineering Chemistry Research, 2016, 55, 4224-4230.	1.8	43
1272	Initial hydration behavior of sodium iodide dimer: photoelectron spectroscopy and ab initio calculations. Physical Chemistry Chemical Physics, 2016, 18, 557-565.	1.3	11
1273	Luminescent dinuclear copper(I) complexes bearing 1,4-bis(diphenylphosphino)butane and functionalized 3-(2-pyridyl)pyrazole mixed ligands. Dalton Transactions, 2016, 45, 696-705.	1.6	44
1274	Prediction of binding modes and affinities of 4-substituted-2,3,5,6-tetrafluorobenzenesulfonamide inhibitors to the carbonic anhydrase receptor by docking and ONIOM calculations. Journal of Molecular Graphics and Modelling, 2016, 63, 38-48.	1.3	15
1275	f-Aromatic cyclic M ₃ (M = Cu, Ag, Au) clusters and their complexation with dimethyl imidazol-2-ylidene, pyridine, isoxazole, furan, noble gases and carbon monoxide. Physical Chemistry Chemical Physics, 2016, 18, 11661-11676.	1.3	49
1276	In silico rational design of ionic liquids for the exfoliation and dispersion of boron nitride nanosheets. Physical Chemistry Chemical Physics, 2016, 18, 1212-1224.	1.3	20
1277	Boron avoids cycloalkane-like structures in the LinBnH _{2n} series. New Journal of Chemistry, 2016, 40, 2007-2013.	1.4	7
1278	Rotational spectroscopy of the atmospheric photo-oxidation product o-toluic acid and its monohydrate. Physical Chemistry Chemical Physics, 2016, 18, 448-457.	1.3	17
1279	About the electronic and photophysical properties of iridium(III)-pyrazino[2,3-f][1,10]-phenanthroline based complexes for use in electroluminescent devices. Physical Chemistry Chemical Physics, 2016, 18, 726-734.	1.3	20
1280	Mutual enhancing effects of the f-hole interactions and halogen/hydrogen-bonded interactions in the iodine-ylide containing complexes. Structural Chemistry, 2016, 27, 927-937.	1.0	4
1281	The spectroscopic (FT-IR, FT-Raman, dispersive Raman and NMR) study of ethyl-6-chloronicotinate molecule by combined density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 153, 754-770.	2.0	11
1282	Experiment and DFT studies on radioiodine removal and storage mechanism by imidazolium-based ionic liquid. Journal of Molecular Graphics and Modelling, 2016, 64, 51-59.	1.3	27
1283	Detailed theoretical investigation of excited-state intramolecular proton transfer mechanism of a new chromophore II. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 154, 130-134.	2.0	9

#	ARTICLE	IF	CITATIONS
1284	First principles study of enhanced CO ₂ adsorption on MOF-253 by salt-insertion. Computational Materials Science, 2016, 111, 79-85.	1.4	7
1285	Synthesis, crystal structure, spectroscopic properties and DFT calculations of a new Schiff base-type Zinc(II) complex. Research on Chemical Intermediates, 2016, 42, 3473-3488.	1.3	42
1286	Structural analysis of (S)-1-((1H-benzo[d][1,2,3]triazol-1-yl)oxy)-3-(4-(2-methoxyphenyl)piperazin-1-yl)propan-2-ol and binding mechanism with α 1A-adrenoceptor: TDDFT calculations, X-ray crystallography and molecular docking. Journal of Molecular Structure, 2016, 1106, 485-490.	1.8	4
1287	Terahertz absorption spectra and potential energy distribution of liquid crystals. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 153, 741-745.	2.0	5
1288	Chalcogen bonds formed through π -holes: SO ₃ complexes with nitrogen and phosphorus bases. Molecular Physics, 2016, 114, 276-282.	0.8	34
1289	Quinoxaline derivatives as corrosion inhibitors for mild steel in hydrochloric acid medium: Electrochemical and quantum chemical studies. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 76, 109-126.	1.3	111
1290	Efficient π -stacking with benzene provides 2D assembly of trans-[PtCl ₂ (p-CF ₃ C ₆ H ₄ CN) ₂]. Journal of Molecular Structure, 2016, 1104, 19-23.	1.8	48
1291	Intramolecular halogen bonds in 1,2-aryldiyne molecules: a theoretical study. Structural Chemistry, 2016, 27, 907-917.	1.0	6
1292	A DFT-D study on the stability and intramolecular interactions of the energetic salts of 3,6-dihydrazido-1,2,4,5-tetrazine. Canadian Journal of Chemistry, 2016, 94, 28-34.	0.6	1
1293	Bond-bending isomerism of Au ₂ I ₃ ⁺ : competition between covalent bonding and aurophilicity. Chemical Science, 2016, 7, 475-481.	3.7	16
1294	A computational study on [(PH ₂ X) ₂] ⁺ homodimers involving intermolecular two-center three-electron bonds. Structural Chemistry, 2016, 27, 753-762.	1.0	10
1295	A computational study on surface-enhanced Raman spectroscopy of para-substituted Benzenethiol derivatives adsorbed on gold nanoclusters. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 152, 278-287.	2.0	17
1296	All-metal binuclear sandwich complexes Al ₄ Ti ₂ Al ₄ : High capacity hydrogen storage through multicenter bonds. International Journal of Hydrogen Energy, 2017, 42, 5440-5446.	3.8	13
1297	Theoretical investigation on photovoltaic properties of PC ₆₁ BM/PPDPP5T system as a promising polymer-based solar cell. Journal of Physical Organic Chemistry, 2017, 30, e3592.	0.9	1
1298	Quantum chemical investigation of structural and electronic properties of trans- and cis-structures of some azo dyes for dye-sensitized solar cells. Computational and Theoretical Chemistry, 2017, 1102, 87-97.	1.1	17
1299	An unprecedented photochromic system with cis-oriented dithienyl-dithiolenes supported by metal chelation. Dalton Transactions, 2017, 46, 2023-2029.	1.6	4
1300	Computational design of three Cu-induced triangular pyrimidines based DNA motifs with improved conductivity. Canadian Journal of Chemistry, 2017, 95, 571-579.	0.6	0
1301	Aluminum Location and Acid Strength in an Aluminum-Rich Beta Zeolite Catalyst: A Combined Density Functional Theory and Solid-State NMR Study. ChemCatChem, 2017, 9, 1494-1502.	1.8	19

#	ARTICLE	IF	CITATIONS
1302	Trapping of organophosphorus chemical nerve agents by pillar[5]arene: A DFT, AIM, NCI and EDA analysis. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2017, 87, 207-218.	0.9	37
1303	Comparison of the molecular interactions of 7- α -carboxyalkyl apigenin derivatives with <i>S. cerevisiae</i> β -glucosidase. <i>Computational Biology and Chemistry</i> , 2017, 67, 182-193.	1.1	0
1304	Effect of additional donor group on the charge transfer/recombination dynamics of a photoactive organic dye: A quantum mechanical investigation. <i>Computational and Theoretical Chemistry</i> , 2017, 1103, 38-47.	1.1	20
1305	Optoelectronic and thermal properties of highly fluorescence emissive 2,2'-distyryl-[3,3'-bithiophenes. <i>Dyes and Pigments</i> , 2017, 140, 222-228.	2.0	6
1306	The influence of inserted thiophene into the (I'-A'-I')-bridge on photovoltaic performances of dye-sensitized solar cells. <i>Materials Chemistry and Physics</i> , 2017, 191, 121-128.	2.0	19
1307	Synthesis, Chemistry, and Electronic Structures of Group 9 Metallaboranes. <i>Inorganic Chemistry</i> , 2017, 56, 1524-1533.	1.9	10
1308	Hydration of the simplest β -keto acid: a rotational spectroscopic and ab initio study of the pyruvic acid-water complex. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4440-4446.	1.3	31
1309	Structural, intramolecular hydrogen bonding and vibrational studies on 3-amino-4-methoxy benzamide using density functional theory. <i>Journal of Chemical Sciences</i> , 2017, 129, 259-269.	0.7	4
1310	Study on effect of lomefloxacin on human holo-transferrin in the presence of essential and nonessential amino acids: Spectroscopic and molecular modeling approaches. <i>International Journal of Biological Macromolecules</i> , 2017, 97, 688-699.	3.6	83
1311	$H_{C(X)X_2}$ (X = Cl, Br) Halogen Bonding of Dihalomethanes. <i>Crystal Growth and Design</i> , 2017, 17, 1353-1362.	1.4	78
1312	Noncovalent interaction assisted fullerene for the transportation of some brain anticancer drugs: A theoretical study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 72, 187-200.	1.3	45
1313	Density functional theory is straying from the path toward the exact functional. <i>Science</i> , 2017, 355, 49-52.	6.0	711
1314	Understanding the mechanism, thermodynamic and kinetic features of the Kukhtin-Ramirez reaction in carbamate synthesis from carbon dioxide. <i>RSC Advances</i> , 2017, 7, 1701-1710.	1.7	14
1315	DFT study of water adsorption on lignite molecule surface. <i>Journal of Molecular Modeling</i> , 2017, 23, 27.	0.8	30
1316	Anion Recognition Based on a Combination of Double-Dentate Hydrogen Bond and Double-Side Anion-Noncovalent Interactions. <i>Journal of Physical Chemistry A</i> , 2017, 121, 892-900.	1.1	24
1317	Intermolecular hydrogen bonding $H\cdots Cl$ in the solid palladium(II)-diaminocarbene complexes. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2017, 232, 299-305.	0.4	20
1318	Preparation of Fe(II)-Al layered double hydroxides: Application to the adsorption/reduction of chromium. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2017, 516, 362-374.	2.3	64
1319	What is the effect of carbon nanotube shape on desalination process? A simulation approach. <i>Desalination</i> , 2017, 407, 103-115.	4.0	36

#	ARTICLE	IF	CITATIONS
1320	Understanding the fragmentation mechanisms of methoxy-, mesyl-, and tosyl-lapachol derivatives by computational chemistry and mass spectrometry analysis. <i>International Journal of Mass Spectrometry</i> , 2017, 418, 92-100.	0.7	6
1321	Ligand-Field-Dependent Behavior of Meta-GGA Exchange in Transition-Metal Complex Spin-State Ordering. <i>Journal of Physical Chemistry A</i> , 2017, 121, 874-884.	1.1	52
1322	A mechanistic study on Decontamination of Methyl Orange Dyes from Aqueous Phase by Mesoporous Pulp Waste and Polyaniline. <i>Environmental Research</i> , 2017, 154, 139-144.	3.7	36
1323	The pyrrole ring η^2 -hapticity bridged binuclear tricarbonyl Mo(O) and W(O) complexes: catalysis of regioselective hydroamination reactions and DFT calculations. <i>Dalton Transactions</i> , 2017, 46, 1840-1847.	1.6	10
1324	Unusual binding modes in the copper(ii) and palladium(ii) complexes of peptides containing both histidyl and cysteinyl residues. <i>New Journal of Chemistry</i> , 2017, 41, 1372-1379.	1.4	8
1325	Theoretical characterization on photoelectric properties of benzothiadiazole- and fluorene-based small molecule acceptor materials for the organic photovoltaics. <i>Journal of Molecular Modeling</i> , 2017, 23, 28.	0.8	16
1326	Contrasting Behavior of the Z Bonds in $X \cdots Z \cdots Y$ Weak Interactions: Z = Main Group Elements Versus the Transition Metals. <i>Inorganic Chemistry</i> , 2017, 56, 1132-1143.	1.9	32
1327	Femtosecond Study of Dimolybdenum Paddlewheel Compounds with Amide/Thioamide Ligands: Symmetry, Electronic Structure, and Charge Distribution in the $1MLCT S_1$ State. <i>Inorganic Chemistry</i> , 2017, 56, 1433-1445.	1.9	7
1328	Function of CN group in organic sensitizers: The first principle study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 179, 227-232.	2.0	4
1329	Ab Initio Calculations of the N-N Bond Dissociation for the Gas-phase RDX and HMX. <i>Scientific Reports</i> , 2017, 7, 40630.	1.6	15
1330	Bonding trends across the series of tricarbonato-actinyl anions $[(AnO)_2(CO)_3]^{3-}$ ($An = U \cdots Cm$): the plutonium turn. <i>Dalton Transactions</i> , 2017, 46, 2542-2550.	1.6	34
1331	Mechanistic insights on DBU catalyzed α -amination of nbs to chalcone driving by water: Multiple roles of water. <i>Journal of Computational Chemistry</i> , 2017, 38, 438-445.	1.5	7
1332	Thermal and Optical Modulation of the Carrier Mobility in OTFTs Based on an Azo-anthracene Liquid Crystal Organic Semiconductor. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 7305-7314.	4.0	34
1333	Bottom-up design of high-energy-density molecules $(N_2CO)_n$ ($n = 2 \cdots 8$). <i>RSC Advances</i> , 2017, 7, 8533-8541.	1.7	2
1334	An <i>ab initio</i> study on properties of cationic chalcogen bonds in $XF_2^+ \cdots Y \cdots NCZ$ ($X = H, CN, F; Y = S, Se; Z = H, Cl, Br$) complexes. <i>Journal of Sulfur Chemistry</i> , 2017, 38, 83-97.	1.0	3
1335	Reaction mechanisms and kinetics of the elimination processes of 2-chloroethylsilane and derivatives: A DFT study using CTST, RRKM, and BET theories. <i>Chemical Physics</i> , 2017, 485-486, 140-148.	0.9	3
1336	Combined DFT and NBO approach to analyze reactivity and stability of $(CuS)_n$ ($n = 1 \cdots 12$) clusters. <i>Computational and Theoretical Chemistry</i> , 2017, 1103, 71-82.	1.1	12
1337	Synthesis, mechanism and efficient modulation of a fluorescence dye by photochromic pyrazolone with energy transfer in the crystalline state. <i>RSC Advances</i> , 2017, 7, 9847-9853.	1.7	5

#	ARTICLE	IF	CITATIONS
1338	Substitution effect on a hydroxylated chalcone: Conformational, topological and theoretical studies. <i>Journal of Molecular Structure</i> , 2017, 1136, 69-79.	1.8	16
1339	Systematic analysis of structural and topological properties: new insights into $\text{PuO}_2(\text{H}_2\text{O})_{n+2}$ ($n = 1, 2, 3, 4, 5, 6, 7$). <i>Journal of Molecular Structure</i> , 2017, 1136, 79-87.	1.7	7
1340	Mechanisms of the transfer hydroformylation catalyzed by rhodium, cobalt, and iridium complexes: Insights from density functional theory study. <i>Journal of Organometallic Chemistry</i> , 2017, 833, 71-79.	0.8	8
1341	How the alkali metal atoms affect electronic structure and the nonlinear optical properties of $\text{C}_{24}\text{N}_{24}$ nanocage. <i>Optik</i> , 2017, 135, 139-152.	1.4	22
1342	Simultaneous CO_2 and SO_2 capture by using ionic liquids: a theoretical approach. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5411-5422.	1.3	18
1343	First-principle studies on the Li^+Te system. <i>Materials Research Express</i> , 2017, 4, 015701.	0.8	0
1344	DFT and PCM-TD-DFT investigation of the electronic structures and spectra of 5-(3-phenyl-2-propenylidene)-2-thioxo-4-thiazolidinone derivatives. <i>Journal of Molecular Structure</i> , 2017, 1134, 840-850.	1.8	13
1345	Trinuclear (aminonitrone) Zn^{II} complexes as key intermediates in zinc(scp)-mediated generation of 1,2,4-oxadiazoles from amidoximes and nitriles. <i>New Journal of Chemistry</i> , 2017, 41, 1940-1952.	1.4	24
1346	Theoretical Design of Perylene Diimide Dimers with Different Linkers and Bridged Positions as Promising Non-Fullerene Acceptors for Organic Photovoltaic Cells. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2125-2134.	1.5	50
1347	Cooperativity between the hydrogen bonding and π -hole interaction in linear $\text{NCX}(\text{NCH})_2$ and $\text{O}_3\text{Z}(\text{NCH})_2$ complexes ($X = \text{Cl, Br; Z} = \text{Ar, Kr}$): a comparative study. <i>Canadian Journal of Chemistry</i> , 2017, 95, 537-546.	0.6	5
1348	A novel diarylethene-hydrazinopyridine-based probe for fluorescent detection of aluminum ion and naked-eye detection of hydroxide ion. <i>Sensors and Actuators B: Chemical</i> , 2017, 245, 263-272.	4.0	52
1349	Mechanistic Study on the Ruthenium-Catalyzed Terminal Alkyne Hydrochlorination. <i>Organometallics</i> , 2017, 36, 523-529.	1.1	11
1350	A ten-electron (10e) thiolate-protected $\text{Au}_{29}(\text{SR})_{19}$ cluster: structure prediction and a gold-atom insertion, thiolate-group elimination mechanism. <i>Nanoscale</i> , 2017, 9, 2895-2902.	2.8	26
1351	Nitrogen doped nanographene structures; study on the adsorption of nucleobases, nucleotides, and their triphosphate derivatives using mixed docking, MD, and QM/MM approaches. <i>Journal of Chemical Physics</i> , 2017, 146, 044105.	1.2	4
1352	Proposal of a simple and effective local reactivity descriptor through a topological analysis of an orbital-weighted Fukui function. <i>Journal of Computational Chemistry</i> , 2017, 38, 481-488.	1.5	58
1353	A Theoretical Perspective on the Photovoltaic Performance of S,N-Heteroacenes: An Even-Odd Effect on the Charge Separation Dynamics. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2574-2587.	1.5	56
1354	Dipolar vinyl sulfur fluorescent dyes. Synthesis and photophysics of sulfide, sulfoxide and sulfone based D^+A compounds. <i>RSC Advances</i> , 2017, 7, 8832-8842.	1.7	14
1355	Theoretical Prediction on $[\text{5}]$ Radialene Sandwich Complexes ($\text{CpM}_2(\text{C}_{10}\text{H}_{10})$) ($\text{Cp} = \text{Ind}^-, \text{Cp}^-, \text{Cp}^+$). <i>Journal of Molecular Structure</i> , 2017, 1134, 850-858.	1.0	14

#	ARTICLE	IF	CITATIONS
1356	An NMR Scale for Measuring the Base Strength of Solid Catalysts with Pyrrole Probe: A Combined Solid-State NMR Experiment and Theoretical Calculation Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3887-3895.	1.5	27
1357	On structure and stability of pyrimidine ylidenes and their homologues. <i>Computational and Theoretical Chemistry</i> , 2017, 1103, 83-91.	1.1	12
1358	Prediction of enthalpies of sublimation of high-nitrogen energetic compounds: Modified Politzer model. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 72, 220-228.	1.3	30
1359	Noncovalent Interactions Accompanying Encapsulation of Resorcinol within Azacalix[4]pyridine Macrocycle. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1814-1824.	1.1	39
1360	Assessment of range-separated exchange functionals and nonempirical functional tuning for calculating the static second hyperpolarizabilities of streptocyanines. <i>Journal of Computational Chemistry</i> , 2017, 38, 594-600.	1.5	6
1361	Interplay between non-covalent pnictogen bonds and halogen bonds interactions in ArH ₂ N---PH ₂ FO---BrF nanostructured complexes: a substituent effects investigation. <i>Structural Chemistry</i> , 2017, 28, 1065-1079.	1.0	5
1362	Thermally Stable Energetic Salts Composed of Heterocyclic Anions and Cations Based on 3,6,7-Triamino-5,7,8-triazolo[5,1-c]triazole: Synthesis and Intermolecular Interaction Study. <i>ChemPlusChem</i> , 2017, 82, 474-482.	1.0	14
1363	Mechanistic insights into biomimetic carbonic anhydrase action catalyzed by doped carbon nanotubes and graphene. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8757-8767.	1.3	9
1364	A comparative study of oxygen-doped and pure beryllium clusters based on structural, energetic and electronic properties. <i>Chemical Physics Letters</i> , 2017, 674, 1-5.	1.2	11
1365	Theoretical study on the bridge comparison of TiO ₂ nanoparticle sensitizers based on phenoxazine in dye-sensitized solar cells. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	9
1366	Constructing a novel nonlinear optical materials: substituents and heteroatoms in π - π systems effect on the first hyperpolarizability. <i>Structural Chemistry</i> , 2017, 28, 1623-1630.	1.0	3
1367	Molecular adsorption of hydrogen peroxide on N- and Fe-doped titania nanoclusters. <i>Applied Surface Science</i> , 2017, 407, 121-129.	3.1	4
1368	A combined experimental and theoretical DFT (B3LYP, CAM-B3LYP and M06-2X) study on electronic structure, hydrogen bonding, solvent effects and spectral features of methyl 1H-indol-5-carboxylate. <i>Journal of Molecular Structure</i> , 2017, 1137, 725-741.	1.8	47
1369	Insights into the enhanced Ce-N triple bond in the HCe-N molecule. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8216-8222.	1.3	10
1370	A Direct Link from the Gas to the Condensed Phase: A Rotational Spectroscopic Study of 2,2,2-Trifluoroethanol Trimers. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 6289-6293.	7.2	52
1371	Hydrogen-Atom Transfer (HAT) Initiated by Intramolecular Ligand-Metal Electron Transfer. <i>Chemistry - A European Journal</i> , 2017, 23, 5520-5528.	1.7	12
1372	Study of the mechanism of the catalytic decomposition of hydrogen iodide (HI) over carbon materials for hydrogen production. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 4977-4986.	3.8	7
1373	Computational investigation of fullerene-DNA interactions: Implications of fullerene's size and functionalization on DNA structure and binding energetics. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 74, 177-192.	1.3	6

#	ARTICLE	IF	CITATIONS
1374	Structural characterization, surface characteristics and non covalent interactions of a heterocyclic Schiff base: Evaluation of antioxidant potential by UV-visible spectroscopy and DFT. <i>Journal of Molecular Structure</i> , 2017, 1137, 569-580.	1.8	23
1375	Anaerobic Dehalogenation of Chloroanilines by <i>Dehalococcoides mccartyi</i> Strain CBDB1 and <i>Dehalobacter</i> Strain 14DCB1 via Different Pathways as Related to Molecular Electronic Structure. <i>Environmental Science & Technology</i> , 2017, 51, 3714-3724.	4.6	21
1376	Insights into the Diels-Alder Reaction between 3-Vinylindoles and Methyleneindolinone without and with the Assistance of Hydrogen-Bonding Catalyst Bisthiourea: Mechanism, Origin of Stereoselectivity, and Role of Catalyst. <i>Journal of Organic Chemistry</i> , 2017, 82, 3046-3061.	1.7	30
1377	Influence of donor and acceptor groups on the S-T energy gap for thermally activated delayed fluorescence emitters. <i>Molecular Physics</i> , 2017, 115, 809-814.	0.8	8
1378	The effect of hydrogen-bonding cooperativity on the strength and properties of π -hole interactions: an <i>ab initio</i> study. <i>Molecular Physics</i> , 2017, 115, 913-924.	0.8	14
1379	Theoretical insights into the ultrafast excited-state intramolecular proton transfer (ESIPT) mechanism in a series of amide-based N-H \cdots N hydrogen-bonding compounds. <i>Organic Electronics</i> , 2017, 45, 1-8.	1.4	42
1380	DFT Investigation of the Kinetics and Mechanism of the Thermal Decomposition of Oxalic Acid. <i>Progress in Reaction Kinetics and Mechanism</i> , 2017, 42, 44-51.	1.1	7
1381	Polymorphic Self-Assemblies of 2,7-Bis(decyloxy)-9-fluorenone at the Solid/Gas Interface: Role of C-H \cdots O \cdots C Hydrogen Bond. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3947-3957.	1.5	20
1382	Probing the influence of carboxyalkyl groups on the molecular flexibility and the charge density of apigenin derivatives. <i>Journal of Molecular Modeling</i> , 2017, 23, 70.	0.8	2
1383	Liquid-phase exfoliation (LPE) of graphite towards graphene: An <i>ab initio</i> study. <i>Journal of Molecular Liquids</i> , 2017, 230, 461-472.	2.3	50
1384	Synthesis of Quaternary Ammonium Salts Based on Diketopyrrolopyrroles Skeletons and Their Applications in Copper Electroplating. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 7793-7803.	4.0	44
1385	Microscopic progression in the free radical addition reaction: modeling, geometry, energy, and kinetics. <i>Journal of Molecular Modeling</i> , 2017, 23, 73.	0.8	7
1386	Theoretical insights into the excited-state intramolecular proton transfer (ESIPT) mechanism in a series of amino-type hydrogen-bonding dye molecules bearing the 10-aminobenzo[h]quinoline chromophore. <i>Dyes and Pigments</i> , 2017, 141, 195-201.	2.0	34
1387	New Cu(II) coordination polymer by chiral tridentate Schiff base ligand. <i>Journal of Molecular Structure</i> , 2017, 1137, 349-353.	1.8	8
1388	The nature of bonding in metal-metal singly bonded coinage metal dimers: Cu ₂ , Ag ₂ and Au ₂ . <i>Computational and Theoretical Chemistry</i> , 2017, 1116, 195-201.	1.1	17
1389	Structural studies of bis(histidinato)nickel(II): Combined experimental and computational studies. <i>Comptes Rendus Chimie</i> , 2017, 20, 467-474.	0.2	2
1390	Theoretical study of the hydrolysis of HOSO+NO ₂ as a source of atmospheric HONO: effects of H ₂ O or NH ₃ . <i>Environmental Chemistry</i> , 2017, 14, 19.	0.7	10
1391	Ultrathin Mg-Al layered double hydroxide prepared by ionothermal synthesis in a deep eutectic solvent for highly effective boron removal. <i>Chemical Engineering Journal</i> , 2017, 319, 108-118.	6.6	70

#	ARTICLE	IF	CITATIONS
1392	Rationalization of the mechanism of in situ Pd(0) formation for cross-coupling reactions from novel unsymmetrical pincer palladacycles using DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2017, 845, 71-81.	0.8	10
1393	Insights into the Photobehavior of Fluorescent Oxazinone, Quinazoline, and Difluoroboron Derivatives: Molecular Design Based on the Structure-Property Relationships. <i>Journal of Physical Chemistry C</i> , 2017, 121, 8091-8108.	1.5	54
1394	On the isomers of pyridine-4-carboxaldoxime and its nitrate salt, X-ray crystal structure and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2017, 1139, 17-30.	1.8	5
1395	Gas-phase COS activation by U ⁺ : Reaction mechanisms and bonding analysis. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750010.	1.8	0
1396	A theoretical study of the H n F4 n Si:N-base (n=4) tetrel-bonded complexes. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	27
1397	Understanding photophysical properties of chiral conjugated corrals for organic photovoltaics. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3495-3502.	2.7	10
1398	Nondoped blue fluorescent OLED based on cyanophenanthrimidazole-styryl-triphenylamine/carbazole materials. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3695.	0.9	13
1399	Computational study on favipiravir adsorption onto undoped- and silicon-decorated C60 fullerenes. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750011.	1.8	25
1400	Mechanochemical mechanism of rapid dechlorination of hexachlorobenzene. <i>Journal of Hazardous Materials</i> , 2017, 333, 116-127.	6.5	37
1401	Computational insights into novel dicobalt polynitrogen: structure, stability, intermolecular interaction, and application. <i>Canadian Journal of Chemistry</i> , 2017, 95, 656-663.	0.6	0
1402	Study on the Catalytic Behavior of Bifunctional Hydrogen-Bonding Catalysts Guided by Free Energy Relationship Analysis of Steric Parameters. <i>Chemistry - A European Journal</i> , 2017, 23, 5488-5497.	1.7	19
1403	The role of hydrogen bond interaction on molecular orientation of alkanolamines through temperature and pressure variation: A mixed molecular dynamics and quantum mechanics study. <i>Computational Materials Science</i> , 2017, 131, 239-249.	1.4	6
1404	Theoretical investigation effects of anchor groups on photovoltaic properties for the C217-based dye sensitizer. <i>Computational and Theoretical Chemistry</i> , 2017, 1105, 89-96.	1.1	10
1405	Why Only Ionic Liquids with Unsaturated Heterocyclic Cations Can Dissolve Cellulose: A Simulation Study. <i>ACS Sustainable Chemistry and Engineering</i> , 2017, 5, 3417-3428.	3.2	80
1406	Identifying electron transfer coordinates in donor-bridge-acceptor systems using mode projection analysis. <i>Nature Communications</i> , 2017, 8, 14554.	5.8	27
1407	High-efficiency organic light-emitting diodes of phosphorescent PtAg ₂ heterotrinnuclear acetylide complexes supported by triphosphine. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3072-3078.	2.7	30
1408	Two novel thorium organic frameworks constructed by bi- and tritopic ligands. <i>Radiochimica Acta</i> , 2017, 105, 531-539.	0.5	1
1409	Ligand size dependence of U-N and U-O bond character in a series of uranyl hexaphyrin complexes: quantum chemical simulation and density based analysis. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7546-7559.	1.3	10

#	ARTICLE	IF	CITATIONS
1410	A DFT study on lignin dissolution in imidazolium-based ionic liquids. RSC Advances, 2017, 7, 12670-12681.	1.7	100
1411	Nature of the interaction between ammonia derivatives and carbon disulfide. A theoretical investigation. International Journal of Quantum Chemistry, 2017, 117, e25369.	1.0	12
1412	Adsorption of various types of amino acids on the graphene and boron-nitride nano-sheet, a DFT-D3 study. Applied Surface Science, 2017, 409, 35-44.	3.1	44
1413	The enhancing effect of a cation- π interaction on the cooperativity of halogen bonds: A computational study. Journal of Molecular Graphics and Modelling, 2017, 73, 200-207.	1.3	3
1414	Topological analysis of steric and relaxation deformation densities. Molecular Physics, 2017, 115, 743-756.	0.8	7
1415	Synthesis, structural characterization, crystal structure and theoretical study of a Pd(II)-salen complex with propylene linkage. Journal of Molecular Structure, 2017, 1137, 310-319.	1.8	4
1416	Silane activation by laser-ablated Be atoms: Formation of HBeSiH ₃ and HBe($\frac{1}{4}$ -H) ₃ Si molecules. Chemical Physics Letters, 2017, 672, 1-6.	1.2	4
1417	Experimental and theoretical investigation of the inhibitory effect of new pyridazine derivatives for the corrosion of mild steel in 1M HCl. Journal of Molecular Structure, 2017, 1136, 127-139.	1.8	87
1418	The enhancing effects of molecule X ($X = \text{PH}_2, \text{Cl}, \text{SHCl}, \text{ClCl}$) on chalcogen-chalcogen interactions in cyclic trimers $Y_3 \cdot \hat{A} \cdot Y_3 \cdot \hat{A} \cdot X$ ($Y = \text{SHCl}, \text{SeHCl}$). International Journal of Quantum Chemistry, 2017, 117, e25354.	1.0	4
1419	Beneficial effects of amino acid-functionalized graphene nanosheets incorporated in the photoanode material of dye-sensitized solar cells: A practical and theoretical study. Applied Surface Science, 2017, 403, 218-229.	3.1	8
1420	Efficient phenanthroimidazole-styryl-triphenylamine derivatives for blue OLEDs: a combined experimental and theoretical study. New Journal of Chemistry, 2017, 41, 2443-2457.	1.4	25
1421	Initial reaction mechanism between HO \cdot and bisphenol \hat{A} : Conformational dependence and the role of nonbond interactions. International Journal of Quantum Chemistry, 2017, 117, e25342.	1.0	4
1422	Adsorption of polycyclic aromatic hydrocarbons onto graphyne: Comparisons with graphene. International Journal of Quantum Chemistry, 2017, 117, e25346.	1.0	23
1423	Van Der Waals heterogeneous layer-by-layer carbon nanostructures involving π - π interactions between CH_2 and CH stacking based on graphene and graphane sheets. Journal of Computational Chemistry, 2017, 38, 730-739.	1.5	14
1424	Structural analyses of two new highly distorted octahedral copper(II) complexes with quinoline-type ligands; Hirshfeld, AIM and NBO studies. Polyhedron, 2017, 127, 36-50.	1.0	23
1425	Highly efficient non-doped blue organic light emitting diodes based on a $\text{D}^{\text{A}}\text{A}^{\text{A}}$ chromophore with different donor moieties. RSC Advances, 2017, 7, 13604-13614.	1.7	12
1426	A general strategy to enhance the alkaline stability of anion exchange membranes. Journal of Materials Chemistry A, 2017, 5, 6318-6327.	5.2	55
1427	Potential of Si-doped boron nitride nanotubes as a highly active and metal-free electrocatalyst for oxygen reduction reaction: A DFT study. Synthetic Metals, 2017, 226, 129-138.	2.1	16

#	ARTICLE	IF	CITATIONS
1428	How does stress affect human being? a molecular dynamic simulation study on cortisol and its glucocorticoid receptor. Saudi Journal of Biological Sciences, 2017, 24, 488-494.	1.8	3
1429	Counterion-induced crystallization of intermetalloid Matryoshka clusters [Sb@Pd ₁₂ @Sb ₂₀] ³⁺ , ⁴⁺ . Dalton Transactions, 2017, 46, 3453-3456.	1.6	22
1430	The S \cdots A \cdots P noncovalent interaction: diverse chalcogen bonds. Journal of Sulfur Chemistry, 2017, 38, 249-263.	1.0	7
1431	Quantum-chemical investigation on 5-fluorouracil anticancer drug. Structural Chemistry, 2017, 28, 1093-1109.	1.0	10
1432	How does the global electron density transfer diminish activation energies in polar cycloaddition reactions? A Molecular Electron Density Theory study. Tetrahedron, 2017, 73, 1718-1724.	1.0	65
1433	Electronic structure theory to decipher the chemical bonding in actinide systems. Coordination Chemistry Reviews, 2017, 344, 150-162.	9.5	16
1434	Design and structural characterization of the all-metal aromatic sandwich species [Bi ₃ Au ₃ Bi ₃] ³⁺ : insight from density functional theory. New Journal of Chemistry, 2017, 41, 2321-2327.	1.4	5
1435	Spirooxazine molecular switches with nonlinear optical responses as selective cation sensors. RSC Advances, 2017, 7, 642-650.	1.7	35
1436	Revealing the Intermolecular Interactions of Asphaltene Dimers by Quantum Chemical Calculations. Energy & Fuels, 2017, 31, 2488-2495.	2.5	59
1437	Mechanistic Insights into the Directed Hydrogenation of Hydroxylated Alkene Catalyzed by Bis(phosphine)cobalt Dialkyl Complexes. Journal of Organic Chemistry, 2017, 82, 2703-2712.	1.7	35
1438	Mechanism, reactivity, and regioselectivity in rhodium-catalyzed asymmetric ring-opening reactions of oxabicyclic alkenes: a DFT Investigation. Scientific Reports, 2017, 7, 40491.	1.6	12
1439	Solvent effects on the intramolecular hydrogen-bond and anti-oxidative properties of apigenin: A DFT approach. Dyes and Pigments, 2017, 141, 179-187.	2.0	42
1440	Reversibility of imido-based ionic liquids: a theoretical and experimental study. RSC Advances, 2017, 7, 11259-11270.	1.7	6
1441	A density functional theory investigation on amantadine drug interaction with pristine and B, Al, Si, Ga, Ge doped C60 fullerenes. Chemical Physics Letters, 2017, 678, 85-90.	1.2	63
1442	A theoretical study on geometry, bonding nature, and stability of several anhydrous and hydrated Ln(III), Gd(III) and Yb(III) complexes in liquid scintillator solvents. Inorganica Chimica Acta, 2017, 463, 20-28.	1.2	2
1443	Characteristics of the molecular electron density, delocalization effect and hydrogen bonding interaction of nitroxoline. Journal of Molecular Structure, 2017, 1141, 524-534.	1.8	1
1444	Photo-degradation ibuprofen by UV/H ₂ O ₂ process: response surface analysis and degradation mechanism. Water Science and Technology, 2017, 75, 2935-2951.	1.2	20
1445	Computational prediction of the endohedral metalloborofullerenes Ti _n @B40 (n=1, 2). Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	13

#	ARTICLE	IF	CITATIONS
1446	Phosphides or nitrides for better NLO properties? A detailed comparative study of alkali metal doped nano-cages. <i>Materials Research Bulletin</i> , 2017, 92, 113-122.	2.7	92
1447	Theoretical insights on a series of difluoramino group-based energetic molecules. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3704.	0.9	5
1448	Impact of Halogenido Coligands on Magnetic Anisotropy in Seven-Coordinate Co(II) Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 5076-5088.	1.9	57
1449	Copper(I)-Catalyzed 1,3-Dipolar Cycloaddition of Ketoneitrone to Dialkylcyanamides: A Step toward Sustainable Generation of 2,3-Dihydro-1,2,4-oxadiazoles. <i>ACS Omega</i> , 2017, 2, 1380-1391.	1.6	32
1450	Exploiting hydrogen bonding interactions to probe smaller linear and cyclic diamines binding to G-quadruplexes: a DFT and molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 11474-11484.	1.3	11
1451	Rotational spectra of two six-membered heterocyclic N-methyl-piperidinol compounds: Conformations by OH rotation, N-methyl inversion, and ring puckering. <i>Journal of Chemical Physics</i> , 2017, 146, 104303.	1.2	4
1452	Computational assessment of nitrogen-rich peracids: a family of peroxide-based energetic materials. <i>RSC Advances</i> , 2017, 7, 21585-21591.	1.7	5
1453	Geometric stability of PtFe/PdFe embedded in graphene and catalytic activity for CO oxidation. <i>Applied Organometallic Chemistry</i> , 2017, 31, e3808.	1.7	9
1454	QTAIM and NCI analysis of intermolecular interactions in steroid ligands binding a cytochrome P450 enzyme "Beyond the most obvious interactions. <i>Computational and Theoretical Chemistry</i> , 2017, 1111, 40-49.	1.1	24
1455	Modulating of the pnictogen-bonding by a H \cdots N interaction: An ab initio study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 165-173.	1.3	13
1456	Theoretical Investigation of the Binding of Nucleobases to Cucurbiturils by Dispersion Corrected DFT Approaches. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4733-4744.	1.2	40
1457	Interplay between the π -tetrel bond and π -halogen bond in PhSiF ₃ \cdots 4-iodopyridine \cdots N-base. <i>RSC Advances</i> , 2017, 7, 21713-21720.	1.7	26
1458	Photo- and electro-luminescence of three TADF binuclear Cu(μ - η^2) complexes with functional tetraamine ligands. <i>Journal of Materials Chemistry C</i> , 2017, 5, 4495-4504.	2.7	61
1459	Influence of denticity and combined soft-hard strategy on the interaction of picolinic-type ligands with NpO ₂ ⁺ . <i>RSC Advances</i> , 2017, 7, 12236-12246.	1.7	3
1460	Heterodimetallaboranes of Group 4 and 9 Metals: Analogues of Pentaborane(11) and Hexaborane(12). <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 4452-4458.	1.0	5
1461	Theoretical study on interactions between Trifluoromethanesulfonate (Triflate) based ionic liquid and thiophene. <i>Journal of Molecular Liquids</i> , 2017, 237, 289-294.	2.3	4
1462	A quantum-chemical insight into the tunable fluorescence color and distinct photoisomerization mechanisms between a novel ESIPT fluorophore and its protonated form. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 183, 123-130.	2.0	21
1463	The role of the long-range exchange corrections in the description of electron delocalization in aromatic species. <i>Journal of Computational Chemistry</i> , 2017, 38, 1640-1654.	1.5	69

#	ARTICLE	IF	CITATIONS
1464	A Fukui function-guided genetic algorithm. Assessment on structural prediction of Si _n (<i>n</i> = 12-20) clusters. <i>Journal of Computational Chemistry</i> , 2017, 38, 1668-1677.	1.5	11
1465	The theoretical study of excited-state intramolecular proton transfer of 2,5-bis(benzoxazol-2-yl)thiophene-3,4-diol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 183, 37-44.	2.0	29
1466	Kinetic Energy Density as a Predictor of Hydrogen-Bonded OH-Stretching Frequencies. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3452-3460.	1.1	25
1467	Redox-Active Macrocycles for Organic Rechargeable Batteries. <i>Journal of the American Chemical Society</i> , 2017, 139, 6635-6643.	6.6	106
1468	Mechanism of the chemical fixation of carbon dioxide with 2-aminobenzonitrile catalyzed by cesium carbonate: A computational study. <i>Molecular Catalysis</i> , 2017, 432, 172-186.	1.0	8
1469	Tuning the electronic and optical properties of diphenylsulphone based thermally activated delayed fluorescent materials via structural modification: A theoretical study. <i>Dyes and Pigments</i> , 2017, 143, 42-47.	2.0	10
1470	Quantitative contribution of molecular orbitals to hydrogen bonding in a water dimer: Electron density projected integral (EDPI) analysis. <i>Chemical Physics Letters</i> , 2017, 678, 98-101.	1.2	5
1471	Interfacial charge-transfer process in nanosemiconductor- N -benzylpiperidine phenanthroimidazole (BDPI)-metal heterostructure: A combined experimental and theoretical studies of BDPI-(FeO) _n composites. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 342, 59-77.	2.0	4
1472	The noble gases adsorption on boron-rich boron nitride nanotubes: A theoretical investigation. <i>Superlattices and Microstructures</i> , 2017, 107, 97-103.	1.4	9
1473	Far-Field Enhancement by Silver Nanoparticles in Organic Light Emitting Diodes Based on Donor-Acceptor Chromophore. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 5325-5338.	1.8	3
1474	Unusual cooperativity effects between halogen bond and donor-acceptor interactions: The role of orbital interaction. <i>Chemical Physics Letters</i> , 2017, 678, 275-282.	1.2	22
1475	NgMCP ⁺ : Noble Gas Bound Half-Sandwich Complexes (Ng = He-Rn, M = Be-Ba, and Cp =) <i>Tj ETQ</i> 1 1 0.784314 rgB	1.1	13
1476	A novel multi-nitrogen 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane-based energetic co-crystal with 1-methyl-3,4,5-trinitropyrazole as a donor: experimental and theoretical investigations of intermolecular interactions. <i>New Journal of Chemistry</i> , 2017, 41, 4165-4172.	1.4	61
1477	Double C-H bond activation of acetylene by atomic boron in forming aromatic cyclic-HBC ₂ BH in solid neon. <i>Chemical Science</i> , 2017, 8, 4443-4449.	3.7	9
1478	Ab initio prediction of the electronic, magnetic and topological properties of Ln ₂ O ₃ clusters. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 265301.	0.7	1
1479	Theoretical study of olefin protonation reactions confined inside mordenite zeolite by energy decomposition analysis. <i>Molecular Catalysis</i> , 2017, 437, 47-56.	1.0	6
1480	Mechanisms and Origins of Chemo- and Regioselectivities of Ru(II)-Catalyzed Decarboxylative C-H Alkenylation of Aryl Carboxylic Acids with Alkynes: A Computational Study. <i>Journal of the American Chemical Society</i> , 2017, 139, 7224-7243.	6.6	134
1481	Exploring electronic properties and NO gas sensitivity of Si-doped SW-BNNTs under axial tensile strain. <i>Journal of Materials Science</i> , 2017, 52, 9739-9763.	1.7	6

#	ARTICLE	IF	CITATIONS
1482	Efficient enhancement of second order nonlinear optical response by complexing metal cations in conjugated 7-substituted coumarin. <i>Organic Electronics</i> , 2017, 47, 152-161.	1.4	17
1483	Double and Triple Si-H-M Bridge Bonds: Matrix Infrared Spectra and Theoretical Calculations for Reaction Products of Silane with Ti, Zr, and Hf Atoms. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3898-3908.	1.1	3
1484	DFT study of CO ₂ and H ₂ O co-adsorption on carbon models of coal surface. <i>Journal of Molecular Modeling</i> , 2017, 23, 187.	0.8	22
1485	Theoretical study of noncovalent interactions in XCN ₃ -YO ₂ H (X = F, Cl, Br, I; Y = P, As, Sb) complexes. <i>Journal of Molecular Modeling</i> , 2017, 23, 188.	0.8	3
1486	Removal of borate by layered double hydroxides prepared through microwave-hydrothermal method. <i>Journal of Water Process Engineering</i> , 2017, 17, 271-276.	2.6	9
1487	Enhancing intermolecular interactions and their anisotropy to build low-impact-sensitivity energetic crystals. <i>CrystEngComm</i> , 2017, 19, 3145-3155.	1.3	38
1488	Electronic structure and rearrangements of anionic [ClMg(̂-2-O ₂ C)] ⁻ and [ClMg(̂-2-CO ₂)] ⁻ complexes: a quantum chemical topology study. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	8
1489	Reactions between hydroxyl-substituted alkylperoxy radicals and Criegee intermediates: correlations of the electronic characteristics of methyl substituents and the reactivity. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15073-15083.	1.3	18
1490	The enhancement mechanism of glycolic acid on the formation of atmospheric sulfuric acid-ammonia molecular clusters. <i>Journal of Chemical Physics</i> , 2017, 146, .	1.2	41
1491	Adsorption mechanism, structural and electronic properties: 4-Phenylpyridine & undoped or doped (B or Si) C ₆₀ . <i>Journal of Molecular Liquids</i> , 2017, 238, 225-228.	2.3	16
1492	Synergetic effect between spin crossover and luminescence in the [Fe(bpp) ₂][BF ₄] ₂ (bpp =) Tj ETQqO O rgBT /Overlock 10 If 50 342 T	2.7	41
1493	Properties of electronically excited states of four squaraine dyes and their complexes with fullerene C ₇₀ : A theoretical investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 184, 82-88.	2.0	4
1494	Iron(II)/copper(I)-mediated stereoselective carbozincation of ynamides. One-pot synthesis of ̂-allyl-tetrasubstituted-enamides. <i>Tetrahedron</i> , 2017, 73, 3415-3422.	1.0	7
1495	Covalent versus Ionic Bonding in Al-C Clusters. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4009-4018.	1.1	19
1496	The effect of relative position of the ̂-spacer center between donor and acceptor on the overall performance of D-̂-A dye: a theoretical study with organic dye. <i>Electrochimica Acta</i> , 2017, 241, 440-448.	2.6	27
1497	Host-Guest Interactions Accompanying the Encapsulation of 1,4-Diazabicyclo[2.2.2]octane within endo-Functionalized Macrocycles. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3792-3802.	1.1	14
1498	Hydrogen bonding and ̂-̂ stacking in nicotinamide/H ₂ O mixtures. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 184, 294-298.	2.0	8
1499	Anion Photoelectron Spectroscopy and Theoretical Investigation on Nb ₂ Si _n (n = 2-12) Clusters. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11851-11861.	1.5	42

#	ARTICLE	IF	CITATIONS
1500	The new competitive mechanism of hydrogen bonding interactions and transition process for the hydroxyphenyl imidazo [1, 2-a] pyridine in mixed liquid solution. <i>Scientific Reports</i> , 2017, 7, 1574.	1.6	31
1501	Reactions of Platinum Carbonyl Chini Clusters with Ag(NHC)Cl Complexes: Formation of Acid-Base Lewis Adducts and Heteroleptic Clusters. <i>Inorganic Chemistry</i> , 2017, 56, 6532-6544.	1.9	16
1502	Structural and electronic analysis of Li/Al layered double hydroxides and their adsorption for CO ₂ . <i>Applied Surface Science</i> , 2017, 416, 411-423.	3.1	26
1503	Unraveling the formation mechanism of subphthalocyanine. Density functional theory studies. <i>Inorganic Chemistry Communication</i> , 2017, 85, 9-15.	1.8	8
1504	AuRnX and XAuRn (X=F and OH). <i>ChemistrySelect</i> , 2017, 2, 3471-3478.	0.7	2
1505	Organoboron copolymers containing thienothiophene and selenophenothiophene analogues: optical, electrochemical and fluoride sensing properties. <i>RSC Advances</i> , 2017, 7, 23197-23207.	1.7	12
1506	Chalcogen bonds tuned by an N-H...O or Ca...H...O interaction: investigation of substituent, cooperativity and solvent effects. <i>Molecular Physics</i> , 2017, 115, 1713-1723.	0.8	12
1507	N ₂ O reduction over a fullerene-like boron nitride nanocage: A DFT study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 2085-2091.	0.9	35
1508	Insights into the structures and electronic properties of Cu _{n+1} and Cu _n S _{1/4} (n=1-12; 1/4=0, 1) clusters. <i>Scientific Reports</i> , 2017, 7, 1345.	1.6	23
1509	Structure and spectroscopic study of aqueous Fe(III)-As(V) complexes using UV-Vis, XAS and DFT-TDDFT. <i>Chemosphere</i> , 2017, 182, 595-604.	4.2	48
1510	The Peculiar Role of the Au ₃ Unit in Au _m Clusters: f-Aromaticity of the Au ₅ Zn ⁺ Ion. <i>Inorganic Chemistry</i> , 2017, 56, 5793-5803.	1.9	27
1511	Synthesis of the Highly Reduced [Fe ₆ C(CO) ₁₅] ⁴⁻ Carbonyl Carbide Cluster and Its Reactions with H ⁺ and [Au(PPh ₃) ₃] ⁺ . <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 3135-3143.	1.0	14
1512	Topological analysis of the metal-metal bond: A tutorial review. <i>Coordination Chemistry Reviews</i> , 2017, 345, 150-181.	9.5	108
1513	Synthesis, structure, spectral properties and theoretical studies of two half-sandwich titanium-complexes with adamantoxy ligands. <i>Journal of Molecular Structure</i> , 2017, 1142, 248-254.	1.8	0
1514	Photophysical and Electroluminescent Properties of PtAg ₂ Acetylide Complexes Supported with <i>meso</i> - and <i>rac</i> -Tetraphosphine. <i>Inorganic Chemistry</i> , 2017, 56, 9461-9473.	1.9	25
1515	Accurate Relative Energies and Binding Energies of Large Ice-Liquid Water Clusters and Periodic Structures. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4030-4038.	1.1	17
1516	External or internal surface of H-ZSM-5 zeolite, which is more effective for the Beckmann rearrangement reaction?. <i>Catalysis Science and Technology</i> , 2017, 7, 2512-2523.	2.1	26
1517	Binding of Small Gas Molecules by Metal-Bipyridyl Monocationic Complexes (Metal = Cu, Ag, Au) and Possible Bond Activations Therein. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3803-3817.	1.1	16

#	ARTICLE	IF	CITATIONS
1518	DFT and TD-DFT theoretical studies on photo-induced electron transfer process on [Cefamandole].C60 nano-complex. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 42-48.	1.3	27
1519	Impact of Dielectric Constant on the Singlet-Triplet Gap in Thermally Activated Delayed Fluorescence Materials. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2393-2398.	2.1	118
1520	Tunnelling and barrier-less motions in the 2-fluoroethanol-water complex: a rotational spectroscopic and ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12221-12228.	1.3	17
1521	Study on molecular structure, spectroscopic properties (FTIR and UV-Vis), NBO, QTAIM, HOMO-LUMO energies and docking studies of 5-fluorouracil, a substance used to treat cancer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 184, 169-176.	2.0	21
1522	The Fractional Occupation Number Weighted Density as a Versatile Analysis Tool for Molecules with a Complicated Electronic Structure. <i>Chemistry - A European Journal</i> , 2017, 23, 6150-6164.	1.7	102
1523	Adsorption/desorption process of formaldehyde onto iron doped graphene: a theoretical exploration from density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4179-4189.	1.3	46
1524	Insight into the structure and stability of Tc and Re DMSA complexes: A computational study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 71, 167-175.	1.3	9
1525	Theoretical insights on the electroluminescent mechanism of thermally activated delayed fluorescence emitters. <i>Organic Electronics</i> , 2017, 41, 17-25.	1.4	65
1526	Structural, spectral, electrochemical and DFT studies of two mononuclear manganese(II) and zinc(II) complexes. <i>Polyhedron</i> , 2017, 122, 228-240.	1.0	103
1527	Properties and separation method of enantiomers of the mono- and bis-substituted derivatives of 3,3',4,4'-tetramethyl-1,1'-diphosphaferrocene: structural analysis using X-ray diffraction and circular dichroism. <i>Tetrahedron: Asymmetry</i> , 2017, 28, 135-145.	1.8	2
1528	Structures, stabilities, and electronic properties of fullerene C ₃₆ with endohedral atomic Sc, Y, and La: A dispersion-corrected DFT study. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25335.	1.0	8
1529	Synthesis and structural studies on Ni(II) dithiocarbamates: Exploring intramolecular Ni-H interactions. <i>Polyhedron</i> , 2017, 123, 453-461.	1.0	14
1530	2,4,6-tris[bis(1H-tetrazol-5-yl)amino]-1,3,5-triazine as a nitrogen-rich material. <i>Journal of Chemical Sciences</i> , 2017, 129, 657-661.	0.7	5
1531	Inhibition activities of catechol diether based non-nucleoside inhibitors against the HIV reverse transcriptase variants: Insights from molecular docking and ONIOM calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 294-305.	1.3	11
1532	A comparative study on the N-heterocyclic carbene adducts of Ir _h -C ₆₀ , D _{5h} -C ₇₀ and Sc ₃ N@Ir _h -C ₈₀ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17598-17606.	1.3	5
1533	Perspective on quantifying electron localization/delocalization, non-linear optical response and vibrational analysis of 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline. <i>Journal of Molecular Structure</i> , 2017, 1146, 797-807.	1.8	4
1534	Atom- and Ion-Centered Icosahedral Shaped Subnanometer-Sized Clusters of Molecular Hydrogen. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15036-15048.	1.5	7
1535	Adsorption of H ₂ on Ga ₂₄ N ₂₄ cluster; A density functional theory investigation. <i>Vacuum</i> , 2017, 143, 209-216.	1.6	3

#	ARTICLE	IF	CITATIONS
1536	Efficient blue organic light-emitting diodes based on pyrene phenanthrimidazole and D-π-A chromophore. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 346, 296-310.	2.0	15
1537	Tunable excited-state intramolecular proton transfer reactions with N H or O H as a proton donor: A theoretical investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 187, 9-14.	2.0	36
1538	Prediction of neutral noble gas compounds LiNgF (Ng = Kr, Xe and Rn). <i>Computational and Theoretical Chemistry</i> , 2017, 1113, 8-13.	1.1	3
1539	Experimental and theoretical investigations on Pd(II) host-guest compound: Deciphering the structural and electronic features of a potential bioactive complex. <i>Journal of Molecular Structure</i> , 2017, 1145, 170-183.	1.8	18
1540	Why Low Valent Lead(II) Hydride Complex Would be a Better Catalyst for CO ₂ Activation than Its 14 Group Analogues?. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12127-12135.	1.5	9
1541	Theoretical Investigation into Suitable Pore Sizes of Membranes for Vanadium Redox Flow Batteries. <i>ChemElectroChem</i> , 2017, 4, 2184-2189.	1.7	27
1542	A Computational Exploration of H ₂ S and CO ₂ Capture by Ionic Liquids Based on ß-Amino Acid Anion and N ⁷ ,N ⁹ -Dimethyladeninium Cation. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4352-4362.	1.1	19
1543	Near UV-Visible electronic absorption originating from charged amino acids in a monomeric protein. <i>Chemical Science</i> , 2017, 8, 5416-5433.	3.7	136
1544	Theoretical insights into the selectivity of 1,6-enyne cycloisomerization on gold clusters: Orbital interaction role. <i>Computational and Theoretical Chemistry</i> , 2017, 1113, 94-100.	1.1	1
1545	Toward a Rigorous Definition of a Strength of Any Interaction Between Bader's Atomic Basins. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4517-4522.	1.1	46
1546	Insights into Glycol Ether-Alkanol Mixtures from a Combined Experimental and Theoretical Approach. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5601-5612.	1.2	6
1547	Computational investigation on the large energy gap between the triplet excited-states in acenes. <i>RSC Advances</i> , 2017, 7, 26697-26703.	1.7	26
1548	Quantum Chemical Spin Densities for Radical Cations of Photosynthetic Pigment Models. <i>Photochemistry and Photobiology</i> , 2017, 93, 815-833.	1.3	9
1549	Copper Crystallization from Aqueous Solution: Initiation and Evolution of the Polynuclear Clusters. <i>Journal of Cluster Science</i> , 2017, 28, 2517-2528.	1.7	3
1550	A DFT analysis of the adsorption of nitrogen oxides on Fe-doped graphene, and the electric field induced desorption. <i>Applied Surface Science</i> , 2017, 420, 446-455.	3.1	65
1551	Exciton coupling between enones: Quassinoids revisited. <i>Chirality</i> , 2017, 29, 476-485.	1.3	16
1552	Investigation of inclusion complexation of acetaminophen with pillar [5]arene: UV-Vis, NMR and quantum chemical study. <i>Journal of Molecular Liquids</i> , 2017, 241, 782-791.	2.3	24
1553	The conversion of donor to acceptor and rational design for diketopyrrolopyrrole-containing small molecule acceptors by introducing nitrogen-atoms for organic solar cells. <i>RSC Advances</i> , 2017, 7, 31800-31806.	1.7	17

#	ARTICLE	IF	CITATIONS
1554	Elaborating the excited-state proton transfer behaviors for novel 3H-MC and P2H-CH. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1935-1942.	2.3	31
1555	Dissecting the accountability of parameterized and parameter-free single-hybrid and double-hybrid functionals for photophysical properties of TADF-based OLEDs. <i>Journal of Chemical Physics</i> , 2017, 146, 234304.	1.2	17
1556	Mutual influence between triel bond and cation-π interactions: an <i>ab initio</i> study. <i>Molecular Physics</i> , 2017, 115, 2999-3010.	0.8	10
1557	Theoretical study on electronic and vibrational properties of hydrogen bonds in glycine-water clusters. <i>Chemical Physics Letters</i> , 2017, 684, 53-59.	1.2	17
1558	Enthalpies of Formation of Hydrazine and Its Derivatives. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5361-5370.	1.1	20
1559	Aromaticity and antiaromaticity of substituted fulvene derivatives: perspectives from the information-theoretic approach in density functional reactivity theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18635-18645.	1.3	43
1560	Double Gold Activation of 1-Ethynyl-2-(Phenylethynyl)Benzene Toward <i>exo</i> and <i>endo</i> Cyclization Reactions. <i>Chemistry - A European Journal</i> , 2017, 23, 13360-13368.	1.7	21
1561	Synthesis and thermal stability of <i>cis</i> -dichloro[(E)-ethyl-2-(2-((8-hydroxyquinolin-2-yl)methylene)hydrazinyl)acetate- η^2 N]-palladium(II) complex. <i>Journal of Thermal Analysis and Calorimetry</i> , 2017, 130, 701-711.	2.0	3
1562	Photoreactions of Porphyrins Initiated by Deep Ultraviolet Single Photons. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4626-4632.	1.1	6
1563	The first Re ^I organometallic complex with an organoimido-polyoxometalate ligand. <i>Dalton Transactions</i> , 2017, 46, 8611-8620.	1.6	4
1564	Gas phase anion photoelectron spectroscopy and theoretical investigation of gold acetylide species. <i>Journal of Chemical Physics</i> , 2017, 146, 194303.	1.2	15
1565	On the Structural and Optoelectronic Properties of Chemically Modified Oligothiophenes with Electron-Withdrawing Substituents for Organic Solar Cell Applications: A DFT/TDDFT Study. <i>Journal of the Physical Society of Japan</i> , 2017, 86, 064802.	0.7	8
1566	Pnicogen bond interaction between PF ₂ Y (Y = C ⁺ N, N ⁺ C) with NH ₃ , CH ₃ OH, H ₂ O, and HF molecules. <i>Structural Chemistry</i> , 2017, 28, 1843-1851.	1.0	3
1567	Transition from metal-ligand bonding to halogen bonding involving a metal as halogen acceptor a study of Cu, Ag, Au, Pt, and Hg complexes. <i>Chemical Physics Letters</i> , 2017, 681, 56-63.	1.2	74
1568	Boron/nitrogen substituted the staggered hetero-dimers: Fascinating intermolecular charge-transfer and large NLO responses. <i>Dyes and Pigments</i> , 2017, 145, 21-28.	2.0	13
1569	A comprehensive density functional theory study on molecular structures of (5, 5) carbon nanotube doped with B, N, Al, Si, P, Co, and Ni. <i>Computational and Theoretical Chemistry</i> , 2017, 1114, 55-64.	1.1	10
1570	Theoretical study of Ni ⁺ assisted C-C and C-H bond activations of propionaldehyde in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2017, 1114, 140-145.	1.1	7
1571	A comprehensive theoretical investigation about the bio-functionalization capability of single walled CNT, BNNT and SiCNT using DNA/RNA nucleobases. <i>Applied Surface Science</i> , 2017, 422, 56-72.	3.1	32

#	ARTICLE	IF	CITATIONS
1572	Selective hydration of asymmetric internal aryl alkynes without directing groups to $\hat{\text{I}}\pm$ -aryl ketones over Cu-based catalyst. <i>New Journal of Chemistry</i> , 2017, 41, 6290-6295.	1.4	15
1573	Synthesis, structural and biological studies of two new Co(III) complexes with tridentate hydrazone ligand derived from the antihypertensive drug hydralazine. <i>Inorganica Chimica Acta</i> , 2017, 466, 16-29.	1.2	19
1574	Experimental, quantum chemical and molecular dynamic simulations studies on the corrosion inhibition of mild steel by some carbazole derivatives. <i>Scientific Reports</i> , 2017, 7, 2436.	1.6	82
1575	Polynitro-Functionalized Dipyrazolo-1,3,5-triazinanes: Energetic Polycyclization toward High Density and Excellent Molecular Stability. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 8834-8838.	7.2	91
1576	Does Confinement Always Lead to Thermodynamically and/or Kinetically Favorable Reactions? A Case Study using Diels-Alder Reactions within ExBox^{+4} and CB[7]. <i>ChemPhysChem</i> , 2017, 18, 2162-2170.	1.0	24
1577	Structure and electronic properties of ion pairs accompanying cyclic morpholinium cation and alkylphosphite anion based ionic liquids. <i>Chemical Physics</i> , 2017, 492, 35-52.	0.9	6
1578	In-situ studies on the micro-structure evolution of $\text{A}_2\text{W}_2\text{O}_7$ (A = Li, Na, K) during melting by high temperature Raman spectroscopy and density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 185, 188-196.	2.0	18
1579	Visualization of weak interactions between quantum dot and graphene in hybrid materials. <i>Scientific Reports</i> , 2017, 7, 417.	1.6	11
1580	Corannulene-fullerene C70 noncovalent interactions and their effect on the behavior of charge transport and optical property. <i>RSC Advances</i> , 2017, 7, 27960-27968.	1.7	7
1581	Computational insights into the $\text{S}_{3\text{transfer}}$ reaction: A special case of double group transfer reaction featuring bicyclically delocalized aromatic transition state geometries. <i>Journal of Computational Chemistry</i> , 2017, 38, 1966-1973.	1.5	3
1582	D $\hat{\text{A}}^{\sim}$ A System: Light Harvesting, Charge Transfer, and Molecular Designing. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12546-12561.	1.5	100
1583	A DFT study of 3d (d $\hat{\text{d}}_{10}$) transition-metal phthalocyanines (TMPcs): Bonding natures, electronic adsorption spectroscopy. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750036.	1.8	0
1584	The crucial role of water clusters $(\text{H}_2\text{O})_n$ ($n = 0\hat{\text{5}}$) on the catalytic oxidation of AsH_3 : An accurate theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 69-79.	1.1	2
1585	Dissociation of H_2 on Mg-coated $\text{B}_{12}\text{C}_6\text{N}_6$. <i>Chinese Physics B</i> , 2017, 26, 068801.	0.7	1
1586	van der Waals DFT ONIOM study of the adsorption of DNA bases on the Cu(111) nanosurface. <i>Applied Surface Science</i> , 2017, 422, 372-387.	3.1	10
1587	Microsolvation of lithium iodide dimer studied by ab initio calculations. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 119-126.	1.1	3
1588	Theoretical evaluation of the organocatalytic behavior of the negatively charged carbon atom in a fused five-member ring in carbon dioxide transformation to methanol. <i>Energy</i> , 2017, 134, 493-503.	4.5	17
1589	Synthesis and characterization of mononuclear ruthenium complexes with carboxylato, chlorido and phosphine ligands. Crystal structures of $[\text{RuCl}_2\{\hat{\text{I}}^2\text{-O}_2\text{O}_2\text{CCCH}_2(\text{CH}_3)\}(\text{PPh}_3)_2]$, $[\text{RuCl}_2(\hat{\text{I}}^2\text{-O}_2\text{O}_2\text{CC}_6\text{H}_4\text{-2-Cl})(\text{PPh}_3)_2]$, and $[\text{Et}_3\text{NH}][\text{RuCl}(\text{SO}_2)(\hat{\text{I}}^2\text{-C}_6\text{H}_4\text{-2-CO}_2)(\text{PPh}_3)_2]$. <i>Inorganica Chimica Acta</i> , 2017, 466, 382-388.	1.2	2

#	ARTICLE	IF	CITATIONS
1590	Halogen Bonding in the Complexes of CH ₃ I and CCl ₄ with Oxygen-Containing Halogen-Bond Acceptors. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5045-5055.	1.1	18
1591	Oxidized and Si-doped graphene: emerging adsorbents for removal of dioxane. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17587-17597.	1.3	18
1592	Interactions between Ketones and Alcohols: Rotational Spectrum and Internal Dynamics of the Acetone-Ethanol Complex. <i>Chemistry - A European Journal</i> , 2017, 23, 11119-11125.	1.7	8
1593	Reaction mechanism of hydrogen cyanide catalyzed by gas-phase titanium. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25412.	1.0	2
1594	Theoretical analysis of the binding of iron(III) protoporphyrin IX to 4-methoxyacetophenone thiosemicarbazone via DFT-D3, MEP, QTAIM, NCI, ELF, and LOL studies. <i>Journal of Molecular Modeling</i> , 2017, 23, 200.	0.8	81
1595	Computational studies on the mechanism and selectivity of Al ₈ O ₁₂ nanocluster for different elimination reactions. <i>Structural Chemistry</i> , 2017, 28, 1895-1906.	1.0	9
1596	Synthesis and evaluation of aromaticity and tautomerization of pyrazolopyridazin(on)es. <i>Journal of Chemical Sciences</i> , 2017, 129, 741-752.	0.7	5
1597	The influence of noncovalent interactions in metal-free organic dye molecules to augment the efficiency of dye sensitized solar cells: A computational study. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25415.	1.0	7
1598	On the role of substituent in noncovalent functionalization of graphene and organophosphor recognition: IQA and SAPT perspective. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25379.	1.0	10
1599	Effect of polyoxometalate in organic-inorganic hybrids on charge transfer and absorption spectra towards sensitizers. <i>Dyes and Pigments</i> , 2017, 142, 379-386.	2.0	20
1600	Molecular recognition of cyclodecapeptides to ibuprofen and naproxen enantiomers: a theoretical study. <i>Structural Chemistry</i> , 2017, 28, 1631-1644.	1.0	7
1601	Theoretical investigation into the influence of molar ratio on binding energy, mechanical property and detonation performance of 1,3,5,7-tetranitro-1,3,5,7-tetrazacyclo octane (HMX)/1-methyl-4,5-dinitroimidazole (MDNI) cocrystal explosive. <i>Computational and Theoretical Chemistry</i> , 2017, 1109, 27-35.	1.1	10
1602	The mechanism of the gas-phase elimination kinetics of the $\hat{1}^2, \hat{1}^3$ -unsaturated aldehyde 2,2-dimethyl-3-butenal: a theoretical study. <i>Molecular Physics</i> , 2017, 115, 1624-1632.	0.8	2
1603	Adducts of Donor-Functionalized Ar ₃ P with the Soft Lewis Acid I ₂ : Probing Simultaneous Lewis Acidity and Basicity at Internally Solvated P(III) Centers. <i>Inorganic Chemistry</i> , 2017, 56, 4622-4634.	1.9	6
1604	Photoactive layer based on T-shaped benzimidazole dyes used for solar cell: from photoelectric properties to molecular design. <i>Scientific Reports</i> , 2017, 7, 45688.	1.6	40
1605	Diiodomethane as a halogen bond donor toward metal-bound halides. <i>CrystEngComm</i> , 2017, 19, 2517-2525.	1.3	64
1606	Silyl Chalconium Ions: Synthesis, Structure and Application in Hydrodefluorination Reactions. <i>Chemistry - A European Journal</i> , 2017, 23, 10068-10079.	1.7	39
1607	A theoretical investigation on doping superalkali for triggering considerable nonlinear optical properties of Si ₁₂ C ₁₂ nanostructure. <i>Journal of Computational Chemistry</i> , 2017, 38, 1574-1582.	1.5	43

#	ARTICLE	IF	CITATIONS
1608	Theoretical insight into the BH ₃ ·HCN adsorption on the Co(100) and Co(110) surfaces as hydrogen storage. <i>Journal of Molecular Modeling</i> , 2017, 23, 126.	0.8	10
1609	A density functional theory study on the interactions between dibenzothiophene and tetrafluoroborate-based ionic liquids. <i>Journal of Molecular Modeling</i> , 2017, 23, 145.	0.8	12
1610	Why does β-cyclodextrin prefer to bind nucleotides with an adenine base rather than other 2-deoxyribonucleoside 5-monophosphates?. <i>Journal of Molecular Modeling</i> , 2017, 23, 149.	0.8	5
1611	Tuning hydrogen bonds via anion-π or lone pair-π interaction: a comparative ab initio study. <i>Structural Chemistry</i> , 2017, 28, 1255-1264.	1.0	14
1612	Cooperativity of adjacent Brønsted acid sites in MFI zeolite channel leads to enhanced polarization and cracking of alkanes. <i>Journal of Catalysis</i> , 2017, 349, 163-174.	3.1	85
1613	Experimental and theoretical study on the molecular structure, covalent and non-covalent interactions of 2,4-dinitrodiphenylamine: X-ray diffraction and QTAIM approach. <i>Journal of Molecular Structure</i> , 2017, 1141, 53-63.	1.8	16
1614	Theoretical analysis of electrochromism under redox of bis(3-thienyl)/(2-thienyl)hexafluorocyclopentene: effects of charged and substituted systems. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 9281-9291.	1.3	3
1615	(N,Se) and (Se,N,Se) Ligands Based on Carborane and Pyridine Fragments – Reactivity of 2,6-bis[(1-methyl-2-imidazolyl)closo-1,10-C ₂ B ₁₀ H ₁₀]SeCH ₂ towards Copper and Silver. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 2643-2652.		
1616	Can Fluorine form Halogen Bond? Investigation of Halogen Bonds through Steric Charge. <i>ChemistrySelect</i> , 2017, 2, 2713-2717.	0.7	8
1617	Computational prediction of endohedral dimetalloborofullerenes M ₂ @B ₈₀ (M = Sc, Y). <i>Chemical Physics Letters</i> , 2017, 676, 89-94.	1.2	16
1618	A computational study on structure and bonding in ion pairs accompanying pyrrolidinium and piperidinium based ionic liquids. <i>Journal of Molecular Liquids</i> , 2017, 234, 227-239.	2.3	7
1619	On the covalence in coinage-metal halides M ₃ X ₃ (M = Cu, Ag and Au, X = F or I). <i>Molecular Physics</i> , 2017, 115, 1544-1554.	0.8	2
1620	Unusual Nonemissive Behavior of Rubrene J-Aggregates: A Rare Violation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3190-3201.	1.2	11
1621	DFT study on the dissolution mechanisms of β-cyclodextrin and chitobiose in ionic liquid. <i>Carbohydrate Polymers</i> , 2017, 169, 227-235.	5.1	35
1622	Theoretical design of three-dimensional non-fullerene acceptor materials based on an arylenediimide unit towards high efficiency organic solar cells. <i>New Journal of Chemistry</i> , 2017, 41, 3857-3864.	1.4	14
1623	Theoretical modulation of singlet/triplet chemiexcitation of chemiluminescent imidazopyrazinone dioxetanone via C8-substitution. <i>Photochemical and Photobiological Sciences</i> , 2017, 16, 897-907.	1.6	21
1624	Computational insights into the concomitant changes of hollow interior evolution in [SbnAunSbn] _m (n=3, 4, 5, 6; m= -3, -2, -1, -2) complex. <i>AIP Advances</i> , 2017, 7, .	0.6	1
1625	Theoretical investigation of the weak interaction between graphene and alcohol solvents. <i>Chemical Physics Letters</i> , 2017, 676, 129-133.	1.2	12

#	ARTICLE	IF	CITATIONS
1626	Design and Applications of <i>N</i> - <i>tert</i> -Butyl Sulfinyl Squaramide Catalysts. <i>Organic Letters</i> , 2017, 19, 1926-1929.	2.4	18
1627	Theoretical Study of the Kinetics and Mechanism of the Thermal Decomposition of 3-Oxetanone in the Gas Phase. <i>Progress in Reaction Kinetics and Mechanism</i> , 2017, 42, 36-43.	1.1	2
1628	Spiro Metalla-aromatics of Pd, Pt, and Rh: Synthesis and Characterization. <i>Journal of the American Chemical Society</i> , 2017, 139, 5039-5042.	6.6	79
1629	Theoretical insights into the π -hole interactions in the complexes containing triphosphorus hydride (P ₃ H ₃) and its derivatives. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 195-202.	0.5	4
1630	Systematic study of imidazoles inhibiting IDO1 via the integration of molecular mechanics and quantum mechanics calculations. <i>European Journal of Medicinal Chemistry</i> , 2017, 131, 152-170.	2.6	13
1631	Sandwich rare earth complexes simultaneously involving aromatic phthalocyanine and antiaromatic hemiporphyrzine ligands showing a predominantly aromatic nature. <i>Chemical Communications</i> , 2017, 53, 3765-3768.	2.2	9
1632	Bond Order Analysis, Packing Ratio, and Electronic Structures of Two Structural Polymorphs Based on Manganese Complexes. <i>Chinese Journal of Chemistry</i> , 2017, 35, 927-930.	2.6	1
1633	Theoretical study on the alkylation of <i>o</i> -xylene with styrene in AlCl ₃ -ionic liquid catalytic system. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 74, 8-15.	1.3	13
1634	Synthesis, characterization and theoretical studies on novel organic-inorganic hybrid ion-gel polymer thin films from a Fe ₂ O ₃ -doped polyvinylpyrrolidone-N-butylpyridinium tetrafluoroborate composite via intramolecular thermal polymerization. <i>RSC Advances</i> , 2017, 7, 16623-16636.	1.7	8
1635	Metal-metal multiple bond in low-valent diuranium porphyrzines and its correlation with metal oxidation state: A relativistic DFT study. <i>Computational and Theoretical Chemistry</i> , 2017, 1108, 29-39.	1.1	6
1636	Cinchona Alkaloid-Squaramide Catalyzed Sulfa-Michael Addition Reaction: Mode of Bifunctional Activation and Origin of Stereinduction. <i>Journal of Organic Chemistry</i> , 2017, 82, 4362-4368.	1.7	57
1637	Cu-wire-mediated dipyrimidine-base pairs the building blocks for conductive and magnetic Cu-DNA nanowires. <i>Journal of Mathematical Chemistry</i> , 2017, 55, 1301-1321.	0.7	3
1638	Photo-induced oxidative damage to dissolved free amino acids by the photosensitizer polycyclic musk tonalide: Transformation kinetics and mechanisms. <i>Water Research</i> , 2017, 115, 339-346.	5.3	17
1639	Computational Study on the Mechanisms of Multiple Complexation of CO and Isonitrile Ligands to Boron. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2688-2697.	1.1	4
1640	A semi-conductive organic-inorganic hybrid emits pure white light with an ultrahigh color rendering index. <i>Journal of Materials Chemistry C</i> , 2017, 5, 4731-4735.	2.7	55
1641	Carbene-aerogen bonds: an <i>ab initio</i> study. <i>Molecular Physics</i> , 2017, 115, 971-980.	0.8	13
1642	Different Ways of Hydrogen Bonding in Water - Why Does Warm Water Freeze Faster than Cold Water?. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 55-76.	2.3	85
1643	Electronic forces as descriptors of nucleophilic and electrophilic regioselectivity and stereoselectivity. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1496-1503.	1.3	49

#	ARTICLE	IF	CITATIONS
1644	Second-order NLO responses of two-cavity inorganic electrides $\text{Li}_{2n}\text{B}_{20}\text{H}_{26}$ ($n = 1, 2$): evolutions with increasing excess electron number and various B–B connection sites of $\text{B}_{20}\text{H}_{26}$. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2557-2566.	1.3	13
1645	High Voltage, Transition Metal Complex Enables Efficient Electrochemical Energy Storage in a Li–K Battery Full Cell. <i>Advanced Functional Materials</i> , 2017, 27, 1604299.	7.8	20
1646	Beyond the electrostatic model: the significant roles of orbital interaction and the dispersion effect in aqueous H_2O systems. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1298-1302.	1.3	7
1647	Cooperation and competition between halogen bonding and van der Waals forces in supramolecular engineering at the aliphatic hydrocarbon/graphite interface: position and number of bromine group effects. <i>Nanoscale</i> , 2017, 9, 237-250.	2.8	36
1648	The electronic density obtained from a QTAIM analysis used as molecular descriptor. A study performed in a new series of DHFR inhibitors. <i>Journal of Molecular Structure</i> , 2017, 1134, 464-474.	1.8	16
1649	Theoretical investigation of gas-phase molecular complex formation between 2-hydroxy thiophenol and a water molecule. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2466-2478.	1.3	8
1650	Tuning the Electron Transport and Electron-Accepting Abilities of Dyes through Introduction of Different π -Conjugated Bridges and Acceptors for Dye-Sensitized Solar Cells. <i>ChemPhysChem</i> , 2017, 18, 366-383.	1.0	33
1651	Stationary Conditions of the Electron Density Along the Reaction Path: Connection with Conceptual DFT and Information Theory. <i>Journal of Physical Chemistry A</i> , 2017, 121, 648-660.	1.1	10
1652	Theoretical Study of the Gaseous Hydrolysis of NO_2 in the Presence of Amines. <i>Journal of Physical Chemistry A</i> , 2017, 121, 226-237.	1.1	22
1653	Benzoindolic squaraine dyes with a large two-photon absorption cross-section. <i>Journal of Materials Chemistry C</i> , 2017, 5, 1224-1230.	2.7	30
1654	Reversible water uptake by a porous molecular crystal from metal complex of gemini surfactant. <i>CrystEngComm</i> , 2017, 19, 802-810.	1.3	4
1655	Edge functionalised & Li-intercalated 555-777 defective bilayer graphene for the adsorption of CO_2 and H_2O . <i>Applied Surface Science</i> , 2017, 400, 375-390.	3.1	14
1656	Theoretical analysis of trends in hydrogen bonding involving halogen acceptors (F^{\sim}At) covalently bonded to a group 14 atom (C^{\sim}Pb). <i>Molecular Physics</i> , 2017, 115, 364-378.	0.8	7
1657	Synthesis, crystal structure and DFT studies of a Zinc(II) complex of 1,3-diaminopropane (Dap), $[\text{Zn}(\text{Dap})(\text{NCS})_2][\text{Zn}(\text{Dap})(\text{NCS})_2]_n$. The additional stabilizing role of S– π chalcogen bond. <i>Journal of Molecular Structure</i> , 2017, 1133, 271-277.	1.8	3
1658	Understanding the Phosphorylation Mechanism by Using Quantum Chemical Calculations and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3565-3573.	1.2	12
1659	Ab initio investigation of possible candidate structures and properties of water cluster $(\text{H}_2\text{O})_7^+$ via particle swarm optimization method. <i>Computational and Theoretical Chemistry</i> , 2017, 1099, 123-132.	1.1	4
1660	Evaluating frontier orbital energy and HOMO/LUMO gap with descriptors from density functional reactivity theory. <i>Journal of Molecular Modeling</i> , 2017, 23, 3.	0.8	75
1661	Theoretical studies on dimerization vs. microhydration of carboxylic acids. <i>Computational and Theoretical Chemistry</i> , 2017, 1099, 185-194.	1.1	9

#	ARTICLE	IF	CITATIONS
1662	Noncovalent interactions from electron density topology and solvent effects on spectral properties of Schiff bases. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 175, 134-144.	2.0	20
1663	Enhancing 4-propylheptane dissociation with nickel nanocluster based on molecular dynamics simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 72, 106-111.	1.3	1
1664	Probing a General Rule towards Thermodynamic Stabilities of Mono BN-doped Lower Polyenes. <i>Chemistry - an Asian Journal</i> , 2017, 12, 605-614.	1.7	5
1665	Microhydration of Neutral and Charged Acetic Acid. <i>Journal of Physical Chemistry A</i> , 2017, 121, 493-504.	1.1	12
1666	Surprising Outcomes of Classic Ring-Expansion Conditions Applied to Octaethyloxochlorin, 3. Schmidt-Reaction Conditions. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 1835-1842.	1.2	11
1667	Insight into electrostatic initiation of nitramine explosives. <i>Journal of Molecular Modeling</i> , 2017, 23, 10.	0.8	10
1668	Characterization of the binding of six actinyls AnO_2^{2+} ($An = U/Np/Pu$) with three expanded porphyrins by density functional theory. <i>New Journal of Chemistry</i> , 2017, 41, 63-74.	1.4	10
1669	Polynitrogen clusters encapsulated inside B ₂₄ N ₂₄ fullerene-like nanocages: Nanoscale high energy materials studied by density functional theory. <i>Inorganica Chimica Acta</i> , 2017, 456, 128-135.	1.2	3
1670	Sensing Ability of Hybrid Cyclic Nanopeptides Based on Thiourea Cryptands for Different Ions, A Joint DFT-D3/MD Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 244-255.	1.1	13
1671	One-Pot Synthesis, Crystal Structure, and Thermal Decomposition Behavior of 1,1-Diamino-4,4,5,5-Tetranitro-2,2-Biimidazole. <i>Journal of Energetic Materials</i> , 2017, 35, 239-249.	1.0	21
1672	Static and Dynamic Study of Disaccharides Trehalose, Maltose and Sucrose. <i>Structural Chemistry</i> , 2017, 28, 911-924.	1.0	4
1673	Photoluminescence and electroluminescence of cationic PtAu ₂ heterotrinnuclear complexes with aromatic acetylides. <i>Dalton Transactions</i> , 2017, 46, 865-874.	1.6	28
1674	Theoretical study on [3]- and [4]radialene complexes CpM(C _{2n} H _{2n}) (n=3, 4; M=Sc ^{1/4} Ni): Special metal-aromatic interaction along with metal-alkene bonds. <i>Journal of Organometallic Chemistry</i> , 2017, 828, 75-82.	0.8	4
1675	Rational synthesis and comparative investigation on a series of fluorinated aryl substituted diketopyrrolopyrrole. <i>Tetrahedron</i> , 2017, 73, 494-499.	1.0	6
1676	A computational study of self-assembled hexapeptide inhibitors against amyloid- β^2 ($A\beta^2$) aggregation. <i>Physical Chemistry Chemical Physics</i> , 2016, 19, 155-166.	1.3	18
1677	Structural variability in Cu(I) and Ag(I) coordination polymers with a flexible dithione ligand: Synthesis, crystal structure, microbiological and theoretical studies. <i>Journal of Solid State Chemistry</i> , 2017, 249, 70-79.	1.4	14
1678	Testing the effectiveness of the isoelectronic substitution principle through the transformation of aromatic osmathiophene derivatives into their inorganic analogues. <i>New Journal of Chemistry</i> , 2017, 41, 1168-1178.	1.4	9
1679	Theory and experiment studies of the 1,4-bis(4-methoxystyryl)benzene as a wavelength shifter of liquid scintillator. <i>Journal of Luminescence</i> , 2017, 183, 442-447.	1.5	2

#	ARTICLE	IF	CITATIONS
1680	Pyrazole cleavage of tris(3,5-dimethylpyrazolyl)borate with Ruthenium(II) complexes: Synthesis, structural characterization and DFT studies. <i>Journal of Molecular Structure</i> , 2017, 1133, 264-270.	1.8	8
1681	Synthesis of heat-resistant benzoxazine-based polyfluorene and its reversible temperature-sensitive fluorescence. <i>Polymer</i> , 2017, 109, 126-136.	1.8	8
1682	Development of a Novel Index for Analysis of Electronically Excited States. <i>ChemPhysChem</i> , 2017, 18, 480-487.	1.0	8
1683	Efficient floating diffuse functions for accurate characterization of the surface-bound excess electrons in water cluster anions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2816-2825.	1.3	3
1684	Electrophilicâ€“Nucleophilic Dualism of Nickel(II) toward Ni-â€“I Noncovalent Interactions: Semicoordination of Iodine Centers via Electron Belt and Halogen Bonding via Îƒ-Hole. <i>Inorganic Chemistry</i> , 2017, 56, 13562-13578.	1.9	84
1685	Probing the Interactions of O ₂ with Small Gold Cluster Au _n ^Q (n = 2â€“10, Q = 0, â€“1): A Neutral Chemisorbed Complex Au ₅ O ₂ Cluster Predicted. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24886-24893.	1.5	24
1686	Unifying Exchange Sensitivity in Transition-Metal Spin-State Ordering and Catalysis through Bond Valence Metrics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5443-5457.	2.3	43
1687	Enantioselective Iridium-Catalyzed Hydrogenation of Î±-Keto Amides to Î±-Hydroxy Amides. <i>Organic Letters</i> , 2017, 19, 5920-5923.	2.4	51
1688	Rotational spectroscopy of the methyl glycidateâ€“water complex: conformation and water and methyl rotor tunnelling motions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29508-29515.	1.3	17
1689	Combined TDDFT and AIM Insights into Photoinduced Excited State Intramolecular Proton Transfer (ESIPT) Mechanism in Hydroxyl- and Amino-Anthraquinone Solution. <i>Scientific Reports</i> , 2017, 7, 13766.	1.6	29
1690	Excited state dynamics for hybridized local and charge transfer state fluorescent emitters with aggregation-induced emission in the solid phase: a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29872-29879.	1.3	36
1691	Density functional theoretical studies on the ring-opening polymerization mechanism of oxetane cation series compounds. <i>RSC Advances</i> , 2017, 7, 49626-49632.	1.7	2
1692	Hierarchical Assembly and Aggregation-Induced Enhanced Emission of a Pair of Isostructural Zn ₁₄ Clusters. <i>Inorganic Chemistry</i> , 2017, 56, 14069-14076.	1.9	29
1693	Intra- and Intermolecular Charge Transfer in a Novel Dimer: Cooperatively Enhancing Second-Order Optical Nonlinearity. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25472-25478.	1.5	19
1694	Encapsulation of creatinine within aryl extended calix[4]pyrrole derivatives: Insights from theory. <i>Journal of Molecular Liquids</i> , 2017, 247, 456-466.	2.3	6
1695	Crystal structure, theoretical and experimental electronic structure and DNA/BSA protein interactions of nickel(II) N ₂ O ₂ tetradentate Schiff base complexes. <i>Polyhedron</i> , 2017, 138, 88-102.	1.0	13
1696	The DFT Calculations of Structures and EPR Parameters for the Dinuclear Paddle-Wheel Copper(II) Complex {Cu ₂ (1/4 ⁻ O ₂ CCH ₃) ₄ }(OCNH ₂ CH ₃) as Powder or Single Crystal. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2017, 72, 985-994.	0.7	8
1697	Tetrahydroisoquinolines functionalized with carbamates as selective ligands of D ₂ dopamine receptor. <i>Journal of Molecular Modeling</i> , 2017, 23, 273.	0.8	9

#	ARTICLE	IF	CITATIONS
1698	Ab initio study of cationic water cluster (H ₂ O) ₉ ⁺ via particle swarm optimization algorithm. Computational and Theoretical Chemistry, 2017, 1120, 102-111.	1.1	3
1699	Hetero Cu(III)–Pd(II) Complex of a Dibenzo[<i>g</i> , <i>p</i>]chrysene-Fused Bis-dicarbocorrole with Stable Organic Radical Character. Journal of the American Chemical Society, 2017, 139, 15232-15238.	6.6	54
1700	Introducing DDEC6 atomic population analysis: part 3. Comprehensive method to compute bond orders. RSC Advances, 2017, 7, 45552-45581.	1.7	327
1701	Two Fox-7-Like High Energy Compounds. ChemistrySelect, 2017, 2, 8738-8744.	0.7	0
1702	Catalytic reduction of NO by CO molecules over Ni-doped graphene: a DFT investigation. New Journal of Chemistry, 2017, 41, 13149-13155.	1.4	23
1703	Theoretical studies on lindqvist polyoxometalates [M ₆ O ₁₉] ⁿ⁻ (M = Mo, W, n=2; M = V, Nb, Ta, n=8) and derivatives: Electronic structures, stability and bonding. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750054.	1.8	6
1704	Way to Highly Emissive Materials: Increase of Rigidity by Introduction of a Furan Moiety in Co-Oligomers. Journal of Physical Chemistry C, 2017, 121, 23359-23369.	1.5	32
1705	Theoretical study of structure, bonding, and electronic behavior of novel sandwich complexes Os ₃ (C ₆ H ₆) _n (n = 1, 2). Russian Journal of Physical Chemistry A, 2017, 91, 2170-2175.	0.1	0
1706	Theoretical Elucidation of the Mechanism and Kinetic Experimental Phenomena on the Esterification of Î±-Tocopherol with Succinic Anhydride: Catalysis of a Histidine Derivative vs an Imidazolium-Based Ionic Liquid. Journal of Organic Chemistry, 2017, 82, 12267-12275.	1.7	9
1707	Theoretical Investigation of an Excited-State Intramolecular Proton-Transfer Mechanism for an Asymmetric Structure of 3,7-Dihydroxy-4-oxo-2-phenyl-4 <i>H</i> -chromene-8-carbaldehyde: Single or Double?. Journal of Physical Chemistry A, 2017, 121, 8807-8814.	1.1	73
1708	Experimental Charge-Density Study of the Intra- and Intermolecular Bonding in TKX-50. Journal of Physical Chemistry A, 2017, 121, 8962-8972.	1.1	16
1709	DFT Modeling of Novel Donor-Acceptor (D-A) Molecules Incorporating 3-hexylthiophene (3HT) for Bulk Heterojunction Solar Cells. ChemistrySelect, 2017, 2, 10082-10090.	0.7	15
1710	Spectroscopic and Theoretical Characterization of Through-Space Conjugation of Foldamers with a Tetraphenylethene Hinge. Chemistry - A European Journal, 2017, 23, 18041-18048.	1.7	27
1711	Insensitive ionic bio-energetic materials derived from amino acids. Scientific Reports, 2017, 7, 12744.	1.6	7
1712	Selective Dispersion of Large-Diameter Semiconducting Carbon Nanotubes by Functionalized Conjugated Dendritic Oligothiophenes for Use in Printed Thin Film Transistors. Advanced Functional Materials, 2017, 27, 1703938.	7.8	22
1713	Concerted Mechanisms of Excited-State Proton Intramolecular Transfer for Bis-2,4-(2-benzoxazolyl)-hydroquinone and Its Derivatives. Journal of Physical Chemistry A, 2017, 121, 8217-8226.	1.1	6
1714	Palladium-catalyzed denitrogenative functionalizations of benzotriazoles with alkenes and 1,3-dienes. Chemical Communications, 2017, 53, 11873-11876.	2.2	33
1715	A systematic investigation of the geometries, electronic and magnetic properties of Al _n As _q (q = 1, 0, +1; n = 1–16) clusters: a DFT calculation. Molecular Physics, 2017, 115, 3033-3043.	0.8	3

#	ARTICLE	IF	CITATIONS
1716	Mechanism and Origins of Stereoinduction in Natural Cinchona Alkaloid Catalyzed Asymmetric Electrophilic Trifluoromethylthiolation of β -Keto Esters with <i>N</i> -Trifluoromethylthiophthalimide as Electrophilic SCF ₃ Source. ACS Catalysis, 2017, 7, 7977-7986.	5.5	35
1717	DFT and AFIR Study on the Mechanism and the Origin of Enantioselectivity in Iron-Catalyzed Cross-Coupling Reactions. Journal of the American Chemical Society, 2017, 139, 16117-16125.	6.6	74
1718	Exploiting electronic strategies to stabilize a planar tetracoordinate carbon in cyclic aromatic hydrocarbons. Chemical Communications, 2017, 53, 12112-12115.	2.2	42
1719	Mechanistic investigation on N ⁺ C ⁺ O relay via non-Brook rearrangement: reaction conditions promote synthesis of furo[3,2-c]pyridinones. Organic and Biomolecular Chemistry, 2017, 15, 9127-9138.	1.5	4
1720	Quantum modeling of the reaction between ozone and hydrogen cyanide. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750063.	1.8	0
1721	Theoretical investigation on the interaction of hypergolic monomethylhydrazine with 1-chloro-1,1-dinitro-2-(N-chloroamidino)ethane using DFT methods. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	0
1722	A biphosphinic ruthenium complex with potent anti-bacterial and anti-cancer activity. New Journal of Chemistry, 2017, 41, 13085-13095.	1.4	22
1723	Activation of acetonitrile by gas-phase uranium: bond structure analysis and spin-flip reaction mechanism. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	1
1724	Local order and vibrational coupling of the C=O Stretching Mode of β -Caprolactone in liquid binary mixtures. Scientific Reports, 2017, 7, 12182.	1.6	18
1725	An Efficient Method for the Synthesis of Boratrane Complexes of Late Transition Metals. Chemistry - A European Journal, 2017, 23, 18264-18275.	1.7	11
1726	Naphthalene Diimide Based n-Type Conjugated Polymers as Efficient Cathode Interfacial Materials for Polymer and Perovskite Solar Cells. ACS Applied Materials & Interfaces, 2017, 9, 36070-36081.	4.0	39
1727	Rigid fused π -spacers in A type molecules for dye-sensitized solar cells: a computational investigation. Journal of Materials Chemistry C, 2017, 5, 11454-11465.	2.7	56
1728	Dinitromethyl-1,2,4-oxadiazole Derivatives from Controllable Cyclization Strategies. Chemistry - A European Journal, 2017, 23, 16401-16407.	1.7	22
1729	A new colorimetric and fluorescent probe with a large stokes shift for rapid and specific detection of biothiols and its application in living cells. Journal of Materials Chemistry B, 2017, 5, 8780-8785.	2.9	26
1730	A carbon-free inorganic-metal complex consisting of an all-nitrogen pentazole anion, a Zn cation and H ₂ O. Dalton Transactions, 2017, 46, 14088-14093.	1.6	76
1731	Synthesis and oxidation of phosphine cations. Dalton Transactions, 2017, 46, 14149-14157.	1.6	11
1732	Theoretical investigation on the electronic properties and UV-Vis absorption spectra of expanded porphyrin mono-Cu(II) complexes. Computational and Theoretical Chemistry, 2017, 1119, 19-25.	1.1	10
1733	Gold Doping of Double-Crown Pd Nanoclusters. Chemistry - A European Journal, 2017, 23, 18187-18192.	1.7	29

#	ARTICLE	IF	CITATIONS
1734	Experimental and Theoretical Study of the Extraction of UO ₂ ²⁺ by Malonamides in Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 12708-12716.	1.8	7
1735	Following the Molecular Mechanism of Decarbonylation of Unsaturated Cyclic Ketones Using Bonding Evolution Theory Coupled with NCI Analysis. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8504-8517.	1.1	40
1736	A novel family of homoleptic copper(I) complexes featuring disubstituted cyanamides: a combined synthetic, structural, and theoretical study. <i>New Journal of Chemistry</i> , 2017, 41, 14557-14566.	1.4	11
1737	The electron density of delocalized bonds (EDDB) applied for quantifying aromaticity. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28970-28981.	1.3	114
1738	Substituent effects on the electronic structures and nonlinear optical properties of Li-doped nano-carbon bowl. <i>Journal of Molecular Modeling</i> , 2017, 23, 316.	0.8	5
1739	Unraveling Excited-Singlet-State Aromaticity via Vibrational Analysis. <i>CheM</i> , 2017, 3, 870-880.	5.8	35
1740	Substituent Effect on Intramolecular Charge Transfer of Symmetric Methoxy-Substituted Bi-1,3,4-oxadiazole Derivatives. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8399-8407.	1.1	17
1741	CO ₂ Complexes with Five-Membered Heterocycles: Structure, Topology, and Spectroscopic Characterization. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9118-9130.	1.1	12
1742	Rotational Spectroscopy of <i>p</i> -Toluic Acid and Its 1:1 Complex with Water. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8625-8631.	1.1	12
1743	Theoretical Study on DBU-Catalyzed Insertion of Isatins into Aryl Difluoronitromethyl Ketones: A Case for Predicting Chemoselectivity Using Electrophilic Parr Function. <i>ACS Omega</i> , 2017, 2, 7029-7038.	1.6	16
1744	Synthesis, Structures, and Characterization of Dimeric Neutral Dithiolato-bridged Tungsten Complexes. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 5434-5441.	1.0	16
1745	Bonding the superalkali M ₃ O (M = Li and K): An effective strategy to improve the electronic and nonlinear optical properties of the inorganic B ₄₀ nanocage. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2017, 94, 204-210.	1.3	17
1746	Kinetics and photophysical behavior of the P,N-Re I complex [P,N-((C ₆ H ₅) ₂ (C ₅ H ₄ N)P)Re(CO) ₃ (O)Tj] ETQ ₀ 000rgB ₃ /Overlock	1.0	3
1747	Mechanism and Origin of Chemical Selectivity in Oxaziridine-Based Methionine Modification: A Computational Study. <i>Journal of Organic Chemistry</i> , 2017, 82, 9765-9772.	1.7	14
1748	Mechanism and Origins of Ligand-Controlled Stereoselectivity of Ni-Catalyzed Suzuki-Miyaura Coupling with Benzylic Esters: A Computational Study. <i>Journal of the American Chemical Society</i> , 2017, 139, 12994-13005.	6.6	99
1749	Synthetic, Structural, and Spectroscopic Characterization of a Novel Family of High-Spin Iron(II) [(¹² -Diketimate)(phosphanylphosphido)] Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 11030-11042.	1.9	14
1750	D ₂ BIA is flexible, not (explicitly) arbitrary and reference/structurally invariant a very effective and improved version of the D ₃ BIA aromaticity index. <i>Journal of Molecular Modeling</i> , 2017, 23, 253.	0.8	3
1751	Effect of functionalization of boron nitride flakes by main group metal clusters on their optoelectronic properties. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 425201.	0.7	6

#	ARTICLE	IF	CITATIONS
1752	Theoretical Insight into Sc ₂ C ₇₆ : Carbide Clusterfullerene Sc ₂ C ₂ @C ₇₄ versus Dimetallofullerene Sc ₂ @C ₇₆ . <i>Inorganic Chemistry</i> , 2017, 56, 10195-10203.	1.9	12
1753	Luminescent Three- and Four-Coordinate Dinuclear Copper(I) Complexes Triply Bridged by Bis(diphenylphosphino)methane and Functionalized 3-(2-Pyridyl)-1,2,4-triazole Ligands. <i>Inorganic Chemistry</i> , 2017, 56, 10311-10324.	1.9	36
1754	Theoretical investigation of the structural, electronic, magnetic and spectral properties of CumX _n (X = Tl, Pb, Bi, Po, At, Rn). <i>Journal of Chemical Physics</i> , 2017, 146, 184701.	1.8	6
1755	Origin of Stereoselectivity of the Photoinduced Asymmetric Phase-Transfer-Catalyzed Perfluoroalkylation of β -Ketoesters. <i>Journal of Organic Chemistry</i> , 2017, 82, 9321-9327.	1.7	36
1756	Simultaneous Occurrence of Quadruple Lewis Acid-Base Interactions between Selenium Atoms in Selenocarbonyl Dimers. <i>ChemPhysChem</i> , 2017, 18, 3498-3503.	1.0	7
1757	Theoretical Study on the Conformational Bioeffect of the Fluorination of Acetylcholine. <i>Molecular Informatics</i> , 2017, 36, 1700084.	1.4	5
1758	Synthesis, structural and spectroscopic features, and investigation of bioactive nature of a novel organic-inorganic hybrid material 1H-1,2,4-triazole-4-ium trioxonitrate. <i>Journal of Molecular Structure</i> , 2017, 1150, 242-257.	1.8	48
1759	Facile activation of alkynes with a boraguanidinato-stabilized germylene: a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2017, 46, 12339-12353.	1.6	10
1760	Calculations of total electron-impact ionization cross sections for Fluoroketone C ₅ F ₁₀ O and Fluoronitrile C ₄ F ₇ N using modified Deutsch-Mark formula. <i>Journal Physics D: Applied Physics</i> , 2017, 50, 445206.	1.3	27
1761	Contribution of Directional Dihydrogen Interactions in the Supramolecular Assembly of Single Crystals: Quantum Chemical and Structural Investigation of C ₁₇ H ₁₇ N ₃ O ₂ Azine. <i>Crystal Growth and Design</i> , 2017, 17, 5145-5153.	1.4	22
1762	Insights into the Reaction Mechanism of Criegee Intermediate CH ₂ OO with Methane and Implications for the Formation of Methanol. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7236-7245.	1.1	31
1763	First hyperpolarizabilities of Pt(4-ethynylbenzo-15-crown-5) ₂ (bpy) derivatives with the complexation of mono-cations (Li ⁺ , Na ⁺ , K ⁺) and di-cations (Mg ²⁺ , Ca ²⁺): development of a cation detector. <i>RSC Advances</i> , 2017, 7, 41830-41837.	1.7	6
1764	Square-planar aminonitronate transition metal complexes (M = CuI, NiII, PdII, and PtII). <i>Inorganica Chimica Acta</i> , 2017, 467, 372-378.	1.2	4
1765	Metal-Ligand Cooperative Reactivity in the (Pseudo)-Dearomatized PN ₂ (P) Systems: The Influence of the Zwitterionic Form in Dearomatized Pincer Complexes. <i>Journal of the American Chemical Society</i> , 2017, 139, 13442-13449.	6.6	63
1766	Phosphorus ylides as a new class of compounds in CO ₂ activation: Thermodynamic and kinetic studies. <i>Journal of CO₂ Utilization</i> , 2017, 21, 459-466.	3.3	12
1767	Theoretical studying of basic photophysical processes in a thermally activated delayed fluorescence copper(I) complex: Determination of reverse intersystem crossing and radiative rate constants. <i>Organic Electronics</i> , 2017, 51, 207-219.	1.4	15
1768	The ground and excited-state electronic structures of sandwich compounds Cp ₂ (ME) ₂ contain an (ME) ₂ four-membered ring (Cp = C ₅ H ₅ ; M = Ni, Pd, Pt; E = O, S, Se, Te). <i>New Journal of Chemistry</i> , 2017, 41, 12028-12034.	1.4	3
1769	Theoretical perspective of the excited state intramolecular proton transfer for a compound with aggregation induced emission in the solid phase. <i>RSC Advances</i> , 2017, 7, 44089-44096.	1.7	18

#	ARTICLE	IF	CITATIONS
1770	Nb ₂ @Au ₆ : a molecular wheel with a short Nb–Nb triple bond coordinated by an Au ₆ ring and reinforced by <i>f</i> aromaticity. <i>Chemical Science</i> , 2017, 8, 7528-7536.	3.7	16
1771	ICT–Isomerization-Induced Turn-On Fluorescence Probe with a Large Emission Shift for Mercury Ion: Application in Combinational Molecular Logic. <i>Inorganic Chemistry</i> , 2017, 56, 11577-11590.	1.9	54
1772	Photoinduced Bimolecular Electron Transfer in Ionic Liquids. <i>Journal of the American Chemical Society</i> , 2017, 139, 14568-14585.	6.6	30
1773	Theoretical investigation on second-order nonlinear optical properties of ruthenium alkynyl–dihydroazulene/vinylheptafulvene complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 77, 363-371.	1.3	3
1774	Synthesis, structural characterization, thermal stability, vibrational spectra and density functional theoretical studies of 1,3-bis(carboxymethyl)imidazolium nitrate ionic liquid. <i>Journal of Molecular Liquids</i> , 2017, 246, 173-177.	2.3	2
1775	Vibrational Characterization of Two-Dimensional Graphdiyne Sheets. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21430-21438.	1.5	16
1776	Atomistic Origins of High Capacity and High Structural Stability of Polymer-Derived SiOC Anode Materials. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 35001-35009.	4.0	34
1777	Theoretical investigation on the mechanism of the OH-initiated degradation process of reactive red 2 azo dye. <i>RSC Advances</i> , 2017, 7, 41799-41811.	1.7	14
1778	Mechanistic Investigation of the Carbon–Iodine Bond Activation on the Niobium–Carbon Cluster. <i>ACS Omega</i> , 2017, 2, 5335-5347.	1.6	2
1779	An assessment of the random-phase approximation functional and characteristics analysis for noncovalent cation– π interactions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26014-26021.	1.3	12
1780	Is there a generalized anomeric effect? Analyses from energy components and information-theoretic quantities from density functional reactivity theory. <i>Chemical Physics Letters</i> , 2017, 687, 131-137.	1.2	27
1781	The role of non-covalent interaction for the adsorption of CO ₂ and hydrocarbons with per-hydroxylated pillar[6]arene: a computational study. <i>New Journal of Chemistry</i> , 2017, 41, 12044-12051.	1.4	32
1782	Theoretically unraveling the separation of Am(<i>iii</i>)/Eu(<i>iii</i>): insights from mixed N,O-donor ligands with variations of central heterocyclic moieties. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26969-26979.	1.3	69
1783	The extent of charge transfer: A qualitative computational study on electronic transitions of unsymmetrical squarylium dyes. <i>Computational and Theoretical Chemistry</i> , 2017, 1118, 123-132.	1.1	1
1784	Formation and Structure of Inhibitive Molecular Film of Oxadiazole on Iron Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21420-21429.	1.5	5
1785	Reactivity of 12-tungstophosphoric acid and its inhibitor potency toward Na ⁺ /K ⁺ -ATPase: A combined 31P NMR study, ab initio calculations and crystallographic analysis. <i>Journal of Inorganic Biochemistry</i> , 2017, 176, 90-99.	1.5	10
1786	Weak hydrogen bond topology in 1,1-difluoroethane dimer: A rotational study. <i>Journal of Chemical Physics</i> , 2017, 147, 094301.	1.2	27
1787	Supramolecular Reversible On–Off Switch for Singlet Oxygen Using Cucurbit[<i>n</i>]uril Inclusion Complexes. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21782-21789.	1.5	29

#	ARTICLE	IF	CITATIONS
1788	An ab initio study on noble gas inserted halogenated acetylene: HNgCCX (Ng = Kr and Xe; X = halogen). Scientific Reports, 2017, 7, 10278.	1.6	2
1789	Cyanosilylation of Aldehydes Catalyzed by MIL-101(Cr): A Theoretical Investigation. ChemistrySelect, 2017, 2, 7813-7820.	0.7	12
1790	Ab initio investigation of structure, spectrum, aromaticity and electronic properties of C ₁₀ carbon cluster. Computational and Theoretical Chemistry, 2017, 1118, 94-106.	1.1	8
1791	Metrics for Molecular Electronic Excitations: A Comparison between Orbital- and Density-Based Descriptors. Journal of Physical Chemistry A, 2017, 121, 7543-7549.	1.1	32
1792	The nature of the Au-N bond in gold complexes with aromatic nitrogen-containing heterocycles: the influence of Au ions on the ligand aromaticity. New Journal of Chemistry, 2017, 41, 12407-12415.	1.4	17
1793	Infrared spectroscopic and theoretical study of the HC _{2n+1} O ⁺ (n = 2-5) cations. Journal of Chemical Physics, 2017, 146, 214301.	1.2	5
1794	Quantum Chemical Insight into La ₂ C ₉₆ : Metal Carbide Fullerene La ₂ C ₂ @C ₉₄ versus Dimetallofullerene La ₂ C ₂ @C ₉₆ . Inorganic Chemistry, 2017, 56, 11883-11890.	1.9	9
1795	A Twisted Bay-Substituted Quaterylene Phosphorescing in the NIR Spectral Region. Helvetica Chimica Acta, 2017, 100, e1700192.	1.0	7
1796	Preparation of Bis(1/4 ₃ -silylyne) Complexes via Consecutive Si-H Bond Cleavage at a Triruthenium Site. Organometallics, 2017, 36, 3774-3783.	1.1	2
1797	Construction of a 9,9-bifluorenylidene-based small molecule acceptor materials by screening conformation, steric configuration and repeating unit number: a theoretical design and characterization. Journal of Materials Chemistry C, 2017, 5, 10343-10352.	2.7	19
1798	DFT study of benzyl alcohol/TiO ₂ interfacial surface complex: reaction pathway and mechanism of visible light absorption. Journal of Molecular Modeling, 2017, 23, 285.	0.8	3
1799	Self-Assembled Donor-Acceptor Chromophores: Evident Layer Effect on the First Hyperpolarizability and Two-Dimensional Charge Transfer Character. Journal of Physical Chemistry C, 2017, 121, 21616-21626.	1.5	17
1800	A comparative theoretical study on the electrical and nonlinear optical properties of Li atom adsorbed on AlN and BN single-walled nanotubes. Journal of Molecular Modeling, 2017, 23, 286.	0.8	9
1801	A theoretical study of the structural and electronic properties of trans and cis structures of chlorprothixene as a nano-drug. Current Applied Physics, 2017, 17, 1754-1764.	1.1	4
1802	Palladium acetate supported on amidoxime-functionalized magnetic cellulose: Synthesis, DFT study and application in Suzuki reaction. Carbohydrate Polymers, 2017, 177, 165-177.	5.1	54
1803	Design of a sub phthalocyanine-based hybrid donor of photovoltaic materials and its theoretical investigation. AIP Conference Proceedings, 2017, , .	0.3	1
1804	A DFT study on the structure and property of novel nitroimidazole derivatives as high energy density materials. Computational and Theoretical Chemistry, 2017, 1118, 39-44.	1.1	4
1805	Structural and Chemical Effects of the P ⁱ Bu ₂ Bridge at Unsaturated Dimolybdenum Complexes Having Hydride and Hydrocarbyl Ligands. Inorganic Chemistry, 2017, 56, 11336-11351.	1.9	13

#	ARTICLE	IF	CITATIONS
1806	Rotational Spectroscopy Probes Water Flipping by Full Fluorination of Benzene. <i>Angewandte Chemie</i> , 2017, 129, 13887-13891.	1.6	13
1807	Ph(R)IF ₆ ⁻ ·HF (R = Me, Et, i Pr, t Bu) interaction: A strong hydrogen bond between hypervalent iodine compounds and HF. <i>Computational and Theoretical Chemistry</i> , 2017, 1118, 45-52.	1.1	2
1808	The effects of structural properties on the methylglyoxal scavenging mechanism of flavonoid aglycones: A quantum mechanical study. <i>Computational and Theoretical Chemistry</i> , 2017, 1118, 26-38.	1.1	9
1809	Rotational Spectroscopy Probes Water Flipping by Full Fluorination of Benzene. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 13699-13703.	7.2	27
1810	Theoretical investigation of the π + π + stacking interactions in substituted pyridinium ion. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 77, 225-231.	1.3	7
1811	The influence of hydrogen bonds on NIAD-4 for use in the optical imaging of amyloid fibrils. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15849-15855.	1.3	5
1812	A molecular electron density theory study of [3+2] cycloaddition reactions of chiral azomethine ylides with 1 ² -nitrostyrene. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	21
1813	Theoretical and experimental approach on the molecular interactions of the DL-Alanine with an electrolytic environment. <i>Chemical Physics Letters</i> , 2017, 687, 73-84.	1.2	5
1814	Molecular engineering of bithiazole-based organic dyes with different electron-rich linkers toward highly efficient dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 349, 171-182.	2.0	3
1815	Synthesis, structure, and photophysics of copper(II) triphenylphosphine complexes with functionalized 3-(2-pyrimidinyl)-1,2,4-triazole ligands. <i>Dalton Transactions</i> , 2017, 46, 13077-13087.	1.6	30
1816	Polyacrylamide-Phytic Acid-Polydopamine Conducting Porous Hydrogel for Efficient Removal of Water-Soluble Dyes. <i>Scientific Reports</i> , 2017, 7, 7878.	1.6	25
1817	The novel link between planar macrocyclic aromatic and third order nonlinear optical properties of metal-bridged polycyclic complexes. <i>Scientific Reports</i> , 2017, 7, 10182.	1.6	19
1818	Theoretical investigation on proton transfer mechanism of extradiol dioxygenase. <i>RSC Advances</i> , 2017, 7, 43197-43205.	1.7	2
1819	Fused 1,2,3-thiaselenazoles Synthesized from 1,2,3-dithiazoles through Selective Chalcogen Exchange. <i>Chemistry - A European Journal</i> , 2017, 23, 17037-17047.	1.7	20
1820	Synthesis of 1,2,3,4-tetrazine 1,3-dioxides Annulated with 1(2)-Aryl-1,2,3-triazoles. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 4963-4971.	1.2	15
1821	Stepwise deprotonation of sumanene: electronic structures, energetics and aromaticity alterations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21575-21583.	1.3	7
1822	Synthesis, Structure, and Properties of Near-Infrared [10]Phenanthrene-Fused BF ₂ Azadipyrromethenes. <i>Chemistry - an Asian Journal</i> , 2017, 12, 2486-2493.	1.7	27
1823	Aryl-Substituted Ruthenium(II) Complexes: A Strategy for Enhanced Photocleavage and Efficient DNA Binding. <i>Inorganic Chemistry</i> , 2017, 56, 9084-9096.	1.9	39

#	ARTICLE	IF	CITATIONS
1824	Transfer Hydrocyanation by Nickel(0)/Lewis Acid Cooperative Catalysis, Mechanism Investigation, and Computational Prediction of Shuttle Catalysts. <i>Organometallics</i> , 2017, 36, 2746-2754.	1.1	29
1825	Catalytic and Enantioselective Diels-Alder Reactions of (<i>E</i>)-4-Oxopent-2-enoates. <i>Organic Letters</i> , 2017, 19, 3986-3989.	2.4	17
1826	Theoretical tuning of the singlet-triplet energy gap to achieve efficient long-wavelength thermally activated delayed fluorescence emitters: the impact of substituents. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21639-21647.	1.3	14
1827	Excited state properties of non-doped thermally activated delayed fluorescence emitters with aggregation-induced emission: a QM/MM study. <i>Journal of Materials Chemistry C</i> , 2017, 5, 8390-8399.	2.7	91
1828	Design of Hexabenzocoronene Derivatives as Non-Fullerene Acceptors in Organic Photovoltaics by Bridging Dimers and Modulating Structural Twists. <i>Solar Rrl</i> , 2017, 1, 1700060.	3.1	22
1829	Weak bonds between molecular tweezers and their guests. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 335-343.	1.1	4
1830	Four-coordinated copper(I) complexes containing variably substituted N-heterocyclic carbenes (NHCs): Synthesis, photophysical properties and theoretical investigation. <i>Journal of Organometallic Chemistry</i> , 2017, 846, 351-359.	0.8	21
1831	Regiocontrolled Electrosynthesis of [60]Fullerene Bisadducts: Photovoltaic Performance and Crystal Structures of C ₆₀ -Quinodimethane Bisadducts. <i>Journal of Organic Chemistry</i> , 2017, 82, 8676-8685.	1.7	15
1832	Theoretical Study of the Ring-Opening of Epoxides Catalyzed by Boronic Acids and Pyridinic Bases. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16300-16307.	1.5	20
1833	Monocyclic aromatic compounds B _n Rg _n ⁽ⁿ⁺²⁾⁺ of boron and rare gases. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19109-19119.	1.3	17
1834	Theoretical study on the cage-like nanostructures formed by amino acids and their potential applications as drug carriers. <i>Molecular Physics</i> , 2017, 115, 3051-3066.	0.8	0
1835	Coaxial Triple-layered versus Helical Be ₆ B ₁₁ ⁺ Clusters: Dual Structural Fluxionality and Multifold Aromaticity. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 10174-10177.	7.2	83
1836	Extraction of U(VI) by the ionic liquid hexyltributylphosphonium bis(trifluoromethylsulfonyl)imides: An experimental and theoretical study. <i>Separation and Purification Technology</i> , 2017, 188, 386-393.	3.9	13
1837	Insight into π -hole interactions containing the inorganic heterocyclic compounds S ₂ N ₂ /SN ₂ P ₂ . <i>Journal of Molecular Modeling</i> , 2017, 23, 233.	0.8	2
1838	Twisted Diarylnitroxides: An Efficient Route for Radical Stabilization. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 4726-4735.	1.2	15
1839	Experimental and theoretical studies on photoluminescent Zn(II) host complex with an open book structure: Implication on potential bioactivity and comparison with its ligand and Zn(II), Pd(II) siblings. <i>Polyhedron</i> , 2017, 135, 278-295.	1.0	19
1840	Synthesis, structural analyses and antimicrobial activity of the water soluble 1D coordination polymer [Ag(3-aminopyridine)]ClO ₄ . <i>Journal of Molecular Structure</i> , 2017, 1149, 58-68.	1.8	15
1841	Solvent Effect Inside the Nanocage of Zeolite Catalysts: A Combined Solid-State NMR Approach and Multiscale Simulation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16921-16931.	1.5	8

#	ARTICLE	IF	CITATIONS
1842	How active sites facilitate charge-transfer interactions of silver and gold clusters with TCNQ?. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21777-21782.	1.3	10
1843	Molecular Dynamics Simulation and Density Functional Theory Study of Chemisorption of Propranolol Optical Isomers on a Uracil-Modified Carbon Paste Electrode. <i>Journal of the Chinese Chemical Society</i> , 2017, 64, 1058-1064.	0.8	3
1844	Strengthening of hydrogen bonding with the push-pull effect. <i>Chemical Physics Letters</i> , 2017, 685, 251-258.	1.2	58
1845	New Theoretical Insights into the Contributions of Poly(methylbenzene) and Alkene Cycles to the Methanol to Propene Process in H-FAU Zeolite. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16216-16237.	1.5	10
1846	Computational studies on the Rh-catalyzed carboxylation of a C(sp ²)-H bond using CO ₂ . <i>Catalysis Science and Technology</i> , 2017, 7, 3539-3545.	2.1	16
1847	The geometric and electronic structures of Al _n Na _m (n = 5, 6; n + m ≤ 10) clusters. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 1-11.	1.1	3
1848	Theoretical investigation of the conformational space of baicalin. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 76, 181-191.	1.3	4
1849	Density Functional Theory Calculation of the Absorption Properties of Brown Carbon Chromophores Generated by Catechol Heterogeneous Ozonolysis. <i>ACS Earth and Space Chemistry</i> , 2017, 1, 353-360.	1.2	25
1850	Preparation and characterization of chemically bonded argon-boroxol ring cation complexes. <i>Chemical Science</i> , 2017, 8, 6594-6600.	3.7	13
1851	A new nonempirical tuning scheme with single self-consistent field calculation: Comparison with global and IP-tuned range-separated functional. <i>Journal of Computational Chemistry</i> , 2017, 38, 2258-2267.	1.5	18
1852	DFT studies on the mechanism of Ag ₂ CO ₃ -catalyzed hydroazidation of unactivated terminal alkynes with TMS ₃ N ₃ : An insight into the silver(I) activation mode. <i>Journal of Computational Chemistry</i> , 2017, 38, 2289-2297.	1.5	8
1853	Exploiting CF Bond of Hexafluorocyclohexane and Decafluoroadamantane Systems to Capture Flue Gases: A Computational Study. <i>ChemistrySelect</i> , 2017, 2, 5775-5782.	0.7	2
1854	Rotational spectroscopic and theoretical study of the perfluorobutyric acid-formic acid complex. <i>Journal of Molecular Spectroscopy</i> , 2017, 335, 88-92.	0.4	8
1855	A zwitterionic pH responsive ES IPT-Based fluorescence Turn-On-Al ³⁺ ion sensing probe and its bioimaging applications. <i>Sensors and Actuators B: Chemical</i> , 2017, 253, 1012-1025.	4.0	22
1856	1,4-Azaborine as a controller of triplet energy, exciton distribution, and aromaticity in [6]cycloparaphenylenes. <i>Journal of Materials Chemistry C</i> , 2017, 5, 9088-9097.	2.7	8
1857	A density functional theory study on the hydrogen bonding interactions between luteolin and ethanol. <i>Journal of Molecular Modeling</i> , 2017, 23, 245.	0.8	7
1858	Structure, electronic properties and electronic excitation analyses of Si ₆₀ Si ₆₀ dimer and Si ₅₉ AlSi ₅₉ P complex. <i>Current Applied Physics</i> , 2017, 17, 1376-1381.	1.1	4
1859	Theoretical prediction of noble gas inserted halocarbenes: FN _g CX (N _g = Kr, and Xe; X = F, Cl, Br, and I). <i>Chemical Physics</i> , 2017, 494, 20-30.	0.9	13

#	ARTICLE	IF	CITATIONS
1860	Ruthenium(II) pentamethylcyclopentadienyl half-sandwich carbene complexes with polypyridyl ligands. <i>Journal of Organometallic Chemistry</i> , 2017, 848, 1-9.	0.8	5
1861	Absorption Spectra for Disordered Aggregates of Chromophores Using the Exciton Model. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3787-3801.	2.3	21
1862	Reductive Activation of C ₇₀ Equatorial Carbons and Structurally Characterized C ₇₀ I ⁻ Adduct with Closed [5,6]-Ring Fusion. <i>Journal of Organic Chemistry</i> , 2017, 82, 9253-9257.	1.7	12
1863	Biopolymer from Tragacanth Gum as a Green Corrosion Inhibitor for Carbon Steel in 1 M HCl Solution. <i>ACS Omega</i> , 2017, 2, 3997-4008.	1.6	77
1864	Derivatization of Phosphine Ligands with Bulky Deltahedral <i>Zintl</i> Clusters—Synthesis of Charge Neutral Zwitterionic Tetrel Cluster Compounds [(Ge ₉ {Si(TMS) ₃ } ₂) ^{+t} Bu ₂ PM(NHC ^{6,6} Dipp) ⁴⁸⁻ (M: Cu, Ag, Au). <i>Journal of the American Chemical Society</i> , 2017, 139, 11933-11940.	6.6	48
1865	The phosphorescence properties of a series of diarylethene-containing platinum complexes: the effect of ligand photoisomerization. <i>Organic Chemistry Frontiers</i> , 2017, 4, 2191-2201.	2.3	11
1866	Ab initio molecular dynamics study of the interaction of plutonium with oxygen in the gas phase. <i>RSC Advances</i> , 2017, 7, 36038-36047.	1.7	2
1867	Deciphering chemical bonding in B _n H _n ²⁺ (n = 2–17): flexible multicenter bonding. <i>RSC Advances</i> , 2017, 7, 36755-36764.	1.7	14
1868	Efficient Near-Infrared (NIR) Organic Light-Emitting Diodes Based on Donor-Acceptor Architecture: An Improved Emissive State from Mixing to Hybridization. <i>Advanced Optical Materials</i> , 2017, 5, 1700441.	3.6	71
1869	Interaction between anti-cancer drug hydroxycarbamide and boron nitride nanotube: A long-range corrected DFT study. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 61-80.	1.1	19
1870	Microscopic Characterization of CO ₂ and H ₂ S Removal by Sulfolane. <i>Energy & Fuels</i> , 2017, 31, 9800-9813.	2.5	8
1871	<i>N</i> - <i>tert</i> -Butyl Sulfinyl Squaramide Receptors for Anion Recognition through Assisted <i>tert</i> -Butyl C–H Hydrogen Bonding. <i>Journal of Organic Chemistry</i> , 2017, 82, 8662-8667.	1.7	26
1872	Promoting Singlet/triplet Exciton Transformation in Organic Optoelectronic Molecules: Role of Excited State Transition Configuration. <i>Scientific Reports</i> , 2017, 7, 6225.	1.6	92
1873	A Direct Link from the Gas to the Condensed Phase: A Rotational Spectroscopic Study of 2,2,2-Trifluoroethanol Trimers. <i>Angewandte Chemie</i> , 2017, 129, 6386-6390.	1.6	31
1874	MNgCCH (M = Cu, Ag, Au; Ng = Xe, Rn): The First Set of Compounds with M–Ng–C Bonding Motif. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6491-6499.	1.1	27
1875	Effect of Ligand Attachment on the C–I Bond Dissociation Process on Aluminum Nanoclusters: A DFT Investigation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17354-17364.	1.5	4
1876	Evaluation of SF ₆ -alternative gas C5-PFK based on arc extinguishing performance and electric strength. <i>Journal Physics D: Applied Physics</i> , 2017, 50, 385202.	1.3	54
1877	Bandgap Engineering in OH-Functionalized Silicon Nanocrystals: Interplay between Surface Functionalization and Quantum Confinement. <i>Advanced Functional Materials</i> , 2017, 27, 1701898.	7.8	15

#	ARTICLE	IF	CITATIONS
1878	A molecular-scale study on the role of lactic acid in new particle formation: Influence of relative humidity and temperature. <i>Atmospheric Environment</i> , 2017, 166, 479-487.	1.9	42
1879	Linear π -hole π -hole intermolecular interactions between carbon monoxide and dihalogen molecules XY (X, Y = Cl, Br). <i>Journal of Molecular Graphics and Modelling</i> , 2017, 76, 419-428.	1.3	6
1880	Analysis and design of resonance Raman reporter molecules by density functional theory. <i>Journal of Raman Spectroscopy</i> , 2017, 48, 1196-1200.	1.2	15
1881	Polynitro-Functionalized Dipyrazolo[1,3,5]triazinanes: Energetic Polycyclization toward High Density and Excellent Molecular Stability. <i>Angewandte Chemie</i> , 2017, 129, 8960-8964.	1.6	22
1882	Cyclopropyl Group: An Excited-State Aromaticity Indicator?. <i>Chemistry - A European Journal</i> , 2017, 23, 13684-13695.	1.7	10
1883	Insights into chemoselective fluorination reaction of alkynals via N-heterocyclic carbene and Brønsted base cooperative catalysis. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	11
1884	Assessment of various DFT, DFT-D, and MP2 methods for studying FOX-7 detonation properties. <i>Journal of Molecular Modeling</i> , 2017, 23, 250.	0.8	19
1885	Gas-phase hydration of glyoxylic acid: Kinetics and atmospheric implications. <i>Chemosphere</i> , 2017, 186, 430-437.	4.2	31
1886	Probing Interligand Electron Transfer in the 1MLCT Excited State of $trans$ - $Mo_2L_2L^2_2$ Compounds: A Comparative Study of Auxiliary Ligands and Solvents. <i>Inorganic Chemistry</i> , 2017, 56, 9660-9668.	1.9	3
1887	"Push-Pull" π - π Systems in Catalysis. <i>ACS Catalysis</i> , 2017, 7, 6430-6439.	5.5	24
1888	An Insoluble Benzoquinone-Based Organic Cathode for Use in Rechargeable Lithium-Ion Batteries. <i>Angewandte Chemie</i> , 2017, 129, 12735-12739.	1.6	36
1889	Reactions of a Ga-Based Frustrated Lewis Pair with $H-X$ ($X = F, I$), Heterocumulenes NCY ($Y = O, S$) and Chalcogens: Adduct Formation and Surprising Stability towards Protolysis. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2017, 643, 1016-1029.	0.6	16
1890	Homolytic Cleavage Reactions of a Neutral Doubly Base Stabilized Diborane(4). <i>Organometallics</i> , 2017, 36, 3163-3170.	1.1	29
1891	Change in optoelectronic properties of $ExBox^{+4}$ on functionalization and guest encapsulation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23373-23385.	1.3	10
1892	Unravelling hydrogen bonding interactions of tryptamine-water dimer from neutral to cation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25260-25269.	1.3	6
1893	Remarkable nonlinear optical response of excess electron compounds: theoretically designed alkali-doped aziridine C_2NH_5 . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23951-23959.	1.3	25
1894	An integrative study to identify novel scaffolds for sphingosine kinase 1 inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2017, 139, 461-481.	2.6	33
1895	Adsorption of 5f-electron atoms (Th-Cm) on graphene surface: An all-electron ZORA-DFT study. <i>Journal of Colloid and Interface Science</i> , 2017, 508, 159-166.	5.0	10

#	ARTICLE	IF	CITATIONS
1896	Theoretical insights into the effect of a conjugated core on the hole transport properties of hole-transporting materials for perovskite solar cells. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24574-24582.	1.3	29
1897	Molecular interactions between 1-butyl-3-methylimidazolium tetrafluoroborate and model naphthenic acids: A DFT study. <i>Journal of Molecular Liquids</i> , 2017, 243, 462-471.	2.3	26
1898	Capturing the Unconventional Metallofullerene $M@C_{66}$ by Trifluoromethylation: A Theoretical Study. <i>ChemPhysChem</i> , 2017, 18, 3007-3011.	1.0	4
1899	Two kinds of $X-H\cdots C(sp^3)$ hydrogen bond formed by the methide anion: Syn- and anti-orientation of monomers. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 141-149.	1.1	7
1900	Electronic Structure and Properties of Berkelium Iodates. <i>Journal of the American Chemical Society</i> , 2017, 139, 13361-13375.	6.6	25
1901	Key role of higher order symmetry and electrostatic ligand field design in the magnetic relaxation of low-coordinate $Er(\text{scp})_3$ complexes. <i>Dalton Transactions</i> , 2017, 46, 11913-11924.	1.6	23
1902	Nucleophilicity and electrophilicity of the $C(sp^3)\cdots H$ bond: methane and ethane binary complexes with iodine. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24555-24565.	1.3	3
1903	Insights into the Adsorption of Resveratrol on Graphene Oxide: A First-Principles Study. <i>ChemistrySelect</i> , 2017, 2, 6895-6900.	0.7	5
1904	Intramolecular hydrogen bonding in conformationally semi-rigid β -acylmethane derivatives: a theoretical NMR study. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 7572-7579.	1.5	2
1905	Testing the ability of rhodanine and 2, 4-thiazolidinedione to interact with the human pancreatic alpha-amylase: electron-density descriptors complement molecular docking, QM, and QM/MM dynamics calculations. <i>Journal of Molecular Modeling</i> , 2017, 23, 252.	0.8	7
1906	Phosphorescent mechanochromism through the contraction of $Ag_{12}Cu_2$ clusters in tetradecanuclear copper-silver acetylide complexes. <i>Journal of Materials Chemistry C</i> , 2017, 5, 8782-8787.	2.7	34
1907	Theoretical study of the stability and properties of magic numbers ($m=5$, $n=2$) and ($m=6$, $n=3$) of bimetallic bismuth-copper nanoclusters; Bi_mCu_n . <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25449.		5
1908	The adsorption of NO, NH ₃ , N ₂ on carbon surface: a density functional theory study. <i>Journal of Molecular Modeling</i> , 2017, 23, 262.	0.8	18
1909	Supramolecular architecture of 5-bromo-7-methoxy-1-methyl-1H-benzimidazole.3H ₂ O: Synthesis, spectroscopic investigations, DFT computation, MD simulations and docking studies. <i>Journal of Molecular Structure</i> , 2017, 1149, 602-612.	1.8	10
1910	DFT study of the interactions between thiophene-based corrosion inhibitors and an Fe ₄ cluster. <i>Journal of Molecular Modeling</i> , 2017, 23, 260.	0.8	8
1911	A theoretical survey of substituent effects on the properties of pnictogen and hydrogen bonds in cationic complexes of PH ₄ ⁺ with substituted benzonitrile. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 77, 64-71.	1.3	1
1912	On the structure of transition metals complexes with the new tridentate dye of thiazole series: Theoretical and experimental studies. <i>Journal of Molecular Structure</i> , 2017, 1149, 669-682.	1.8	33
1913	The Many Facets of Chalcogen Bonding: Described by Vibrational Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6845-6862.	1.1	95

#	ARTICLE	IF	CITATIONS
1914	Influence of axial tensile strain on the electronic and structural properties as well as NO gas sensitivity and reactivity of C-doped SW-BNNTs. <i>Surface Science</i> , 2017, 665, 62-82.	0.8	2
1915	The important role of superalkalis on the static first hyperpolarizabilities of new electrides: Theoretical investigation on superalkali-doped hexamethylenetetramine (HMT). <i>Synthetic Metals</i> , 2017, 232, 39-45.	2.1	25
1916	From blue to full color – theoretical design and characterization of a series of Ir(III) complexes containing azoline ligand with potential application in OLEDs. <i>Dalton Transactions</i> , 2017, 46, 11491-11502.	1.6	13
1917	Microhydration of oxalic acid leading to dissociation. <i>Molecular Physics</i> , 2017, 115, 3224-3233.	0.8	3
1918	An Insoluble Benzoquinone-Based Organic Cathode for Use in Rechargeable Lithium-Ion Batteries. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 12561-12565.	7.2	177
1919	A theoretical exploration of the effect of fluorine and cyano substitutions in diketopyrrolopyrrole-based polymer donor for organic solar cells. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 77, 9-16.	1.3	12
1920	Non-covalent green functionalization of boron nitride nanotubes with tunable aryl alkyl ionic liquids: A quantum chemical approach. <i>Journal of Molecular Liquids</i> , 2017, 243, 22-40.	2.3	13
1921	How do ligands influence the quantum yields of cyclometalated platinum(II) complexes, a theoretical research study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23454-23460.	1.3	5
1922	Microhydration of a benzoic acid molecule and its dissociation. <i>New Journal of Chemistry</i> , 2017, 41, 7195-7202.	1.4	10
1923	A Novel Supported Liquid Membrane Based on Binary Metal Chloride Deep Eutectic Solvents for Ethylene/Ethane Separation. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 15153-15162.	1.8	32
1924	Trends in Metallophilic Bonding in Pd-Zn and Pd-Cu Complexes. <i>Organometallics</i> , 2017, 36, 4854-4863.	1.1	26
1925	First-principle study of structural, electronic and magnetic properties of (FeC) _n (n=8) and (FeC) ₈ TM _{1.6} (TM=V, Cr, Mn and Co) clusters. <i>Scientific Reports</i> , 2017, 7, 17516.	1.6	8
1926	Planar Octagonal Tetranuclear Cobaltacarborane Macrocycle [(I ⁵⁺ -C ₅ Me ₅)Co(2,3-Et ₂ C ₂ B ₄ H ₃ -5-C ₇) ₄] ⁺ for 2D Nonlinear Optics: Ultra-High-Response and Multistate Controlled Cubic NLO Switch. <i>Journal of Physical Chemistry C</i> , 2017, 121, 28462-28474.	1.5	19
1927	Synergistic Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Cyanoesterification: Effect of Lewis Acid. <i>Organometallics</i> , 2017, 36, 4713-4720.	1.1	11
1928	Systematic Coupled Cluster Study of Noncovalent Interactions Involving Halogens, Chalcogens, and Pnicogens. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9544-9556.	1.1	72
1929	The π-π stacking of tanshinone I and isotanshinone I with phenylalanine: The effects of isomerization, complexation and environment. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750067.	1.8	1
1930	Theoretical investigation of the effects of the molar ratio and solvent on the formation of the pyrazole-nitroamine cocrystal explosive 3,4-dinitropyrazole (DNP)/2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (CL-20). <i>Journal of Molecular Modeling</i> , 2017, 23, 353.	0.8	13
1931	Growth morphology of CL-20/HMX cocrystal explosive: insights from solvent behavior under different temperatures. <i>Journal of Molecular Modeling</i> , 2017, 23, 360.	0.8	25

#	ARTICLE	IF	CITATIONS
1932	Chiral intertwined spirals and magnetic transition dipole moments dictated by cylinder helicity. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13097-13101.	3.3	210
1933	NMR Chemical Shift of a Helium Atom as a Probe for Electronic Structure of FH, F ⁺ , (FHF) ⁻ , and FH ₂ ⁺ . Journal of Physical Chemistry A, 2017, 121, 9654-9662.	1.1	6
1934	Exploring what prompts ITIC to become a superior acceptor in organic solar cell by combining molecular dynamics simulation with quantum chemistry calculation. Physical Chemistry Chemical Physics, 2017, 19, 31227-31235.	1.3	39
1935	Absorption and Mid-IR SHG in Two-Dimensional Halogen and Hydrogen Saturated Silicene Series. Journal of Physical Chemistry C, 2017, 121, 27139-27146.	1.5	10
1936	Functionalized deltahedral Zintl complexes Ge ₉ R ₃ (R = CF ₃ , CN). Journal of Physical Chemistry C, 2017, 121, 27147-27154.	2.2	26
1937	Theoretical investigation on the covalence in AgRnX and XAgRn (X = F, I). Journal of Molecular Modeling, 2017, 23, 350.	0.8	2
1938	Synthesis meets theory: Past, present and future of rational chemistry. Physical Sciences Reviews, 2017, 2, .	0.8	3
1939	Toward a quantitative evaluation of the strength of Cp ₂ M ⁺ -borate interactions. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	1
1940	Circular cationic compounds B ₃ R _n ⁺ of triangular ion B ₃ ⁺ trapping rare gases. Chemical Research in Chinese Universities, 2017, 33, 958-964.	1.3	1
1941	Experimental and Computational Thermochemical Study of Maleic Anhydride and Vinylene Carbonate. Journal of Physical Chemistry A, 2017, 121, 9474-9484.	1.1	5
1942	Unveiling Mechanism of a Quinine-Squaramide Catalyzed Enantioselective Aza-Friedel-Crafts Reaction between Cyclic Trifluoromethyl Ketimine and Naphthol: A DFT Study. Journal of Organic Chemistry, 2017, 82, 13109-13114.	1.7	10
1943	Impact of substitution and self-aggregation on photoelectric and charge transfer characteristics in JD21 analogues. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	1
1944	Influence of Relativistic Effects on Bonding Modes in M(II) Dinuclear Complexes (M = Au, Ag, and Cu). Inorganic Chemistry, 2017, 56, 14624-14631.	1.9	21
1945	Exploring Quantum Chemical Descriptors and Molecular Docking Approach for Designing Antagonist Search Model for the Glycine/NMDA Receptor Site. ChemistrySelect, 2017, 2, 10476-10483.	0.7	1
1946	Electrochemical and theoretical studies of the interactions of a pyridyl-based corrosion inhibitor with iron clusters (Fe ₁₅ , Fe ₃₀ , Fe ₄₅ , and Fe ₆₀). Journal of Molecular Modeling, 2017, 23, 342.	0.8	16
1947	Inorganic benzenes as the noncovalent interaction donor: a study of the π-hole interactions. Journal of Molecular Modeling, 2017, 23, 335.	0.8	2
1948	A Systematic Theoretical Study of UC ₆ : Structure, Bonding Nature, and Spectroscopy. Inorganic Chemistry, 2017, 56, 13794-13800.	1.9	14
1949	Computational Study on ¹³ C-H Functionalization of ^{1,2} -Unsaturated Ester Catalyzed by N-Heterocyclic Carbene: Mechanisms, Origin of Stereoselectivity, and Role of Catalyst. Journal of Organic Chemistry, 2017, 82, 13043-13050.	1.7	55

#	ARTICLE	IF	CITATIONS
1950	Infrared Spectroscopic and Electronic Structure Investigations of Beryllium Halide Molecules, Cations, and Anions in Noble Gas Matrices. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8843-8855.	1.1	8
1951	The Polarization of Polycyclic Aromatic Hydrocarbons Curved by Pentagon Incorporation: The Role of the Flexoelectric Dipole. <i>Journal of Physical Chemistry C</i> , 2017, 121, 27154-27163.	1.5	48
1952	Theoretical aspects of the enhancement of metal binding affinity by intramolecular hydrogen bonding and modulating pK_a values. <i>New Journal of Chemistry</i> , 2017, 41, 15110-15119.	1.4	8
1953	Nonconventional Hydrogen Bonds between Silver Anion and Nucleobases: Size-Selected Anion Photoelectron Spectroscopy and Density Functional Calculations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8973-8981.	1.1	10
1954	$B_{12}F_{20}^{+}$ ($n=1-6$) series: when do boron double chain nanoribbons become global minima?. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31655-31665.	1.3	5
1955	The nature of the multicenter bonding in $[TCNE]_2^{2+}$ dimer: $4c/2e$, $12c/2e$, or $20c/2e$?. <i>RSC Advances</i> , 2017, 7, 49526-49531.	1.7	6
1956	Reactivity and regioselectivity in Diels-Alder reactions of anion encapsulated fullerenes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30393-30401.	1.3	19
1957	Coordination Polymerization of Metal Azides and Powerful Nitrogen-Rich Ligand toward Primary Explosives with Excellent Energetic Performances. <i>Chemistry of Materials</i> , 2017, 29, 9725-9733.	3.2	92
1958	Synthesis, crystal structures, quantum chemical studies and corrosion inhibition potentials of 4-(((4-ethylphenyl)imino)methyl)phenol and (E)-4-((naphthalen-2-ylimino) methyl) phenol Schiff bases. <i>Journal of Molecular Structure</i> , 2017, 1147, 252-265.	1.8	33
1959	Environmentally-relevant concentrations of Al(III) and Fe(III) cations induce aggregation of free DNA by complexation with phosphate group. <i>Water Research</i> , 2017, 123, 58-66.	5.3	30
1960	Modeling cooperative effects in halogen-bonded infinite linear chains. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18529-18538.	1.3	9
1961	Understanding the behavior of caffeine on a boron-doped diamond surface: voltammetric, DFT, QTAIM and ELF studies. <i>New Journal of Chemistry</i> , 2017, 41, 7766-7774.	1.4	18
1962	Anomeric effect revisited: Perspective from information-theoretic approach in density functional reactivity theory. <i>Chemical Physics Letters</i> , 2017, 684, 97-102.	1.2	15
1963	Discovery of potent IDO1 inhibitors derived from tryptophan using scaffold-hopping and structure-based design approaches. <i>European Journal of Medicinal Chemistry</i> , 2017, 138, 199-211.	2.6	14
1964	DFT/TDDFT Study on the Sensing Mechanism of a Fluorescent Probe for Hydrogen Sulfide: Excited State Intramolecular Proton Transfer Coupled Twisted Intramolecular Charge Transfer. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5245-5256.	1.1	57
1965	Sulfonamide vs. sulfonimide: tautomerism and electronic structure analysis of N-heterocyclic arenesulfonamides. <i>New Journal of Chemistry</i> , 2017, 41, 8118-8129.	1.4	18
1966	Tanshinone I and isotanshinone I: The effects of media, isomerization and complexation on structural and electronic parameters. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 276-283.	1.1	1
1967	A combined experimental and theoretical approach for structural, spectroscopic, NLO, NBO, thermal and photophysical studies of new fluorescent 5-amino-1-(7-chloroquinolin-4-yl)-1H-1,2,3-triazole-4-carbonitrile using density functional theory. <i>Journal of Molecular Structure</i> , 2017, 1147, 725-734.	1.8	13

#	ARTICLE	IF	CITATIONS
1968	Copper(II) Binding Sites in N-Terminally Acetylated β -Synuclein: A Theoretical Rationalization. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5711-5719.	1.1	14
1969	Computational study on NHC-catalyzed enantioselective and chemoselective fluorination of aliphatic aldehydes. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1987-1998.	2.3	47
1970	Metal-mediated reactions between dialkylcyanamides and acetamidoxime generate unusual (nitrosoguanidinate)nickel(σ) complexes. <i>Dalton Transactions</i> , 2017, 46, 10090-10101.	1.6	46
1971	Perspective on carbazole-based organic compounds as emitters and hosts in TADF applications. <i>Journal of Materials Chemistry C</i> , 2017, 5, 8622-8653.	2.7	262
1972	Stabilities and interactions of CuRnX and XCuRn ($\text{X}=\text{F}, \text{Cl}, \text{Br}, \text{I}$): ab initio calculations. <i>Molecular Physics</i> , 2017, 115, 3128-3135.	0.8	1
1973	Combined Theoretical and Experimental Studies of Nickel-Catalyzed Cross-Coupling of Methoxyarenes with Arylboronic Esters via C–O Bond Cleavage. <i>Journal of the American Chemical Society</i> , 2017, 139, 10347-10358.	6.6	87
1974	Halogen and chalcogen bonding in dichloromethane solvate of cyclometalated iridium(III) isocyanide complex. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2017, 232, 797-805.	0.4	27
1975	Magnetic nanoparticle-supported tetrazole-functionalized palladium catalyst: synthesis, DFT study and application for Sonogashira and Heck cross-coupling reactions. <i>Research on Chemical Intermediates</i> , 2017, 43, 6737-6761.	1.3	22
1976	Effect of Different Substituted Groups on Excited-State Intramolecular Proton Transfer of 1-(Acylamino)-anthraquinons. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14779-14786.	1.5	72
1977	Highly Efficient Thermally Activated Delayed Fluorescence from an Excited-State Intramolecular Proton Transfer System. <i>ACS Central Science</i> , 2017, 3, 769-777.	5.3	148
1978	Asymmetric triiodide-diiodine interactions in the crystal of (Z)-4-chloro-5-((2-((4-chloro-5H-1,2,3-dithiazol-5-ylidene)amino)phenyl)amino)-1,2,3-dithiazol-1-ium oligoiodide. <i>Structural Chemistry</i> , 2017, 28, 1927-1934.	1.0	14
1979	Tuning Light Absorption in Platinum(II) Terpyridyl π -Conjugated Complexes: A First-Principle Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5533-5539.	1.1	0
1980	Synthesis, characterization, thermal properties and theoretical investigation on Bis(guanidinium) 4,4'-Azo-1H-1,2,4-triazol-5-one. <i>Journal of Molecular Structure</i> , 2017, 1147, 754-762.	1.8	4
1981	Hydrogen bond strengthening induces fluorescence quenching of PRODAN derivative by turning on twisted intramolecular charge transfer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 187, 68-74.	2.0	27
1982	An octupolar bis(porphyrinato) terbium(III) complex with the highest off-resonant hyperpolarizability. <i>RSC Advances</i> , 2017, 7, 22855-22859.	1.7	2
1983	Structural Asymmetry-Facilitated Tunability of Spin Distribution in the (10, 0) Carbon Nanotube Induced by Charging. <i>Journal of Electronic Materials</i> , 2017, 46, 3857-3861.	1.0	2
1984	DFT studies of the substituent effects of dimethylamino on non-heme active oxidizing species: iron(V)-oxo species or iron(IV)-oxo acetate aminopyridine cation radical species?. <i>Journal of Biological Inorganic Chemistry</i> , 2017, 22, 987-998.	1.1	19
1985	Intramolecular C–O–S(C) chalcogen bonds: A theoretical study of the effects of substituents and intermolecular hydrogen bonds. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 190-196.	1.1	8

#	ARTICLE	IF	CITATIONS
1986	Strategy for extractant residual reduction: Experimental and computational investigation of fluorinated phosphate. <i>Fluid Phase Equilibria</i> , 2017, 449, 167-174.	1.4	6
1987	Recognition of switching on or off fluorescence emission spectrum on the Schiff-bases as a Mg ²⁺ chemosensor: A first principle DFT and TD-DFT study. <i>Journal of Molecular Structure</i> , 2017, 1147, 815-820.	1.8	20
1988	Mechanism of the Copper/TEMPO-Catalyzed Aerobic Oxidation of Alcohols. <i>Chemistry - A European Journal</i> , 2017, 23, 1368-1378.	1.7	45
1989	The study on interactions between 1-ethyl-3-methylimidazolium chloride and benzene/pyridine/pyrrole/thiophene. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3663.	0.9	4
1990	Theoretical investigation on the spectroscopic properties of furylfulgide with different substituents and design of novel bis-furylfulgimide photochromes. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25327.	1.0	1
1991	Kinetic and mechanistic study on the pyrolysis of 1,3-dihydroisothianaphthene-2,2-dioxide toward benzocyclobutene using RRKM and BET theories. <i>Chemical Physics</i> , 2017, 483-484, 12-25.	0.9	7
1992	Theoretical study of YD2-o-C8-based derivatives as promising sensitizers for dye-sensitized solar cells. <i>Journal of Materials Science</i> , 2017, 52, 1235-1245.	1.7	18
1993	Copper(I) iodide supported on modified cellulose-based nano-magnetite composite as a biodegradable catalyst for the synthesis of 1,2,3-triazoles. <i>Applied Organometallic Chemistry</i> , 2017, 31, e3660.	1.7	33
1994	Molecular Dimensions and Porous Structure of Activated Carbons for Sorption of Xylene and Isooctane. <i>Chemical Engineering and Technology</i> , 2017, 40, 6-17.	0.9	8
1995	Specific Intermolecular Interactions in the Supramolecular Structure of 5-Hydroxy-6-Methyluracil: A DFT Study of the Hydrogen-bonded Dimers. <i>Journal of the Chinese Chemical Society</i> , 2017, 64, 143-151.	0.8	6
1996	Unveiling the three-center hydrogen bond dynamic behavior in ground and excited states. <i>Journal of Luminescence</i> , 2017, 182, 15-21.	1.5	7
1997	A computational investigation on the influence of different spacer groups in the bithiazole-based organic dye sensitizers on the short-circuit photocurrent densities of dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 333, 70-78.	2.0	23
1998	A Computational Study of Density of Some High Energy Molecules. <i>Propellants, Explosives, Pyrotechnics</i> , 2017, 42, 204-212.	1.0	7
1999	Cyclopentadithiophene bridged organic sensitizers with different auxiliary acceptor for high performance dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2017, 137, 165-173.	2.0	19
2000	Theoretical study of zinc porphyrin-based dyes for dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 333, 200-207.	2.0	12
2001	Geometries, stabilities and electronic properties of copper and selenium doped copper clusters: Density functional theory study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2017, 86, 303-310.	1.3	14
2002	Glucose derivatives substitution and cyclic peptide diameter effects on the stability of the self-assembled cyclic peptide nanotubes; a joint QM/MD study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 71, 28-39.	1.3	13
2003	Theoretical Screening of Novel 5-picrylamino-1,2,3,4-tetrazole (PAT) and 5,5-dicyano-2-styphnylamino-1,2,3,4-tetrazole (SAT) Derivatives: A New Molecular Design Strategy of Multi-Nitrogen Energetic Materials by Introducing Intermolecular Hydrogen Bonds and π - π Stacking Interactions. <i>Polycyclic Aromatic Compounds</i> , 2017, 37, 327-344.	1.4	4

#	ARTICLE	IF	CITATIONS
2005	Exploring the effect of vibronic contributions on light harvesting efficiency of NKX-2587 derivatives through vibrationally resolved electronic spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 171, 406-414.	2.0	5
2006	Reactivity, vibrational spectroscopy, internal rotation and thermochemical aspects of methylarsine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 171, 383-394.	2.0	9
2007	Theoretical studies on nitrogen-rich furoxan-based heterocyclic derivatives. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3627.	0.9	7
2008	Protein Arrangement Effects on the Exciton Dynamics in the PE555 Complex. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3228-3236.	1.2	13
2009	Computational Methodologies for Developing Structure-Morphology-Performance Relationships in Organic Solar Cells: A Protocol Review. <i>Chemistry of Materials</i> , 2017, 29, 346-354.	3.2	61
2010	Intermolecular hydrogen bonding, structural and vibrational assignments of 2, 3, 4, 5-tetrafluorobenzoic acid using density functional theory. <i>Journal of Molecular Structure</i> , 2017, 1128, 534-543.	1.8	5
2011	Theoretical design of push-pull porphyrin dyes with π -bridge modification for dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 332, 232-240.	2.0	18
2012	Bimetallic Fe-Au Carbonyl Clusters Derived from Collman's Reagent: Synthesis, Structure and DFT Analysis of $\text{Fe}(\text{CO})_4(\text{AuNHC})_2$ and $[\text{Au}_3\text{Fe}_2(\text{CO})_8(\text{NHC})_2]^+$. <i>Journal of Cluster Science</i> , 2017, 28, 703-723.	1.7	23
2013	Experimental and theoretical analysis of organic dyes having a double D-A configurations for dye-sensitized solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 173, 361-368.	2.0	5
2014	Moisture removal mechanism of low-rank coal by hydrothermal dewatering: Physicochemical property analysis and DFT calculation. <i>Fuel</i> , 2017, 187, 242-249.	3.4	90
2015	Alkali-earth metal bridges formed in biofilm matrices regulate the uptake of fluoroquinolone antibiotics and protect against bacterial apoptosis. <i>Environmental Pollution</i> , 2017, 220, 112-123.	3.7	13
2016	A systematic study of phenoxazine-based organic sensitizers for solar cells. <i>Dyes and Pigments</i> , 2017, 137, 12-23.	2.0	61
2017	A DFT study on electronic and optical properties of aspirin-functionalized B12N12 fullerene-like nanocluster. <i>Structural Chemistry</i> , 2017, 28, 735-748.	1.0	68
2018	Effect of the species and number of heteroatom on the interaction energy and charge transfer between crown ether and alkali metal ions. <i>Structural Chemistry</i> , 2017, 28, 749-756.	1.0	3
2019	Halobenzene activation by heterofullerenes: computational investigation of oxidative addition activity. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3628.	0.9	2
2020	Decomposition of acetaminophen in water by a gas phase dielectric barrier discharge plasma combined with TiO ₂ -rGO nanocomposite: Mechanism and degradation pathway. <i>Journal of Hazardous Materials</i> , 2017, 323, 719-729.	6.5	91
2021	Molecular structure of gaseous isatin as studied by electron diffraction and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2017, 1132, 44-49.	1.8	7
2022	Theoretical Investigation of the ES IPT Mechanism for the 1-Hydroxy-9H-fluoren-9-one and 1-Hydroxy-11H-benzo[b]fluoren-11-one Chromophores. <i>Journal of Cluster Science</i> , 2017, 28, 1191-1200.	1.7	20

#	ARTICLE	IF	CITATIONS
2023	The role of non-covalent interaction in the hexadentate coordination environment on the magnetic behavior of binuclear helical complex [Ni ₂ (L) ₂] ⁴⁺ : A broken-symmetry approach. <i>Polyhedron</i> , 2017, 122, 172-178.	1.0	1
2024	In silico insight into ammonia adsorption on pristine and X-doped phosphorene (X = B, C, N, O, Si, and) <i>TJ ETQq1 1 0.784314 1.0 BT / Over</i>	3.1	27
2025	Quantum Chemical Approach for Determining Degradation Pathways of Phenol by Electrical Discharge Plasmas. <i>Plasma Chemistry and Plasma Processing</i> , 2017, 37, 5-28.	1.1	7
2026	An ab initio study on anionic aerogen bonds. <i>Chemical Physics Letters</i> , 2017, 667, 337-344.	1.2	17
2027	Role of intermolecular interaction in crystal packing: A competition between halogen bond and electrostatic interaction. <i>Journal of Molecular Structure</i> , 2017, 1131, 250-257.	1.8	5
2028	Metal-mediated generation of triazapentadienate-terminated di- and trinuclear μ_4 -pyrazolate Ni ^{II} species and control of their nuclearity. <i>New Journal of Chemistry</i> , 2017, 41, 316-325.	1.4	31
2029	An ab initio study on substituent and cooperative effects in bifurcated fluorine bonds. <i>Molecular Physics</i> , 2017, 115, 278-287.	0.8	5
2030	Alternative Mechanistic Strategy for Enzyme Catalysis in a Ni-Dependent Lactate Racemase (LarA): Intermediate Destabilization by the Cofactor. <i>Chemistry - A European Journal</i> , 2017, 23, 3623-3630.	1.7	28
2031	Binuclear trivalent and tetravalent uranium halides and cyanides supported by cyclooctatetraene ligands. <i>Radiochimica Acta</i> , 2017, 105, 21-32.	0.5	1
2032	A theoretical study on the efficiency and role of guanidines-based organic superbases on carbon dioxide utilization in quinazoline-2,4(1H, 3H)-diones synthesis. <i>Structural Chemistry</i> , 2017, 28, 675-686.	1.0	13
2033	A new dithienylethene dimer with terminal tertiary amine redox centers: Electrochemical, UV-vis-NIR spectral and electronic transfer charges induced by a stepwise photochromic process. <i>Dyes and Pigments</i> , 2017, 136, 669-677.	2.0	7
2034	Improved lithium adsorption in boron- and nitrogen-substituted graphene derivatives. <i>Journal of Materials Science</i> , 2017, 52, 815-831.	1.7	21
2035	Characterization and intramolecular bonding patterns of busulfan: Experimental and quantum chemical approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 173, 390-399.	2.0	10
2036	Computational study on fused five membered heterocyclic compounds containing tertiary oxygen. <i>Journal of Molecular Structure</i> , 2017, 1129, 98-104.	1.8	6
2037	The X ⁺ -A ⁻ -A ⁻ -benzohydrazide complexes: the interplay between anion- π and H-bond interactions. <i>Structural Chemistry</i> , 2017, 28, 687-695.	1.0	4
2038	Nature and strength of weak intermolecular interactions with metal atoms in crystals of square-planar nickel(ii) complexes. <i>Russian Chemical Bulletin</i> , 2017, 66, 1550-1556.	0.4	2
2039	Supramolecular stereoelectronic effect in hemiketals. <i>Mendeleev Communications</i> , 2017, 27, 595-598.	0.6	3
2040	Polymorphism of a widely used building block for halogen-bonded assemblies: 1,3,5-trifluoro-2,4,6-triiodobenzene. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2017, 73, 667-673.	0.2	4

#	ARTICLE	IF	CITATIONS
2041	Evaluation of Structural Isomers, Molecular Interactions, Reactivity Descriptors, and Vibrational Analysis of Tretinoin. <i>Analytical Sciences</i> , 2017, 33, 83-87.	0.8	2
2042	A series of energetic metal pentazolate hydrates. <i>Nature</i> , 2017, 549, 78-81.	13.7	340
2043	Trends in Geometric, Energetic, Electronic, and Magnetic Properties of Vanadium-Copper Clusters Cu_nV with $n = 1-12$: Density Functional Calculations. <i>Russian Journal of Physical Chemistry A</i> , 2017, 91, 2558-2568.	0.1	0
2044	Structural and Electronic Properties of Co_nC_3 and Co_nC_4 ($n=1-4$) Clusters: Mass-Selected Anion Photoelectron Spectroscopy and Density Functional Theory Calculations. <i>Chinese Journal of Chemical Physics</i> , 2017, 30, 717-726.	0.6	5
2045	Modeling Photovoltaic Performances of BTBPD-PC61BM System via Density Functional Theory Calculations. <i>Chinese Journal of Chemical Physics</i> , 2017, 30, 268-276.	0.6	2
2046	Infrared Spectra and Theoretical Calculations of BS2 and BS2 $\hat{=}$: Strong Pseudo Jahn-Teller Effect. <i>Chinese Journal of Chemical Physics</i> , 2017, 30, 678-684.	0.6	6
2047	Density functional theory study of organic small molecules for renewable energy system. , 2017, , .		2
2048	Intramolecular Hydrogen Bonding Involving Organic Fluorine: NMR Investigations Corroborated by DFT-Based Theoretical Calculations. <i>Molecules</i> , 2017, 22, 423.	1.7	55
2049	Halogen Bonds Formed between Substituted Imidazoliums and N Bases of Varying N-Hybridization. <i>Molecules</i> , 2017, 22, 1634.	1.7	18
2050	Nucleophilicities of Lewis Bases B and Electrophilicities of Lewis Acids A Determined from the Dissociation Energies of Complexes $B\hat{=}A$ Involving Hydrogen Bonds, Tetrel Bonds, Pnictogen Bonds, Chalcogen Bonds and Halogen Bonds. <i>Molecules</i> , 2017, 22, 1786.	1.7	30
2051	Synthesis, Analysis, Cholinesterase-Inhibiting Activity and Molecular Modelling Studies of 3-(Dialkylamino)-2-hydroxypropyl 4-[(Alkoxy-carbonyl)amino]benzoates and Their Quaternary Ammonium Salts. <i>Molecules</i> , 2017, 22, 2048.	1.7	9
2052	Non-Fullerene Acceptor-Based Solar Cells: From Structural Design to Interface Charge Separation and Charge Transport. <i>Polymers</i> , 2017, 9, 692.	2.0	29
2053	Mechanistic Insight into the 2 $\hat{=}$ Alcohol Oxidation Mediated by an Efficient CuI/L-Proline-TEMPO Catalyst $\hat{=}$ A Density Functional Theory Study. <i>Catalysts</i> , 2017, 7, 264.	1.6	3
2054	Synthesis, Crystal Structure and Hirshfeld Topology Analysis of Polymeric Silver(I) Complex with s-Triazine-Type Ligand. <i>Crystals</i> , 2017, 7, 160.	1.0	1
2055	Crystallographic and computational study of a network composed of $[ZnCl_4]^{2-}$ anions and triply protonated 4 $\hat{=}$ -functionalized terpyridine cations. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2017, 73, 1121-1130.	0.2	5
2056	Synthesis, Crystal Structure, and DFT Study of Ethyl 1-(2-(Hydroxyimino)-2-phenylethyl)-3-phenyl-1H-pyrazole-5-carboxylate. <i>Journal of Chemistry</i> , 2017, 2017, 1-9.	0.9	4
2057	Theoretical study for tuning the HOMO level of the donor to increase the efficiency through open-circuit voltage of small molecule solar cells. , 2017, , .		0
2058	Solvent/co-solvent effects on the electronic properties and adsorption mechanism of anticancer drug Thioguanine on Graphene oxide surface as a nanocarrier: Density functional theory investigation and a molecular dynamics. <i>Applied Surface Science</i> , 2017, 422, 1030-1041.	3.1	55

#	ARTICLE	IF	CITATIONS
2059	Modulated structure to maximize the open-circuit voltage with moderate band-gap of small molecule organic solar cells-DFT approach. , 2017, , .		0
2060	Reduction potential tuning of first row transition metal MIII/MII (M = Cr, Mn, Fe, Co, Ni) hexadentate complexes for viable aqueous redox flow battery catholytes: A DFT study. <i>Electrochimica Acta</i> , 2017, 246, 156-164.	2.6	8
2061	A theoretical study on the ESPT mechanism for a novel Bisâ€HPBT fluorophore. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3821.	0.9	10
2062	Energetics and electronic structures of nitrogen chains encapsulated in zigzag carbon nanotube. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 103, 444-451.	1.3	19
2063	Experimental and theoretical studies on vanadium bromoperoxidase activity of alkyne arm dioxidovanadium(V) complex: Crystal structure, spectral studies, and DFT calculations. <i>Polyhedron</i> , 2018, 145, 191-199.	1.0	6
2064	A model of atoms in molecules based on potential acting on one electron in a molecule: I. Partition and atomic charges obtained from ab initio calculations. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25610.	1.0	13
2065	Insight into the thermodynamically preferred V3N@I(31924)-C80 and acknowledged VxSc3-xN@I(31924)-C80 (x=0, 1 and 2). <i>Carbon</i> , 2018, 132, 312-322.	5.4	9
2066	Structural and spectrophotometric characterization of 2-[4-(dimethylamino)styryl]-1-ethylquinolinium iodide as a reagent for sequential injection determination of tungsten. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 196, 398-405.	2.0	19
2067	Heterobimetallic [NiFe] Complexes Containing Mixed CO/CN^{â€“} Ligands: Analogs of the Active Site of the [NiFe] Hydrogenases. <i>Inorganic Chemistry</i> , 2018, 57, 2558-2569.	1.9	14
2068	Computational studies on horseshoe shape pocket of human orexin receptor type 2 and boat conformation of suvorexant by molecular dynamics simulations. <i>Chemical Biology and Drug Design</i> , 2018, 92, 1221-1231.	1.5	4
2069	Boron Carbonyl Analogues of Hydrocarbons: An Infrared Photodissociation Spectroscopic Study of B₃(CO)_n (<i>n</i> = 4â€“6). <i>Journal of Physical Chemistry A</i> , 2018, 122, 2688-2694.	1.1	6
2070	Controlling the spin state of diphenylcarbene via halogen bonding: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25616.	1.0	4
2071	Accurate description of excited state intramolecular proton transfer that involves zwitterionic state using optimally tuned rangeâ€separated timeâ€dependent density functional theory. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25618.	1.0	17
2072	Characterization of point defects in monolayer arsenene. <i>Applied Surface Science</i> , 2018, 443, 74-82.	3.1	31
2073	The physicochemical properties and tyrosinase inhibitory activity of ectoine and its analogues: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2018, 1130, 6-14.	1.1	5
2074	A computational study on the strength and nature of bifurcated aerogen bonds. <i>Chemical Physics Letters</i> , 2018, 698, 1-6.	1.2	17
2075	Redox-switchable structures and NLO property: Li2 doped into the cavity of pyridine helix. <i>Organic Electronics</i> , 2018, 57, 68-73.	1.4	12
2076	Intramolecular Hydrogen Bonding Appetency for Conformational Penchants in Oxalohydrazide Fluoro Derivatives: NMR, MD, QTAIM, and NCI Studies. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2703-2713.	1.1	7

#	ARTICLE	IF	CITATIONS
2077	Spontaneous disproportionation of lithium biphenyl in solution: a combined experimental and theoretical study. <i>New Journal of Chemistry</i> , 2018, 42, 5168-5177.	1.4	9
2078	Nature of Bonding in Bowl-Like B ₃₆ Cluster Revisited: Concentric (6+18) Double Aromaticity and Reason for the Preference of a Hexagonal Hole in a Central Location. <i>Chemistry - an Asian Journal</i> , 2018, 13, 1148-1156.	1.7	11
2079	Understanding the Effect of Solvent on the Growth and Crystal Morphology of MTNP/CL ₂₀ Cocrystal Explosive: Experimental and Theoretical Studies. <i>Crystal Research and Technology</i> , 2018, 53, 1700299.	0.6	18
2080	Kinetic and mechanistic insight into the formation of amphetamine using the Leuckart-Wallach reaction and interaction of the drug with Cp-CpG base-pair step of DNA: a DFT study. <i>Monatshefte für Chemie</i> , 2018, 149, 1045-1057.	0.9	6
2081	Nature of bonding and cooperativity in linear DMSO clusters: A DFT, AIM and NCI analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 81, 50-59.	1.3	58
2082	Implications of monomer deformation for tetrel and pnictogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8832-8841.	1.3	67
2083	A cation-selective and anion-controlled benzothiazolyl-attached macrocycle for NLO-based cation detection: variational first hyperpolarizabilities. <i>New Journal of Chemistry</i> , 2018, 42, 6091-6100.	1.4	12
2084	Screening of different interactions in oxo-manganese porphyrin dimers containing axial N-donor ligands: a theoretical study. <i>RSC Advances</i> , 2018, 8, 9770-9774.	1.7	5
2085	C ⁺ N coordination bonds in (CCC) ⁺ N + ⁺ (L) complexes. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1. 0.5		13
2086	Simple electron donor molecules based on triphenylamine and carbazole derivatives. <i>Dyes and Pigments</i> , 2018, 153, 275-283.	2.0	23
2087	Mechanistic insights into asymmetric reductive coupling of isoquinolines by a chiral diboron with DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 97-104.	0.8	13
2088	Intermolecular forces in 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide + ethanol mixtures. <i>Journal of Molecular Liquids</i> , 2018, 258, 1-9.	2.3	19
2089	Insights into the effect of donor ability on photophysical properties of dihydroindeno[2,1-c <i>i</i>]fluorene-based imide derivatives. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7514-7522.	1.3	22
2090	Computational Studies on the Sc _n N _m (n+m=10) Clusters: Structure, Electronic and Vibrational Properties. <i>Journal of Cluster Science</i> , 2018, 29, 459-468.	1.7	3
2091	Steric Crowding in Tetrel Bonds. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2550-2562.	1.1	55
2092	Theoretical Insights into Monometallofullerene Th@C ₇₆ : Strong Covalent Interaction between Thorium and the Carbon Cage. <i>Inorganic Chemistry</i> , 2018, 57, 2961-2964.	1.9	22
2093	Electronic Structure and Bonding Situation in M ₂ O ₂ (M = Be, Mg, Ca) Rhombic Clusters. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2816-2822.	1.1	34
2094	Phosphorene as a Template Material for Physisorption of DNA/RNA Nucleobases and Resembling of Base Pairs: A Cluster DFT Study and Comparisons with Graphene. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4870-4880.	1.5	55

#	ARTICLE	IF	CITATIONS
2095	Recognition of Melamine by Chromium Tricarbonyl (Thio)barbituric Acid Derivatives: Theoretical Insight into Multiple Hydrogen-Bond Modes. <i>ChemistrySelect</i> , 2018, 3, 2404-2415.	0.7	0
2096	Theoretical studies on glycolysis of poly(ethylene terephthalate) in ionic liquids. <i>RSC Advances</i> , 2018, 8, 8209-8219.	1.7	35
2097	Noble gas supported boron-pentagonal clusters B ₅ N _g n ³⁺ : exploring the structures and bonding. <i>Journal of Molecular Modeling</i> , 2018, 24, 90.	0.8	3
2098	Synthesis, molecular structure, Hirshfeld surface, spectral investigations and molecular docking study of 3-(5-bromo-2-thienyl)-1-(4-fluorophenyl)-3-acetyl-2-pyrazoline (2) by DFT method. <i>Journal of Molecular Structure</i> , 2018, 1164, 420-437.	1.8	15
2099	Effect of conjugation and aromaticity of 3,6 di-substituted carbazoles on triplet energy and the implication of triplet energy in multiple-cyclic aromatic compounds. <i>RSC Advances</i> , 2018, 8, 9850-9857.	1.7	15
2100	Solid-State Photodimerization of Azaanthracene Derivative Based on a [4+4] Cycloaddition. <i>Asian Journal of Organic Chemistry</i> , 2018, 7, 906-909.	1.3	7
2101	Theoretical study of an anti-Markovnikov addition reaction catalyzed by β -cyclodextrin. <i>Journal of Molecular Modeling</i> , 2018, 24, 77.	0.8	3
2102	Mechanistic insights into the selective hydrogenation of resorcinol to 1,3-cyclohexanedione over Pd/rGO catalyst through DFT calculation. <i>Chinese Journal of Chemical Engineering</i> , 2018, 26, 2542-2548.	1.7	6
2103	Photophysical properties of 2,6-unsubstituted 1,4-dihydropyridines: Experimental and theoretical studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 358, 51-60.	2.0	7
2104	A highly selective fluorescent probe for cyanide ion and its detection mechanism from theoretical calculations. <i>Talanta</i> , 2018, 185, 1-6.	2.9	28
2105	Third-Order Nonlinear Optical Properties of Endohedral Fullerene (H ₂) ₂ @C ₇₀ and (H ₂ O) ₂ @C ₇₀ Accompanied by the Prospective of Novel (HF) ₂ @C ₇₀ . <i>Journal of Physical Chemistry C</i> , 2018, 122, 6835-6845.	1.5	24
2106	Halides Held by Bifurcated Chalcogen-Hydrogen Bonds. Effect of $\frac{1}{4}$ (S, N-H) Cl Contacts on Dimerization of Cl(carbene)Pd ^{II} Species. <i>Inorganic Chemistry</i> , 2018, 57, 3420-3433.	1.9	66
2107	Reaction Electronic Flux Perspective on the Mechanism of the Zimmerman Di- π -methane Rearrangement. <i>Journal of Organic Chemistry</i> , 2018, 83, 5969-5974.	1.7	11
2108	Enantiocontrol by assembled attractive interactions in copper-catalyzed asymmetric direct alkylation of β -ketoesters with terminal alkynes: OH ³ -CH ² O two-point hydrogen bonding combined with dispersive attractions. <i>Chemical Science</i> , 2018, 9, 3484-3493.	3.7	43
2109	Tris-amidoximate uranyl complexes <i>via</i> β -binding mode coordinated in aqueous solution shown by X-ray absorption spectroscopy and density functional theory methods. <i>Journal of Synchrotron Radiation</i> , 2018, 25, 514-522.	1.0	12
2110	Effect of surface vacancies on the adsorption of Pd and Pb on MgO(100). <i>Monatshefte für Chemie</i> , 2018, 149, 1009-1015.	0.9	0
2111	Identifying Strong Covalent Interactions with Pauli Energy. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3087-3095.	1.1	36
2112	Tipping the Balance between Ligand and Metal Protonation due to Relativistic Effects: Unusually High Proton Affinity in Gold(I) Pincer Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 6047-6051.	1.7	12

#	ARTICLE	IF	CITATIONS
2113	Bond Ellipticity Alternation: An Accurate Descriptor of the Nonlinear Optical Properties of π -Conjugated Chromophores. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1377-1383.	2.1	22
2114	Fixation of nitrous oxide (N_2O) by 1, 4, 2, 5-diazadiborinine: A DFT study. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25593.	1.0	14
2115	Investigation on the electronic structures and nonlinear optical properties of alkali metal atom doped all-cis-1,2,3,4,5,6-hexafluorocyclohexane. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25619.	1.0	20
2116	Extractive Distillation Approach to the Removal of Dimethyl Disulfide from Methyl Tert-Butyl Ether: Combined Computational Solvent Screening and Experimental Process Investigation. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 3348-3358.	1.8	13
2117	A porous rhodium(III)-porphyrin metal-organic framework as an efficient and selective photocatalyst for CO ₂ reduction. <i>Applied Catalysis B: Environmental</i> , 2018, 231, 173-181.	10.8	126
2118	Can Remote N-Heterocyclic Carbenes Coordinate with Main Group Elements? Synthesis, Structure, and Quantum Chemical Analysis of N^+ -Centered Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 6418-6425.	1.7	21
2119	Predicting ion mobility collision cross sections directly from standard quantum chemistry software. <i>Journal of Mass Spectrometry</i> , 2018, 53, 432-434.	0.7	2
2120	Spectroscopic, structural and theoretical investigation of 1,3-bis(3-hydroxymethylpyridinium)propane dibromide, tetrabromozincate and tetrabromocuprate. <i>Journal of Molecular Structure</i> , 2018, 1163, 345-356.	1.8	2
2121	Experimental and theoretical elucidation of structural and antioxidant properties of vanillylmandelic acid and its carboxylate anion. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 198, 61-70.	2.0	28
2122	A novel <i>N</i> -methylimidazolium-based poly(ionic liquid) to recover trace tetrachloroaurate from aqueous solution based on multiple supramolecular interactions. <i>Inorganic Chemistry Frontiers</i> , 2018, 5, 922-931.	3.0	17
2123	Characterisation of superalkaline-earth-metal halides, hydroxide and chalcogenides. <i>Molecular Physics</i> , 2018, 116, 1871-1882.	0.8	1
2124	Physical mechanism of photoinduced intermolecular charge transfer enhanced by fluorescence resonance energy transfer. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13558-13565.	1.3	37
2125	Ring closure of polynitroazoles via an N,N -alkylene bridge: towards high thermally stable energetic compounds. <i>Journal of Materials Chemistry A</i> , 2018, 6, 8382-8387.	5.2	40
2126	Defect Structures, Electronic Properties, UV-Vis, and EPR Parameters for Rh^{2+} Centers in LiD: A DFT Study. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1800026.	0.7	2
2127	Structure-property relationship of phosphine oxide based thermally activated delayed fluorescence molecules: First-principles study. <i>Organic Electronics</i> , 2018, 59, 7-14.	1.4	6
2128	Excimer formation and evolution of excited state properties in discrete dimeric stacking of an anthracene derivative: a computational investigation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12129-12137.	1.3	95
2129	From Open-Shell Singlet Diradicaloid to Closed-Shell Global Antiaromatic Macrocycles. <i>Angewandte Chemie</i> , 2018, 130, 7284-7288.	1.6	13
2130	Structural Memory Effect of Mg-Al and Zn-Al layered Double Hydroxides in the Presence of Different Natural Humic Acids: Process and Mechanism. <i>Langmuir</i> , 2018, 34, 5386-5395.	1.6	77

#	ARTICLE	IF	CITATIONS
2131	Understanding Am ³⁺ /Cm ³⁺ separation with H ₄ TPAEN and its hydrophilic derivatives: a quantum chemical study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14031-14039.	1.3	23
2132	La ⁺ bonded dimetallofullerenes [La ₂ @C _{2n}] ⁺ : species for stabilizing C _{2n} (2n = 92-96) besides La ₂ C ₂ @C _{2n} . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14671-14678.	1.3	10
2133	The role of fluorine-substitution on the Ir-bridge in constructing effective thermally activated delayed fluorescence molecules. <i>Journal of Materials Chemistry C</i> , 2018, 6, 5536-5541.	2.7	29
2134	Spectroscopic and Electronic Analysis of Chelation Reactions of Galangin and Related Flavonoids with Nickel(II). <i>Journal of Chemical & Engineering Data</i> , 2018, 63, 1488-1497.	1.0	9
2135	Ab initio investigation of the lower-energy candidate structures for (H ₂ O) ₁₀₊ water cluster. <i>Structural Chemistry</i> , 2018, 29, 1273-1285.	1.0	4
2136	A first principle study of benzimidazobenzophenanthrolin and tetraphenyldibenzoperiflanthene to design and construct novel organic solar cells. <i>Physica B: Condensed Matter</i> , 2018, 542, 32-36.	1.3	26
2137	Three new dihydro- β -agarofuran sesquiterpenes from the seeds of <i>Maytenus boaria</i> . <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 564-570.	0.2	3
2138	Secondary Oxide Phosphines to Promote Tandem Acyl-Alkyl Coupling/Hydrogen Transfer to Afford (Hydroxyalkyl)rhodium Complexes. <i>Theoretical and Experimental Studies. Inorganic Chemistry</i> , 2018, 57, 5307-5319.	1.9	6
2139	Mechanism of Photoinduced Triplet Intermolecular Hydrogen Transfer between Cycloxydim and Chlorothalonil. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4285-4293.	1.1	3
2140	Synthesis, structures and luminescence properties of amine-bis(N-heterocyclic carbene) copper and silver complexes. <i>Dalton Transactions</i> , 2018, 47, 6742-6753.	1.6	22
2141	Quest for Insight into Ultrashort C-H...H Proximities in Molecular Iron Maiden. <i>Journal of Organic Chemistry</i> , 2018, 83, 5114-5122.	1.7	8
2142	Insight into the Extraction Mechanism of Americium(III) over Europium(III) with Pyridylpyrazole: A Relativistic Quantum Chemistry Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4499-4507.	1.1	32
2143	The structure-electrochemical property relationship of quinone electrodes for lithium-ion batteries. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13478-13484.	1.3	59
2144	Insight into the mechanism of methanol assistance with syngas conversion over partially hydroxylated γ -Al ₂ O ₃ (110) surface in slurry bed. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12845-12857.	1.3	8
2145	Slow Magnetic Relaxation in a Palladium-Gadolinium Complex Induced by Electron Density Donation from the Palladium Ion. <i>Chemistry - A European Journal</i> , 2018, 24, 9285-9294.	1.7	34
2146	Static second hyperpolarizability of inverse sandwich compounds (M ₁ -C ₅ H ₅ -M ₂) of alkali (M ₁ = Li, Na, K) and alkaline earth metals (M ₂ = Be, Mg, Ca). <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13331-13339.	1.3	2
2147	From Open-Shell Singlet Diradicaloid to Closed-Shell Global Antiaromatic Macrocycles. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 7166-7170.	7.2	29
2148	Theoretical study on complexes and reactions of boron isotopic exchange separation with fluorinated anisoles as novel donors. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2018, 316, 587-594.	0.7	3

#	ARTICLE	IF	CITATIONS
2149	Theoretical Studies on Aromaticity of Spiro Metallaaromatics of (C ₁₀ H ₁₀ M) ₂ (M=Ni, Pd, Pt). <i>Chemical Research in Chinese Universities</i> , 2018, 34, 470-474.	1.3	1
2150	Effect of (super) alkali doping and boron substitution on the nonlinear optical property of biphenalenyl diradical $\dot{\text{I}}\epsilon$ dimer: A theoretical study. <i>Optik</i> , 2018, 165, 319-331.	1.4	8
2151	Critical Role of Molecular Electrostatic Potential on Charge Generation in Organic Solar Cells. <i>Chinese Journal of Chemistry</i> , 2018, 36, 491-494.	2.6	163
2152	Chemistry of Triple-Decker Sandwich Complexes Containing Four-Membered Open B ₂ E ₂ Rings (E = S or Se). <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 2045-2053.	1.0	16
2153	Yoink: An interaction-based partitioning API. <i>Journal of Computational Chemistry</i> , 2018, 39, 799-806.	1.5	13
2154	Exploring Chimeric Calix[4]tetrolarene Molecular Scaffolds: Theoretical Investigations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4189-4197.	1.1	4
2155	Repair Activity of <i>trans</i> -Resveratrol toward 2-Deoxyguanosine Radicals. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4397-4406.	1.2	2
2156	Halogen, Chalcogen, and Pnictogen Bonding Involving Hypervalent Atoms. <i>Chemistry - A European Journal</i> , 2018, 24, 8167-8177.	1.7	68
2157	All-Optical Switching and Two-States Light-Controlled Coherent-Incoherent Random Lasing in a Thiophene-Based Donor-Acceptor System. <i>ChemPhysChem</i> , 2018, 19, 1605-1616.	1.0	16
2158	Substituent regulated photoluminescent thermochromism in a rare type of octahedral Cu ₄ clusters. <i>New Journal of Chemistry</i> , 2018, 42, 8426-8437.	1.4	18
2159	Doping of the first row transition metals onto B ₁₂ N ₁₂ nanocage: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2018, 1132, 1-11.	1.1	52
2160	Esterification of Aryl and Alkyl Amides Enabled by Tailor-Made and Proposed Nickel Catalyst: Insights from Theoretical Investigation. <i>Journal of Organic Chemistry</i> , 2018, 83, 5009-5018.	1.7	17
2161	High-resolution X-ray diffraction determination of the electron density of 1-(8-PhSC ₁₀ H ₆)SS(C ₁₀ H ₆)SPh-8-1 with the QTAIM approach: evidence for S ₄ $\dot{\text{I}}f(4c^{-}6e)$ at the naphthalene <i>peri</i> -positions. <i>RSC Advances</i> , 2018, 8, 9651-9660.	1.7	12
2162	Double-helix P _n Li _n chains: novel potential nonlinear optical materials. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12618-12623.	1.3	8
2163	Understanding the hydrogen transfer mechanism for the biodegradation of 2,4,6-trinitrotoluene catalyzed by pentaerythritol tetranitrate reductase: molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12157-12165.	1.3	11
2164	Probing the structural evolution and bonding properties of PtnC ₂ ⁿ /O (n = 1-7) clusters by density functional calculations. <i>Chemical Physics Letters</i> , 2018, 699, 218-222.	1.2	6
2165	Theoretical studies on the structural and spectra properties of two C ₇₄ fullerenes and the chlorinated species C ₇₄ Cl ₁₀ . <i>Molecular Physics</i> , 2018, 116, 1772-1781.	0.8	6
2166	The Evolution of Electronic and Magnetic Properties of the Chain and Sheet Assemblies Based on Planar Tetracoordinate Carbon C ₂ Al ₄ (CH ₃) ₈ . <i>Journal of Physical Chemistry A</i> , 2018, 122, 4181-4188.	1.1	0

#	ARTICLE	IF	CITATIONS
2167	Elucidating the key role of fluorine in improving the charge mobility of electron acceptors for non-fullerene organic solar cells by multiscale simulations. <i>Journal of Materials Chemistry C</i> , 2018, 6, 4912-4918.	2.7	35
2168	Investigation of carbon monoxide catalytic oxidation on vanadium-embedded graphene. <i>Monatshefte für Chemie</i> , 2018, 149, 1349-1356.	0.9	7
2169	Quantum mechanical determination of atomic polarizabilities of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10992-10996.	1.3	47
2170	The design of rigid cyclic tripyrrins: the importance of intermolecular interactions on aggregation and luminescence. <i>Organic Chemistry Frontiers</i> , 2018, 5, 1877-1885.	2.3	11
2171	Quantum Chemistry Study on the Extraction of Trivalent Lanthanide Series by Cyanex301: Insights from Formation of Inner- and Outer-Sphere Complexes. <i>ACS Omega</i> , 2018, 3, 4070-4080.	1.6	17
2172	Mechanism of generation of closo-decaborato amidrazones. Intramolecular non-covalent H \cdots N(Ph) interaction determines stabilization of the configuration around the amidrazone C \equiv N bond. <i>New Journal of Chemistry</i> , 2018, 42, 8693-8703.	1.4	52
2173	Effect of electron-withdrawing terminal group on BDT-based donor materials for organic solar cells: a theoretical investigation. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	17
2174	Adaptive aromaticity in S ₀ and T ₁ states of pentalene incorporating 16 valence electron osmium. <i>Communications Chemistry</i> , 2018, 1, .	2.0	43
2175	Effect of Magnesium Bond on the Competition Between Hydrogen and Halogen Bonds and the Induction of Proton and Halogen Transfer. <i>ChemPhysChem</i> , 2018, 19, 1456-1464.	1.0	11
2176	Tautomeric preferences of the cis and trans isomers of axitinib. <i>Chemical Physics</i> , 2018, 507, 10-18.	0.9	4
2177	Remote modulation of singlet \rightarrow triplet gaps in carbenes. <i>Chemical Physics Letters</i> , 2018, 694, 48-52.	1.2	4
2178	Prediction of Henry's law constant of CO ₂ in ionic liquids based on SEP and S _{if} -profile molecular descriptors. <i>Journal of Molecular Liquids</i> , 2018, 262, 139-147.	2.3	25
2179	Unveiling the mechanism of the promising two-dimensional photoswitch " Hemithioindigo. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 200, 1-9.	2.0	3
2180	Influence of substituents and cooperativity in doubly hydrogen-bonded complexes of 2-pyridone and oxalic acid. <i>Molecular Physics</i> , 2018, 116, 1862-1870.	0.8	1
2181	Probing the geometric structures and electronic properties of anionic and neutral Pt ₃ C ₂ clusters by density functional calculations. <i>Chemical Physics Letters</i> , 2018, 694, 70-74.	1.2	7
2182	Description of an unusual hydrogen bond between carborane and a phenyl group. <i>Journal of Organometallic Chemistry</i> , 2018, 865, 114-127.	0.8	42
2183	Theoretical investigation on the ground state properties of the hexaamminecobalt(III) and nitro \rightarrow nitrito linkage isomerism in pentaamminecobalt(III) in vacuo. <i>RSC Advances</i> , 2018, 8, 3328-3342.	1.7	11
2184	Conformational preferences and isomerization upon excitation/ionization of 2-methoxypyridine and 2-N-methylaminopyridine. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6211-6226.	1.3	3

#	ARTICLE	IF	CITATIONS
2185	Doubly hybrid density functionals that correctly describe both density and energy for atoms. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 2287-2292.	3.3	36
2186	The Nature of Ion-Pair Recognition by Tetra-phosphonate Calix[4]pyrroles. Advanced Theory and Simulations, 2018, 1, 1700010.	1.3	4
2187	Probing the Most Aromatic and Antiaromatic Pyrrolium Rings by Maximizing Hyperconjugation and Push-Pull Effect. Chemistry - an Asian Journal, 2018, 13, 1419-1423.	1.7	21
2188	Prediction of the electron redundant SinNn fullerenes. Physica E: Low-Dimensional Systems and Nanostructures, 2018, 99, 208-214.	1.3	5
2189	Improving the first hyperpolarizability of anthracene through interaction with HX molecules (X F, Cl). Journal of Molecular Graphics and Modelling, 2018, 196, 353-365.	2.0	4
2190	DFT investigation on the selective complexation of Fe ³⁺ and Al ³⁺ with hydroxypyridinones used for treatment of the aluminium and iron overload diseases. Journal of Molecular Graphics and Modelling, 2018, 80, 182-189.	1.3	11
2191	On the interaction of anisole and thioanisole derivatives with gold clusters studied by DFT. Computational and Theoretical Chemistry, 2018, 1126, 54-64.	1.1	6
2192	DFT simulation, quantum chemical electronic structure, spectroscopic and structure-activity investigations of 4-acetylpyridine. Journal of Molecular Structure, 2018, 1161, 55-65.	1.8	22
2193	Stable and Inert Yttrium(III) Complexes with PycLen-Based Ligands Bearing Pendant Picolinate Arms: Toward New Pharmaceuticals for ¹⁷⁷ Lu-Radiotherapy. Inorganic Chemistry, 2018, 57, 2051-2063.	1.9	25
2194	Mechanism of Aerobic Alcohol Oxidation Mediated by Water-Soluble Cu ^{II} -TEMPO Catalyst in Water: A Density Functional Theory Study. ChemistrySelect, 2018, 3, 1268-1274.	0.7	3
2195	Protonation of Patented Blue V in aqueous solutions: theoretical and experimental studies. Journal of Chemical Sciences, 2018, 130, 1.	0.7	16
2196	Structural analysis of zwitterionic liquids vs. homologous ionic liquids. Journal of Chemical Physics, 2018, 148, 193807.	1.2	24
2197	Spatially resolved characterization of electron localization and delocalization in molecules: Extending the Kohn-Resta approach. International Journal of Quantum Chemistry, 2018, 118, e25600.	1.0	7
2198	Determination of molar enthalpy of sublimation in case of orotic acid as obtained from experimental and computational data. Chemical Physics Letters, 2018, 695, 107-111.	1.2	3
2199	Relaxed structure of typical nitro explosives in the excited state: Observation, implication and application. Chemical Physics Letters, 2018, 698, 200-205.	1.2	6
2200	The estimation of H-bond and metal ion-ligand interaction energies in the G-Quadruplex Mn^{2+} complexes. Journal of Molecular Structure, 2018, 1161, 246-253.	1.8	6
2201	3-Methylthio-4-phenyl-5-phenylamino-1,2,4-triazole hexabromotellurate: X-ray and computational study. Journal of Molecular Structure, 2018, 1161, 226-236.	1.8	25
2202	Experimental and Theoretical Study for Vapor Phase Aldol Condensation of Methyl Acetate and Formaldehyde over Alkali Metal Oxides Supported on SBA-15. Industrial & Engineering Chemistry Research, 2018, 57, 2773-2786.	1.8	30

#	ARTICLE	IF	CITATIONS
2203	Theoretical Insight into the Mechanism and Origin of Ligand-Controlled Regioselectivity in Homogeneous Gold-Catalyzed Intramolecular Hydroarylation of Alkynes. <i>Journal of Organic Chemistry</i> , 2018, 83, 2763-2772.	1.7	30
2204	Distribution of the unpaired electron in neutral bis(phthalocyaninato) yttrium double-deckers: An experimental and theoretical combinative investigation. <i>Journal of Porphyrins and Phthalocyanines</i> , 2018, 22, 165-172.	0.4	4
2205	Structure and stability of AlnMgm ($n=4, 8, 16, 3$) clusters: Genetic algorithm and density functional theory approach. <i>Computational and Theoretical Chemistry</i> , 2018, 1128, 15-23.	1.1	7
2206	Proton-coupled electron transfer in dye-sensitized solar cells: a theoretical perspective. <i>Structural Chemistry</i> , 2018, 29, 983-997.	1.0	12
2207	Systematic Characterization of Gas Phase Binary Pre-Nucleation Complexes Containing $H_2SO_4 + X$, [$X = NH_3, (CH_3)_2NH, (CH_3)_3N, H_2O, (CH_3)_2OH, (CH_3)_2O, HF, CH_3F, PH_3, (CH_3)_2PH, (CH_3)_3P,$		

#	ARTICLE	IF	CITATIONS
2221	H ₂ MBH ₂ and M(1/4-H) ₂ BH ₂ Molecules Isolated in Solid Argon: Interelement M-B and M-H-B Bonds (M = Ge, Sn). <i>Inorganic Chemistry</i> , 2018, 57, 2218-2227.	1.9	8
2222	Electron Precise Group 5 Dimetallaheteroboranes [{CpV(1/4-EPh)} ₂ {1/4- \uparrow ² : \uparrow ² -BH ₃ E}] and [{CpNb(1/4-EPh)} ₂ {1/4- \uparrow ² : \uparrow ² -B ₂ H ₄ E}] (E = S or Se). <i>Inorganic Chemistry</i> , 2018, 57, 985-994.	1.9	17
2223	Reconsideration of the Detection and Fluorescence Mechanism of a Pyrene-Based Chemosensor for TNT. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1400-1405.	1.1	32
2224	Donor Engineering for NIR-II Molecular Fluorophores with Enhanced Fluorescent Performance. <i>Journal of the American Chemical Society</i> , 2018, 140, 1715-1724.	6.6	379
2225	Prediction of Intramolecular Charge-Transfer Excitation for Thermally Activated Delayed Fluorescence Molecules from a Descriptor-Tuned Density Functional. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7816-7823.	1.5	36
2226	Interactions of Biodegradable Ionic Liquids with a Model Naphthenic Acid. <i>Scientific Reports</i> , 2018, 8, 176.	1.6	9
2227	A fully analytical integration of properties over the 3D volume of the $\langle i \rangle^2$ sphere in topological atoms. <i>Journal of Computational Chemistry</i> , 2018, 39, 604-613.	1.5	5
2228	Ab initio calculations, structure, NBO and NCI analyses of X H \cdots E interactions. <i>Chemical Physics Letters</i> , 2018, 693, 202-209.	1.2	15
2229	Adsorption characteristics of green 5-arylaminoethylene pyrimidine-2,4,6-triones on mild steel surface in acidic medium: Experimental and computational approach. <i>Results in Physics</i> , 2018, 8, 657-670.	2.0	38
2230	Three-dimensional nanopores on monolayer graphene for hydrogen storage. <i>Materials Chemistry and Physics</i> , 2018, 209, 134-145.	2.0	6
2231	Hydrogen storage of Li ₄ B ₃₆ cluster. <i>Scientific Reports</i> , 2018, 8, 1940.	1.6	26
2232	Phosphoric acid as a precursor to chemicals traditionally synthesized from white phosphorus. <i>Science</i> , 2018, 359, 1383-1385.	6.0	91
2233	Design Strategy for Improving Optical and Electrical Properties and Stability of Lead-Halide Semiconductors. <i>Journal of the American Chemical Society</i> , 2018, 140, 2805-2811.	6.6	210
2234	Exploring the ESIPT dynamical processes of two novel chromophores: symmetrical structure CHC and asymmetric structure CHN. <i>Organic Chemistry Frontiers</i> , 2018, 5, 1330-1341.	2.3	22
2235	Can water continuously oxidize the PuO molecule? Mechanisms, topological analysis and rate constant calculations. <i>RSC Advances</i> , 2018, 8, 4295-4303.	1.7	4
2236	Nitrogen doped nanohoops as promising CO ₂ capturing devices. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8607-8615.	1.3	7
2237	Expansion of the (BB) \cdots Ru metallacycle with coinage metal cations: formation of B \cdots M \cdots Ru \cdots B (M = Cu, Ag). <i>Journal of Physical Chemistry C</i> , 2018, 122, 3000-3003.	3.7	30
2238	Charge-transfer channel in quantum dot-graphene hybrid materials. <i>Nanotechnology</i> , 2018, 29, 145202.	1.3	8

#	ARTICLE	IF	CITATIONS
2257	Activation and diffusion of ammonia borane hydrogen on gold tetramers. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25567.	1.0	5
2258	A quantum chemistry study for 1-ethyl-3-Methylimidazolium ion liquids with aprotic heterocyclic anions applied to carbon dioxide absorption. <i>Fluid Phase Equilibria</i> , 2018, 459, 208-218.	1.4	8
2259	Cholinesterase-inhibitory effect and in silico analysis of alkaloids from bulbs of <i>Hieronymiella</i> species. <i>Phytomedicine</i> , 2018, 39, 66-74.	2.3	27
2260	Hydroxyl radical dominated degradation of aquatic sulfamethoxazole by FeO/bisulfite/O ₂ : Kinetics, mechanisms, and pathways. <i>Water Research</i> , 2018, 138, 323-332.	5.3	236
2261	A mechanism study on the hydrogen evolution reaction catalyzed by molybdenum disulfide complexes. <i>Chemical Communications</i> , 2018, 54, 1113-1116.	2.2	15
2262	A nanowire array with two types of bromoplumbate chains and high anisotropic conductance. <i>Dalton Transactions</i> , 2018, 47, 1023-1026.	1.6	15
2263	Synthesis, crystal structure and magnetic properties of diaquabis(2,6-diamino-7 <i>H</i> -purin-1-ium-1 <i>β</i> -N) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 502 Td (⁹)₂bis(4,4-oxydib) Structural Chemistry, 2018, 74, 37-44.	0.2	1
2264	Lanthanide metals in the boron cages: Computational prediction of M@B_{<i>n</i>} (M=Eu, Yb) Tj ETQq1 1,0.7843 14	1.0	13
2265	Evaluation of non-covalent interactions of chlorambucil (monomer and dimer) and its interaction with biological targets: Vibrational frequency shift, electron density topological and automated docking analysis. <i>Arabian Journal of Chemistry</i> , 2018, 11, 591-608.	2.3	3
2266	Comparison for f-hole and e-hole tetrel-bonded complexes involving F ₂ C CFTF ₃ (T C, Si, and Ge): Substitution, hybridization, and solvation effects. <i>Journal of Fluorine Chemistry</i> , 2018, 207, 38-44.	0.9	16
2267	Synthesis, Structure, and Cytotoxicity of a New Sulphonyl-bridged Thiadiazolyl-β-D-glucosaminide Conjugate: The Relevance of Sâ€¦â€¦â€¦N Interaction. <i>Chemistry - A European Journal</i> , 2018, 24, 3251-3262.	1.7	9
2268	Time dependent-density functional theory (TD-DFT) and experimental studies of UV-Visible spectra and cyclic voltammetry for Cu(II) complex with Et ₂ DTC. <i>Journal of Molecular Structure</i> , 2018, 1157, 463-468.	1.8	7
2269	Understanding and Measurement for the Binding Energy of Hydrogen bonds of Biomass-Derived Hydroxyl Compounds. <i>Journal of Physical Chemistry A</i> , 2018, 122, 843-848.	1.1	16
2270	Theoretical insights into the 1D charge transport properties in a series of hexaazatrinaphthylene-based discotic molecules. <i>Journal of Computational Chemistry</i> , 2018, 39, 773-779.	1.5	8
2271	The influence of the double-ring nanotubes diameter of Bn (n=14, 20, 24 and 32) on the electronic and structural properties due to lithium atom doping: quantum chemistry approach. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	0
2272	Molecular interactions in the complexes of toluene with butyronitrile: A DFT approach. <i>Journal of Molecular Structure</i> , 2018, 1157, 654-659.	1.8	8
2273	Understanding the thermodynamic and kinetic performances of the substituted phosphorus ylides as a new class of compounds in carbon dioxide activation. <i>Energy</i> , 2018, 145, 329-337.	4.5	6
2274	A theoretical guide for screening ionic liquid extractants applied in the separation of a binary alcohol-ester azeotrope through a DFT method. <i>Journal of Molecular Liquids</i> , 2018, 251, 51-60.	2.3	44

#	ARTICLE	IF	CITATIONS
2275	Crystal structure, magnetism, and luminescent properties of two isostructural pcu MOFs based on a triangular ligand. <i>Journal of Molecular Structure</i> , 2018, 1159, 5-9.	1.8	5
2276	Excited-state intramolecular proton transfer in non-fused five- and fused six-membered ring pyrrole-pyridine hydrogen bond systems. <i>Organic Electronics</i> , 2018, 54, 177-183.	1.4	32
2277	Synthesis and characterization of diruthenaborane analogues of pentaborane(11) and hexaborane(10). <i>Journal of Organometallic Chemistry</i> , 2018, 865, 29-36.	0.8	6
2278	Self-Attractive Hartree Decomposition: Partitioning Electron Density into Smooth Localized Fragments. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 92-103.	2.3	7
2279	Steric charge. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1408-1420.	1.3	35
2280	On the covalence in H ₂ AuX (X=I). <i>International Journal of Hydrogen Energy</i> , 2018, 43, 1709-1717.	3.8	6
2281	Electronic structure, spectral characteristics and physicochemical properties of linear, branched and cyclic alkyl group substituted 1-alkyl-3-butylimidazolium cation based ionic liquids. <i>Journal of Molecular Liquids</i> , 2018, 251, 394-406.	2.3	11
2282	Theoretical Study of Low Viscous Ionic Liquids at the Graphene Interface. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1645-1656.	1.5	15
2283	Periodic Trends in the Binding of a Phosphine-Ethered Ketone Ligand to Fe, Co, Ni, and Cu. <i>Chemistry - A European Journal</i> , 2018, 24, 5163-5172.	1.7	12
2284	Strategical Designing of Donor-Acceptor Based Organic Molecules for Tuning Their Linear Optical Properties. <i>Journal of Physical Chemistry A</i> , 2018, 122, 492-504.	1.1	17
2285	A Systematic DFT Study of Some Plausible Zn(II) and Al(III) Interaction Sites in N-Terminally Acetylated β -Synuclein. <i>Journal of Physical Chemistry A</i> , 2018, 122, 690-699.	1.1	9
2286	Molecular Recognition, Conformational Behavior, and Spectral Characteristics of Oxatub[4]arene Macrocyclic. <i>Journal of Physical Chemistry A</i> , 2018, 122, 714-723.	1.1	2
2287	Intermediates for Larger Endohedral Metallofullerenes: Theoretical Characterization of M@C ₄₄ Species. <i>Journal of Physical Chemistry C</i> , 2018, 122, 798-807.	1.5	8
2288	Cationic (λ^5 -C ₅ Me ₄ Rh ^{III}) Complexes with Metalated Aryl Phosphines Featuring λ^4 -Phosphorus plus Pseudo-Allylic Coordination. <i>Organometallics</i> , 2018, 37, 11-21.	1.1	10
2289	Low temperature X-ray structure analyses combined with NBO studies of a new heteroleptic octa-coordinated Holmium(III) complex with N,N,N-tridentate hydrazono-phthalazine-type ligand. <i>Journal of Molecular Structure</i> , 2018, 1157, 222-229.	1.8	5
2290	Nature and Value of Freely Dissolved EPS Ecosystem Services: Insight into Molecular Coupling Mechanisms for Regulating Metal Toxicity. <i>Environmental Science & Technology</i> , 2018, 52, 457-466.	4.6	77
2291	Theoretical Insights Into the Excited State Double Proton Transfer Mechanism of Deep Red Pigment Alkannin. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1200-1208.	1.1	159
2292	Fusing a Planar Group to a Bowl: Electronic and Molecular Structure, Aromaticity and Solid-State Packing of Naphthocorannulene and its Anions. <i>Chemistry - A European Journal</i> , 2018, 24, 3455-3463.	1.7	35

#	ARTICLE	IF	CITATIONS
2293	Theoretical study on benzoheterocycle based energetic materials, effect of heterocyclic-fused, conjugation, hydrogen bond, and substitutional group on the detonation performance. <i>Journal of Molecular Modeling</i> , 2018, 24, 40.	0.8	4
2294	Combined spectroscopic, molecular docking and quantum mechanics study of β^2 -casein and p-coumaric acid interactions following thermal treatment. <i>Food Chemistry</i> , 2018, 252, 163-170.	4.2	60
2295	Crystal lattice free volume in a study of initiation reactivity of nitramines: Friction sensitivity. <i>Defence Technology</i> , 2018, 14, 132-136.	2.1	7
2296	Cost-effective synthesis of carbazole/triphenylsilyl host materials with multiple π - π conjugation for blue phosphorescent organic light-emitting diodes. <i>Dyes and Pigments</i> , 2018, 151, 187-193.	2.0	10
2297	Solution conformations for the flexible 1-chloro-1,1-difluoro-2-pentanol unveiled using multinuclear magnetic resonance. <i>Tetrahedron</i> , 2018, 74, 880-883.	1.0	3
2298	Stereocontrol through Synergistic Catalysis in the Enantioselective α -Alkenylation of Aldehyde: A Computational Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 1304-1311.	1.7	1
2299	Excited State Properties of a Thermally Activated Delayed Fluorescence Molecule in Solid Phase Studied by Quantum Mechanics/Molecular Mechanics Method. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2358-2366.	1.5	68
2300	A theoretical study on La-activated bicyclo-oligomerization of acetylene to form naphthalene in gas phase using density functional theory (DFT). <i>Structural Chemistry</i> , 2018, 29, 171-178.	1.0	3
2301	Experimental and theoretical studies on the structural, spectroscopic and hydrogen bonding on 4-nitro- <i>n</i> -(2,4-dinitrophenyl) benzenamine. <i>Journal of Molecular Structure</i> , 2018, 1158, 139-144.	1.8	0
2302	Structural Evolution of $B_{20}Si_{10}N_{12}$ Clusters: Size-Selected Anion Photoelectron Spectroscopy and Theoretical Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2391-2401.	1.5	31
2303	Attraction or repulsion? Theoretical assessment of bulky alkyl groups by employing dispersion-corrected DFT. <i>RSC Advances</i> , 2018, 8, 2240-2247.	1.7	8
2304	Redox reactive (RNC) Cu_{II} species stabilized in the solid state via halogen bond with I_{20} . <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2018, 233, 371-377.	0.4	40
2305	Design and Assembly of Covalently Functionalised Polyoxofluorovanadate Molecular Hybrids. <i>Chemistry - A European Journal</i> , 2018, 24, 3836-3845.	1.7	9
2306	The influence of the negative hyperconjugation is relevant for the analysis of the π - π^* conjugation with the mono-substitution and di-substitution of $H_2C=$ by $O=$ and/or $HN=$ in trans-but-1,3-diene?. <i>Structural Chemistry</i> , 2018, 29, 847-857.	1.0	18
2307	Aerogen bonds formed between $AeOF_2$ ($Ae = Kr, Xe$) and diazines: comparisons between σ -hole and π -hole complexes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4676-4687.	1.3	36
2308	Strong C H/O interactions between polycyclic aromatic hydrocarbons and water: Influence of aromatic system size. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 80, 121-125.	1.3	10
2309	Central-metal effect on intramolecular vibrational energy transfer of $M(CO)_5Br$ ($M = Mn$). <i>Tj ETQq0 0 0 rgBT /Overlock 10 T</i> 3637-3647.	1.3	10
2310	The selective adsorption of formaldehyde and methanol over Al- or Si-decorated graphene oxide: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 80, 25-31.	1.3	49

#	ARTICLE	IF	CITATIONS
2311	Matrix-Infrared Spectra and Structures of HMâ€“SiH ₃ (M = Ge, Sn, Pb, Sb, Bi, Te Atoms). <i>Journal of Physical Chemistry A</i> , 2018, 122, 81-88.	1.1	7
2312	Base-Free Aerobic Oxidation of Alcohols over Copper-Based Complex under Ambient Condition. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 2362-2369.	3.2	26
2313	Theoretical investigations on the unsymmetrical effect of Î²-link Znâ€“porphyrin sensitizers on the performance for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3741-3751.	1.3	24
2314	Valence bonds in elongated boron clusters. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25575.	1.0	8
2315	Where Does the Density Localize in the Solid State? Divergent Behavior for Hybrids and DFT+U. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 670-683.	2.3	57
2316	Enantioselective Regiodivergent Synthesis of Chiral Pyrrolidines with Two Quaternary Stereocenters via Ligand-Controlled Copper(I)-Catalyzed Asymmetric 1,3-Dipolar Cycloadditions. <i>Journal of the American Chemical Society</i> , 2018, 140, 2272-2283.	6.6	108
2317	The effect of twisted Dâ€“Dâ€“Î“ configuration on electron transfer and photo-physics characteristics. <i>Molecular Physics</i> , 2018, 116, 1179-1191.	0.8	2
2318	Theoretical study on the charge transport in single crystals of TCNQ, F ₂ -TCNQ and F ₄ -TCNQ. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3784-3794.	1.3	27
2319	An investigation about the structures, thermodynamics and kinetics of the formic acid involved molecular clusters. <i>Chemical Physics</i> , 2018, 507, 44-50.	0.9	7
2320	Two heptacoordinated manganese(II) complexes of giant pentadentate s-triazine bis-Schiff base ligand: Synthesis, crystal structure, biological and DFT studies. <i>Inorganica Chimica Acta</i> , 2018, 479, 275-285.	1.2	21
2321	Electronic and structural properties of Li _n @Be ₂ B ₈ (n=14) and Li _n @Be ₂ B ₃₆ (n=21) nanoflakes shed light on possible anode materials for Li-based batteries. <i>Journal of Computational Chemistry</i> , 2018, 39, 1795-1805.	1.5	4
2322	Stimuli-responsive luminescent coumarin thiazole hybrid dye: Mechanism of excited-state intramolecular double proton transfer. <i>Journal of Luminescence</i> , 2018, 201, 189-195.	1.5	35
2323	Gravimetric, Electrochemical, Surface Morphology, DFT, and Monte Carlo Simulation Studies on Three N-Substituted 2-Aminopyridine Derivatives as Corrosion Inhibitors of Mild Steel in Acidic Medium. <i>Journal of Physical Chemistry C</i> , 2018, 122, 11870-11882.	1.5	85
2324	Highly Stable [C ₆₀ AuC ₆₀] ⁺ Dumbbells. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2703-2706.	2.1	10
2325	Theoretical study on the optical and electronic properties of graphene quantum dots doped with heteroatoms. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 15244-15252.	1.3	83
2326	Belamchinenin A, an unprecedented tricyclic-fused triterpenoid with cytotoxicity from <i>Belamcanda chinensis</i> . <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 3754-3759.	1.5	11
2327	Revealing Factors Influencing the Fluorine-Centered Non-Covalent Interactions in Some Fluorine-Substituted Molecular Complexes: Insights from First-Principles Studies. <i>ChemPhysChem</i> , 2018, 19, 1486-1499.	1.0	21
2328	An <i>ab initio</i> study on coinage atom-inserted cyanide/isocyanide: XMCN/XMNC (M = coinage) <i>TJ ETQq1 1 0.784314 rgBT /Overl</i>	1.7	2

#	ARTICLE	IF	CITATIONS
2329	Short-Lived Orthobenzynes Complexes with Early Transition Metals of Group IV. First Direct Characterization and Electronic Cartography by Coupling FVT/UVâ€PES with Calculations. European Journal of Inorganic Chemistry, 2018, 2018, 2717-2729.	1.0	4
2330	The possibility of iron chelation therapy in the presence of different HPOs; a molecular approach to the non-covalent interactions and binding energies. Journal of Molecular Structure, 2018, 1166, 448-455.	1.8	13
2331	DFT studies for three Cu(II) coordination polymers: Geometrical and electronic structures, g factors and UVâ€visible spectra. Chemical Physics, 2018, 508, 20-25.	0.9	12
2332	AlN and AlP doped graphene quantum dots as novel drug delivery systems for 5-fluorouracil drug: Theoretical studies. Journal of Fluorine Chemistry, 2018, 211, 81-93.	0.9	95
2333	Improvement of photovoltaic performances by optimizing ï€-conjugated bridge for the C217-based dyes: A theoretical perspective. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 360, 137-144.	2.0	2
2334	Structural and luminescent properties of a new 1D Cadmium(II) coordination polymer: A combined effort with experiment & theory. Journal of Molecular Structure, 2018, 1167, 187-193.	1.8	14
2335	An open library of relativistic core electron density function for the QTAIM analysis with pseudopotentials. Journal of Computational Chemistry, 2018, 39, 1697-1706.	1.5	9
2336	Red photo- and electroluminescent half-lantern cyclometalated dinuclear platinum(II) complex. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 795-802.	0.4	8
2337	Strong Preference of the Redox-Neutral Mechanism over the Redox Mechanism for the Ti^{IV} Catalysis Involved in the Carboamination of Alkyne with Alkene and Diazene. Chemistry - A European Journal, 2018, 24, 7010-7025.	1.7	12
2338	Synthesis, Spectra, and Theoretical Investigations of 1,3,5-Triazines Compounds as Ultraviolet Rays Absorber Based on Time-Dependent Density Functional Calculations and three-Dimensional Quantitative Structure-Property Relationship. Journal of Fluorescence, 2018, 28, 707-723.	1.3	11
2339	Co(III) complexes based on ï±-N-heterocyclic thiosemicarbazone ligands: DNA binding, DNA cleavage, and topoisomerase I/II inhibitory activity studies. Journal of Molecular Structure, 2018, 1167, 33-43.	1.8	22
2340	Conformational and electronic properties of hydroquinone adsorption on C60 fullerenes: Doping atom, solvent and basis set effects. Journal of Molecular Structure, 2018, 1167, 227-231.	1.8	18
2341	Theoretical investigation of M@Pb₁₂^{2âˆ-2} and M@Sn₁₂^{2âˆ-2} Zintl clusters (M = Lrⁿ⁺, Luⁿ⁺,) Tj ETQq0 0 0 rgBTJ/Overlock 10 Tf 50 20, 15253-15272.	1.3	13
2342	Maximum bonding fragment orbitals for deciphering complex chemical interactions. Physical Chemistry Chemical Physics, 2018, 20, 13792-13809.	1.3	14
2343	Efficient Absorption of CO₂ by Introduction of Intramolecular Hydrogen Bonding in Chiral Amino Acid Ionic Liquids. Energy & Fuels, 2018, 32, 6130-6135.	2.5	47
2344	Study on the mechanism of platinum(II)-catalyzed asymmetric ring-opening addition of oxabicyclic alkenes with arylboronic acids. Physical Chemistry Chemical Physics, 2018, 20, 14105-14116.	1.3	3
2345	Structural variation determined by length-matching effects: towards the formation of flexible porous molecular crystals. CrystEngComm, 2018, 20, 2648-2652.	1.3	0
2346	Fluorinated graphene as an anticancer nanocarrier: an experimental and DFT study. Journal of Materials Chemistry B, 2018, 6, 2769-2777.	2.9	38

#	ARTICLE	IF	CITATIONS
2347	Systematic Experimental and Computational Studies of Substitution and Hybridization Effects in Solid-State Halogen Bonded Assemblies. <i>Crystal Growth and Design</i> , 2018, 18, 3244-3254.	1.4	20
2348	Role of Carbonaceous Aerosols in Catalyzing Sulfate Formation. <i>ACS Catalysis</i> , 2018, 8, 3825-3832.	5.5	59
2349	Theoretical design of new small molecules with a low band-gap for organic solar cell applications: DFT and TD-DFT study. <i>Computational Materials Science</i> , 2018, 150, 54-61.	1.4	41
2350	Mechanochemical formation of chlorinated phenoxy radicals and their roles in the remediation of hexachlorobenzene contaminated soil. <i>Journal of Hazardous Materials</i> , 2018, 352, 172-181.	6.5	40
2351	Tuning the BODIPY core for its potential use in DSSC: a quantum chemical approach. <i>Bulletin of Materials Science</i> , 2018, 41, 1.	0.8	19
2352	The effect of benzoannulation on intermolecular hydrogen bond and proton transfer of 2-methyl-3-hydroxy-1H-quinolone in methanol: A TD-DFT study. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3803.	1.0	5
2353	Delocalization of frontier orbitals induced red emission for heptazine based thermally activated delayed fluorescence molecule: First-principles study. <i>Chemical Physics Letters</i> , 2018, 698, 187-194.	1.2	6
2354	Ambient Degradation of Perylene Diimide-Based Organic Transistors: Hidden Role of Ozone and External Electric Field. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7067-7074.	1.5	2
2355	Investigation of rotameric conformations of substituted imidazo-[1,2-a]pyrazine: experimental and theoretical approaches. <i>RSC Advances</i> , 2018, 8, 9707-9717.	1.7	4
2356	Implicit and explicit host effects on excitons in pentacene derivatives. <i>Journal of Chemical Physics</i> , 2018, 148, 104108.	1.2	12
2357	Unexpected solvent effects on the UV/Vis absorption spectra of o-cresol in toluene and benzene: in contrast with non-aromatic solvents. <i>Royal Society Open Science</i> , 2018, 5, 171928.	1.1	16
2358	Comment on "Synthesis and characterization of the pentazolite anion cyclo-N ₅ ⁻ in (N ₅) ₆ (H ₃ O) ₃ (NH ₄) ₄ Cl· Science, 2018, 359, .	6.0	15
2359	One pot synthesis of two Mn(II) perchlorate complexes with s-triazine NNN-pincer ligand; molecular structure, Hirshfeld analysis and DFT studies. <i>Journal of Molecular Structure</i> , 2018, 1164, 344-353.	1.8	23
2360	The [4+4] thermocyclization of 9-anthraldehyde: synthesis, crystal structure, experimental and theoretical UV spectra, natural bonding orbital analysis and prediction of third-order nonlinear optical properties. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 480-486.	0.2	0
2361	Structure and Bonding in CE ₅ ⁺ (E=Al ⁺ Tl) Clusters: Planar Tetracoordinate Carbon versus Pentacoordinate Carbon. <i>Chemistry - an Asian Journal</i> , 2018, 13, 1467-1473.	1.7	30
2362	Comparing the substituent effects about ESIPT process for HBO derivatives. <i>Computational and Theoretical Chemistry</i> , 2018, 1131, 51-56.	1.1	10
2363	Theoretical screening and design of SM315-based porphyrin dyes for highly efficient dye-sensitized solar cells with near-IR light harvesting. <i>Dyes and Pigments</i> , 2018, 155, 292-299.	2.0	41
2364	Dielectron Clathrate Hydrates with Unique Superexchange Spin Couplings. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7635-7641.	1.5	4

#	ARTICLE	IF	CITATIONS
2365	Mechanism of Charged, Neutral, Mono-, and Polyatomic Donor Ligand Coordination to Perchlorinated Cyclohexasilane ($\text{Si}_6\text{Cl}_{12}$). <i>Journal of Physical Chemistry A</i> , 2018, 122, 4067-4075.	1.1	6
2366	Insight into selectivity: uptake studies of radionuclides $^{90}\text{Sr}^{2+}$, $^{137}\text{Cs}^{+}$, and $^{233}\text{UO}_2^{2+}$ with bis-amidoxime polymers. <i>Dalton Transactions</i> , 2018, 47, 5348-5358.	1.6	5
2367	Chiral polymorphism in the self-assemblies of achiral molecules induced by multiple hydrogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11160-11173.	1.3	9
2368	Comparative conformational studies of 3,4,6-tri-O-acetyl-1,5-anhydro-2-deoxyhex-1-enitols at the DFT level. <i>Carbohydrate Research</i> , 2018, 462, 13-27.	1.1	23
2369	Noncovalent Interactions Descriptor Based on the Source Function of Individual Localized Molecular Orbitals in Whole Space. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3850-3857.	1.1	2
2370	Using machine learning and quantum chemistry descriptors to predict the toxicity of ionic liquids. <i>Journal of Hazardous Materials</i> , 2018, 352, 17-26.	6.5	76
2371	Solvent effects on excited state intramolecular proton transfer mechanism in 4-(N,N-dimethylamino)-3-hydroxyflavone. <i>Organic Electronics</i> , 2018, 57, 292-297.	1.4	21
2372	Theoretical studies on the synergistic extraction of Am^{3+} and Eu^{3+} with CMPO HDEHP and CMPO HEH[EHP] systems. <i>Dalton Transactions</i> , 2018, 47, 5474-5482.	1.6	23
2373	Combining first-principles and data modeling for the accurate prediction of the refractive index of organic polymers. <i>Journal of Chemical Physics</i> , 2018, 148, 241712.	1.2	33
2374	Hydrogen-bonding interactions between 1-butyl-2,3-dimethylimidazolium tetrafluoroborate and dimethyl sulphoxide. <i>Journal of Molecular Structure</i> , 2018, 1164, 70-76.	1.8	17
2375	Electron-Transfer-Enhanced Cation Cation Interactions in Homo- and Heterobimetallic Actinide Complexes: A Relativistic Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2018, 57, 3893-3902.	1.9	7
2376	A joint QM/MD study on $\hat{1}^{\pm}$, $\hat{1}^2$ - and $\hat{1}^3$ -cyclodextrins in selective complexation with cathinone. <i>Supramolecular Chemistry</i> , 2018, 30, 687-696.	1.5	13
2377	Dependence of UV Visible Absorption Characteristics on the Migration Distance and the Hyperconjugation Effect of a Methine Chain. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7831-7837.	1.5	16
2378	Intramolecular hydrogen bond directed stable conformations of benzoyl phenyl oxalamides: unambiguous evidence from extensive NMR studies and DFT-based computations. <i>RSC Advances</i> , 2018, 8, 11230-11240.	1.7	18
2379	Porous Anionic Uranyl Organic Networks for Highly Efficient Cs^{+} Adsorption and Investigation of the Mechanism. <i>Inorganic Chemistry</i> , 2018, 57, 4419-4426.	1.9	70
2380	Intermolecular interactions between π - and σ -holes of bromopentafluorobenzene and pyridine: computational and experimental investigations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11386-11395.	1.3	15
2381	Intermolecular interactions and molecular docking investigations on 4-methoxybenzaldehyde. <i>Computational Materials Science</i> , 2018, 149, 291-300.	1.4	63
2382	Theoretical studies on the potentials of some nanocages ($\text{Al}_{12}\text{N}_{12}$, $\text{Al}_{12}\text{P}_{12}$, $\text{B}_{12}\text{N}_{12}$, $\text{Be}_{12}\text{O}_{12}$, $\text{C}_{12}\text{Si}_{12}$,) <i>Tj ETQq1 1 0.784314 rgB</i> of Molecular Liquids, 2018, 260, 138-148.	2.3	58

#	ARTICLE	IF	CITATIONS
2383	Excited-state intramolecular proton transfer mechanism for 2-(quinolin-2-yl)-3-hydroxychromone: A detailed time-dependent density functional theory study. <i>Journal of Molecular Liquids</i> , 2018, 260, 447-457.	2.3	25
2384	The potential role of malonic acid in the atmospheric sulfuric acid - Ammonia clusters formation. <i>Chemosphere</i> , 2018, 203, 26-33.	4.2	39
2385	Hydride donating abilities of the tetracoordinated boron hydrides. <i>Journal of Organometallic Chemistry</i> , 2018, 865, 247-256.	0.8	18
2386	Quantum-Chemical Simulation of the Solvent Effect on Spontaneous Emission of Singlet Oxygen. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2018, 124, 32-42.	0.2	2
2387	3D-QSAR study of steroidal and azaheterocyclic human aromatase inhibitors using quantitative profile of protein-ligand interactions. <i>Journal of Cheminformatics</i> , 2018, 10, 2.	2.8	14
2388	Theoretical investigation on the effect of fluorine and carboxylate substitutions on the performance of benzodithiophene-diketopyrrolopyrrole-based polymer solar cells. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	3
2389	Hydrogen storage property of alkali and alkaline-earth metal atoms decorated C ₂₄ fullerene: A DFT study. <i>Chemical Physics</i> , 2018, 505, 26-33.	0.9	81
2390	Microwave spectroscopy of 2-(trifluoromethyl)pyridine-water complex: Molecular structure and hydrogen bond. <i>Journal of Chemical Physics</i> , 2018, 148, 044306.	1.2	9
2391	Theoretical insight into phosphoric acid-catalyzed asymmetric conjugate addition of indolizines to α,β -unsaturated ketones. <i>Chinese Chemical Letters</i> , 2018, 29, 1237-1241.	4.8	26
2392	Unravelling the nature of binding of cubane and substituted cubanes within cucurbiturils: A DFT and NCI study. <i>Journal of Molecular Liquids</i> , 2018, 260, 18-29.	2.3	52
2393	DFT and TD-DFT study of the adsorption and detection of sulfur mustard chemical warfare agent by the C ₂₄ , C ₁₂ Si ₁₂ , Al ₁₂ N ₁₂ , Al ₁₂ P ₁₂ , Be ₁₂ O ₁₂ , B ₁₂ N ₁₂ and Mg ₁₂ O ₁₂ nanocages. <i>Journal of Molecular Structure</i> , 2018, 1164, 227-238.	1.8	52
2394	Theoretical Investigation on Ni-Catalyzed C(sp ³)-F Activation and Ring Contraction of Tetrahydropyrans: Exploration of an S _N 2 Pathway. <i>Organometallics</i> , 2018, 37, 1114-1122.	1.1	8
2395	Theoretical design and prediction of properties for dinitromethyl, fluorodinitromethyl, and (difluoroamino)dinitromethyl derivatives of triazole and tetrazole. <i>RSC Advances</i> , 2018, 8, 10215-10227.	1.7	27
2396	Narrow bandgap non-fullerene acceptor based on a thiophene-fused benzothiadiazole unit with a high short-circuit current density of over 20 mA cm ⁻² . <i>Journal of Materials Chemistry A</i> , 2018, 6, 6393-6401.	5.2	59
2397	O ₂ adsorbed on Pt _n clusters: Structure and optical absorption. <i>AIP Advances</i> , 2018, 8, 035307.	0.6	4
2398	Functionalized carbon black nanoparticles used for separation of emulsified oil from oily wastewater. <i>Journal of Dispersion Science and Technology</i> , 2018, 39, 497-506.	1.3	30
2399	Electron velocity map imaging and theoretical study on CuXH (X = O and S) anions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 188, 85-89.	2.0	6
2400	Photoexcitation effect on the adsorption of hazardous gases on silica surface. <i>Journal of Hazardous Materials</i> , 2018, 341, 93-101.	6.5	36

#	ARTICLE	IF	CITATIONS
2401	The hydrogen-bonded complexes of the 5-fluorouracil with the DNA purine bases: a comprehensive quantum chemical study. <i>Structural Chemistry</i> , 2018, 29, 69-80.	1.0	3
2402	Formation and estimated toxicity of trihalomethanes, haloacetonitriles, and haloacetamides from the chlor(am)ination of acetaminophen. <i>Journal of Hazardous Materials</i> , 2018, 341, 112-119.	6.5	84
2403	The excited-state intramolecular proton transfer in N H-type dye molecules with a seven-membered-ring intramolecular hydrogen bond: A theoretical insight. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 421-426.	2.0	8
2404	Synthesis and structure analysis of ferrocene-containing pseudopeptides. <i>Peptide Science</i> , 2018, 110, e23072.	1.0	7
2405	DFT study on the selective complexation of B ₁₂ N ₁₂ nanocage with alkali metal ions. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2018, 193, 178-184.	0.8	16
2406	Cl ^{δ-} as the halogen bond acceptor: studies on strong halogen bonds. <i>Structural Chemistry</i> , 2018, 29, 503-511.	1.0	1
2407	Spectroscopic investigations using density functional theory on 2-methoxy-4(phenyliminomethyl)phenol: A non linear optical material. <i>Journal of Molecular Structure</i> , 2018, 1155, 249-259.	1.8	5
2408	Optical backbone-sidechain charge transfer transitions in proteins sensitive to secondary structure and modifications. <i>Faraday Discussions</i> , 2018, 207, 115-135.	1.6	17
2409	Adsorption modes of molecular iodine on defected boron nitrides: A DFT study. <i>Applied Surface Science</i> , 2018, 434, 604-612.	3.1	16
2410	Structures and nonlinear optical properties of alkali atom/superalkali doped pyridinic vacancy graphene. <i>Optik</i> , 2018, 154, 411-420.	1.4	10
2411	Molecular structure, electronic properties, and charge transfer analysis of clopenthixol as a nano-drug with quantum chemical calculations. <i>Canadian Journal of Physics</i> , 2018, 96, 312-327.	0.4	6
2412	Molecular acidity: An accurate description with information-theoretic approach in density functional reactivity theory. <i>Journal of Computational Chemistry</i> , 2018, 39, 117-129.	1.5	67
2413	Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative. <i>Journal of Molecular Structure</i> , 2018, 1155, 184-195.	1.8	16
2414	Insight into the σ -hole electrons tetrel bonds between F ₂ ZO (Z = C, Si, Ge) and unsaturated hydrocarbons. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25521.	1.0	13
2415	Comparison of Various Means of Evaluating Molecular Electrostatic Potentials for Noncovalent Interactions. <i>Journal of Computational Chemistry</i> , 2018, 39, 500-510.	1.5	27
2416	New theoretically predicted RDX and HMX based high energy density molecules. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25528.	1.0	16
2417	Cd(II) and Ni(II) complexes from aroyl hydrazones: Unravelling the intermolecular interactions and electronic, crystal structures through experimental and theoretical studies. <i>Inorganica Chimica Acta</i> , 2018, 469, 264-279.	1.2	23
2418	Determination of pKa and the corresponding structures of quinclorac using combined experimental and theoretical approaches. <i>Journal of Molecular Structure</i> , 2018, 1152, 53-60.	1.8	11

#	ARTICLE	IF	CITATIONS
2419	Environment-dependent conformation investigation of 3-amino-1,2,4-triazole (3-AT): Raman Spectroscopy and density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 478-485.	2.0	15
2420	Theoretical investigation of twisted charge-transfer-promoted intramolecular proton transfer in the excited state of 4- β -dimethylaminoflavonol in a highly polar solvent. <i>Journal of Luminescence</i> , 2018, 194, 785-790.	1.5	41
2421	The molecular structure of 5-X-isatines where (X = F, Cl, and Br) determined by gas-phase electron diffraction with theoretical calculations. <i>Journal of Molecular Structure</i> , 2018, 1152, 361-367.	1.8	4
2422	Synthesis, photophysical properties, and computational studies of four-coordinate copper(I) complexes based on benzimidazolylidene N-heterocyclic carbene (NHC) ligands bearing aryl substituents. <i>Journal of Molecular Structure</i> , 2018, 1153, 12-19.	1.8	15
2423	Synergistic effect of fluorinated hexane as diluent of fluorinated octanol for salicylic acid extraction. <i>Journal of Industrial and Engineering Chemistry</i> , 2018, 58, 311-318.	2.9	0
2424	The effect of the hydrogen fluoride chain on the aromaticity of C ₆ H ₆ in the C ₆ H ₆ ·(HF) _n complexes. <i>Molecular Physics</i> , 2018, 116, 313-322.	0.8	1
2425	Mechanistic and kinetic study on the catalytic hydrolysis of COS in small clusters of sulfuric acid. <i>Environmental Pollution</i> , 2018, 232, 615-623.	3.7	26
2426	Adsorption orientation effects of porphyrin dyes on the performance of DSSC: Comparison of benzoic acid and tropolone anchoring groups binding onto the TiO ₂ anatase (101) surface. <i>Applied Surface Science</i> , 2018, 433, 1137-1147.	3.1	20
2427	Crystal structure and bio-catalytic potential of oxovanadium(IV) Schiff base complexes derived from 2-hydroxy-4-(prop-2-yn-1-yloxy)benzaldehyde and alicyclic/aromatic diamines. <i>Inorganica Chimica Acta</i> , 2018, 469, 503-514.	1.2	14
2428	DFT calculations for anharmonic force field and spectroscopic constants of YC ₂ and its ¹³ C isotopologues. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 191, 382-388.	2.0	8
2429	Solvent extraction of americium(III) and europium(III) with 2,6-bis(5,6-diethyl-1,2,4-triazin-3-yl) pyridine in ionic liquids: Experimental study and molecular dynamics simulation. <i>Separation and Purification Technology</i> , 2018, 192, 302-308.	3.9	25
2430	Mn ²⁺ promoted Cr(VI) reduction with oxalic acid: The indispensable role of In-situ generated Mn ³⁺ . <i>Journal of Hazardous Materials</i> , 2018, 343, 356-363.	6.5	57
2431	Spectral analysis and quantum chemical studies of chair and twist-boat conformers of cycloheximide in gas and solution phases. <i>Journal of Molecular Structure</i> , 2018, 1154, 428-436.	1.8	2
2432	Asymmetrical semisphere nanopores on monolayer graphene for gas permeation. <i>Journal of Materials Science</i> , 2018, 53, 1962-1977.	1.7	3
2433	Experimental and theoretical analysis of a rare nitrato bridged 3d-4f complex containing LaZn ₂ core synthesized from a Zn(II) metalloligand. <i>Journal of Molecular Structure</i> , 2018, 1153, 85-95.	1.8	8
2434	Understanding of the conformational flexibility and electrostatic properties of coumarin derivatives in the active site of <i>S. cerevisiae</i> β -glucosidase. <i>Medicinal Chemistry Research</i> , 2018, 27, 607-617.	1.1	1
2435	The keto-enol equilibrium and thermal conversion kinetics of 2- and 4-hydroxyacetophenone in the gas phase: a DFT study. <i>Molecular Physics</i> , 2018, 116, 194-203.	0.8	2
2436	N ₂ O + CO reaction over single Ga or Ge atom embedded graphene: A DFT study. <i>Surface Science</i> , 2018, 667, 105-111.	0.8	12

#	ARTICLE	IF	CITATIONS
2437	Rational Design and Synthesis of Unsaturated Seâ€Containing Osmacycles with Ĩfâ€Aromaticity. Chemistry - A European Journal, 2018, 24, 2389-2395.	1.7	35
2438	Exploring hydride-Ĩ interactions and their tuning by Ĩf-hole bonds: an ab initio study. Molecular Physics, 2018, 116, 118-128.	0.8	1
2439	Fe-doped graphene nanosheet as an adsorption platform of harmful gas molecules (CO, CO ₂ , SO ₂ and Tj ETQq0 0.0 rgBT /Overlock 10	3.1	180
2440	Experimental and theoretical insight into the cooperativity effect in composite wax powder and ternary complex of coronene with CH₄ and Mⁿ⁺ (Mⁿ⁺ =) Tj ETQq1 1 0.784314 rgBT /Overlock 1	0.8	5
2441	Intermolecular vibrational modes and H-bond interactions in crystalline urea investigated by terahertz spectroscopy and theoretical calculation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 189, 528-534.	2.0	25
2442	Synthesis and properties of novel heat-resistant fluorescent conjugated polymers with bisindolylmaleimide. Chinese Chemical Letters, 2018, 29, 513-516.	4.8	2
2443	Synthesis, X-ray structure and topology (AIM and Hirshfeld) analyses of the new square planar [Ag(pyridine-2-aldoxime) 2]ClO 4 complex; A comparative study with its nitrate analogue. Journal of Molecular Structure, 2018, 1151, 204-217.	1.8	6
2444	Influence of vibronic contribution on light harvesting efficiency of NKX-2587 derivatives with oligothiophene as Ĩ-conjugated linker. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 189, 454-462.	2.0	3
2445	Comparison for Ĩf-hole and Ĩ-hole tetrel-bonded complexes involving cyanoacetaldehyde. Molecular Physics, 2018, 116, 222-230.	0.8	22
2446	Screening benzylpentazoles for replacing PhN5 as cyclo-N5 â” precursor by theoretical calculation. Structural Chemistry, 2018, 29, 267-274.	1.0	7
2447	A series of bowl-shaped PDI dimers designed for organic photovoltaic cells through engineering N-annulated bridge towards potential alternatives of PDI bridged dimer acceptors. Dyes and Pigments, 2018, 148, 394-404.	2.0	17
2448	Application of calculated NMR parameters, aromaticity indices and wavefunction properties for evaluation of corrosion inhibition efficiency of pyrazine inhibitors. Journal of Molecular Structure, 2018, 1151, 34-40.	1.8	11
2449	New insights into the chlorination of sulfonamide: Smiles-type rearrangement, desulfation, and product toxicity. Chemical Engineering Journal, 2018, 331, 785-793.	6.6	37
2450	Reactions involving some gas molecules through sequestration on Al₁₂Be cluster: An electron density based study. Journal of Computational Chemistry, 2018, 39, 535-545.	1.5	5
2451	Hostâ€guest interactions between octa acid and cations/nucleobases. Journal of Computational Chemistry, 2018, 39, 161-175.	1.5	12
2452	Understanding the anchoring effect of Graphene, BN, C2N and C3N4 monolayers for lithiumâ” polysulfides in Liâ”S batteries. Applied Surface Science, 2018, 434, 596-603.	3.1	78
2453	On the properties and structure of 2-hydroxyethylammonium formate ionic liquid. Journal of Molecular Liquids, 2018, 249, 233-244.	2.3	28
2454	A catalyst-free achieving of N-doped carbon nanotubes: The healing of single-vacancy defects by NO molecule. Chemical Physics Letters, 2018, 691, 172-177.	1.2	4

#	ARTICLE	IF	CITATIONS
2455	Benzimidazobenzothiazole-based highly-efficient thermally activated delayed fluorescence emitters for organic light-emitting diodes: A quantum-chemical TD-DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 192, 297-303.	2.0	5
2456	The role of the π -holes in stability of non-bonded chalcogenide π -benzene interactions: the ground and excited states. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 299-306.	1.3	10
2457	Raman spectra of thiolated arsenicals with biological importance. <i>Talanta</i> , 2018, 179, 520-530.	2.9	9
2458	(Rg π = π He π ¼ Rn, $\langle i \rangle n \langle /i \rangle \pi$ = π 1 π “4): In quest of the potential trapping ability of the aromatic ring. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25530.	1.0	8
2459	Reactivity of the coumarine derivative towards cartilage proteins: combined NBO, QTAIM, and molecular docking study. <i>Monatshefte für Chemie</i> , 2018, 149, 159-166.	0.9	8
2460	B(C6F5)3 Promotes the catalytic activation of [N,S]-ferrocenyl nickel complexes in ethylene oligomerization. <i>Applied Catalysis A: General</i> , 2018, 550, 228-235.	2.2	8
2461	Thermodynamics of aqueous perfluorooctanoic acid (PFOA) and 4,8-dioxo-3H-perfluorononanoic acid (DONA) from DFT calculations: Insights into degradation initiation. <i>Chemosphere</i> , 2018, 193, 1063-1070.	4.2	20
2462	π -N chalcogen bonded complexes of carbon disulfide with diazines. Theoretical study. <i>Chemical Physics</i> , 2018, 500, 37-44.	0.9	12
2463	Effect of mono-vacant defects on the opto-electronic properties of ionic liquid functionalized hexagonal boron-nitride nanosheets. <i>Journal of Molecular Liquids</i> , 2018, 249, 1172-1182.	2.3	17
2464	Application of terahertz spectroscopy and theoretical calculation in dimethylurea isomers investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 192, 336-342.	2.0	8
2465	Stable NCNgNSi (Ng=Kr, Xe, Rn) Compounds with Covalently Bound C π Ng π N Unit: Possible Isomerization of NCNSi through the Release of the Noble Gas Atom. <i>Chemistry - A European Journal</i> , 2018, 24, 2879-2887.	1.7	20
2466	The π - π Tetrel Bond and its Influence on Hydrogen Bonding and Proton Transfer. <i>ChemPhysChem</i> , 2018, 19, 736-743.	1.0	46
2467	Do surfaces of positive electrostatic potential on different halogen derivatives in molecules attract? like attracting like!. <i>Journal of Computational Chemistry</i> , 2018, 39, 343-350.	1.5	33
2468	Experimental and spin-orbit coupled TDDFT predictions of photophysical properties of three-coordinate mononuclear and four-coordinate binuclear copper(I) complexes with thioamidines and bulky triarylphosphanes. <i>Inorganica Chimica Acta</i> , 2018, 471, 680-690.	1.2	5
2469	On lithium doping in two stable nano-flakes of the B24: The double-ring versus the quasiplanar configuration. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 79, 213-222.	1.3	0
2470	Intramolecular HB Interactions Evidenced in Dibenzoyl Oxalamide Derivatives: NMR, QTAIM, and NCI Studies. <i>Journal of Physical Chemistry A</i> , 2018, 122, 199-208.	1.1	15
2471	Noble gas encapsulated B ₄₀ cage. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1953-1963.	1.3	41
2472	Impact of position and number of nitrogen atom substitution on the curvature and hydrogen adsorption properties of metallized borophene. <i>Journal of Materials Science</i> , 2018, 53, 4540-4553.	1.7	11

#	ARTICLE	IF	CITATIONS
2473	Blue-to-green electrophosphorescence from iridium(III) complexes with cyclometalated pyrimidine ligands. <i>Dyes and Pigments</i> , 2018, 150, 284-292.	2.0	20
2474	Distinct interface behaviors of Ni(II) on graphene oxide and oxidized carbon nanotubes triggered by different topological aggregations. <i>Nanoscale</i> , 2018, 10, 1383-1393.	2.8	20
2475	Decorating Zintl polyanions with alkali metal cations: A novel strategy to design superatom cations with low electron affinity. <i>Journal of Alloys and Compounds</i> , 2018, 740, 400-405.	2.8	19
2476	Electronic properties of DNA: Description of weak interactions in TATA-box-like chains. <i>Biophysical Chemistry</i> , 2018, 233, 26-35.	1.5	3
2477	Insight into the new excited-state intramolecular proton transfer (ESIPT) mechanism of N,N'-bis(salicylidene)-p-phenylenediamine (p-BSP). <i>Chemical Physics</i> , 2018, 501, 53-59.	0.9	16
2478	Interaction of Elemental Mercury with a Diverse Series of π -Organic Substrates Probed by Computational Methods: Is Mercury Fixation Possible?. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 451-461.	1.2	5
2479	Structure, aromaticity and reactivity of corannulene and its analogues: a conceptual density functional theory and density functional reactivity theory study. <i>Molecular Physics</i> , 2018, 116, 956-968.	0.8	18
2480	DFT calculations of the defect structures, electronic structures, and EPR parameters for three Rh^{2+} centers in $AgCl$. <i>Magnetic Resonance in Chemistry</i> , 2018, 56, 196-209.	1.1	3
2481	Anionic tetrel bonds: An ab initio study. <i>Chemical Physics Letters</i> , 2018, 691, 394-400.	1.2	31
2482	Does gold cluster promote or scavenge radicals? A controversy at DFT. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3776.	0.9	3
2483	Bonding of Butylparaben, Bis(2-ethylhexyl)-phthalate, and Perfluorooctanesulfonic Acid to DNA: Comparison with Benzo[a]pyrene Shows Low Probability for Strong Noncovalent DNA Intercalation. <i>Chemical Research in Toxicology</i> , 2018, 31, 22-36.	1.7	3
2484	Uncovering the impact of β -capsule TM shaped amine-type ligands on Am(III)/Eu(III) separation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1030-1038.	1.3	24
2485	The strengthening effect of a halogen, chalcogen or pnictogen bonding on halogen- π interaction: a comparative ab initio study. <i>Molecular Physics</i> , 2018, 116, 526-535.	0.8	6
2486	Modification on C217 by auxiliary acceptor toward efficient sensitiser for dye-sensitised solar cells: a theoretical study. <i>Molecular Physics</i> , 2018, 116, 536-545.	0.8	6
2487	Trade-Off Hidden in Condensed State Solvation: Multiradiative Channels Design for Highly Efficient Solution-Processed Purely Organic Electroluminescence at High Brightness. <i>Advanced Functional Materials</i> , 2018, 28, 1704927.	7.8	105
2488	N-doped cycloparaphenylenes: Tuning electronic properties for applications in thermally activated delayed fluorescence. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25562.	1.0	9
2489	Isolation of strawberry anthocyanins using high-speed counter-current chromatography and the copigmentation with catechin or epicatechin by high pressure processing. <i>Food Chemistry</i> , 2018, 247, 81-88.	4.2	30
2490	Low coordinated mononuclear erbium(III) single-molecule magnets with C_{3v} symmetry: a method for altering single-molecule magnet properties by incorporating hard and soft donors. <i>Dalton Transactions</i> , 2018, 47, 302-305.	1.6	40

#	ARTICLE	IF	CITATIONS
2491	Computational Kinetic Modeling of the Catalytic Cycle of Glutathione Peroxidase Nanomimic: Effect of Nucleophilicity of Thiols on the Catalytic Activity. <i>Journal of Physical Chemistry A</i> , 2018, 122, 364-374.	1.1	9
2492	ForceGen: atomic covalent bond value derivation for Gromacs. <i>Journal of Molecular Modeling</i> , 2018, 24, 5.	0.8	13
2493	Zeolite-Y entrapped metallo-pyrazolone complexes as heterogeneous catalysts: Synthesis, catalytic aptitude and computational investigation. <i>Microporous and Mesoporous Materials</i> , 2018, 261, 275-285.	2.2	12
2494	Confinement induced thermodynamic and kinetic facilitation of some Diels-Alder reactions inside a CB[7] cavitand. <i>Journal of Computational Chemistry</i> , 2018, 39, 151-160.	1.5	34
2495	Theoretical confirmation of existence of X ⁻ Au non-covalent contacts. <i>Inorganica Chimica Acta</i> , 2018, 471, 126-129.	1.2	14
2496	Molecular docking, vibrational, structural, electronic and optical studies of {4-(2,6)-dichlorophenyl amino 2-methylidene 4-oxobutanoic acid and 4-(2,5)-dichlorophenyl amino 2-methylidene 4-oxobutanoic acid} A comparative study. <i>Journal of Molecular Structure</i> , 2018, 1155, 21-38.	1.8	6
2497	Exploring more effective polymer donors for the famous non-fullerene acceptor ITIC in organic solar cells by increasing electron-withdrawing ability. <i>Organic Electronics</i> , 2018, 53, 308-314.	1.4	27
2498	A combinational molecular design to achieve highly efficient deep-blue electrofluorescence. <i>Journal of Materials Chemistry C</i> , 2018, 6, 745-753.	2.7	45
2499	Mechanism and Origin of the Stereoselectivity in the Palladium-Catalyzed <i>trans</i> Hydroboration of Internal 1,3-Enynes with an Azaborine-Based Phosphine Ligand. <i>Chemistry - A European Journal</i> , 2018, 24, 178-186.	1.7	35
2500	1D Chains of Diruthenium Tetracarbonyl Sawhorse Complexes. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 54-61.	1.0	4
2501	Ion-pair recognition based on halogen bonding: a case of the crown-ether receptor with iodo-triazole moiety. <i>Structural Chemistry</i> , 2018, 29, 533-540.	1.0	7
2502	Hydrogen bonding interaction of ascorbic acid with nicotinamide: Experimental and theoretical study. <i>Journal of Molecular Liquids</i> , 2018, 249, 9-15.	2.3	16
2503	Theoretical study of the CO, NO, and N ₂ adsorptions on Li-decorated graphene and boron-doped graphene. <i>Canadian Journal of Chemistry</i> , 2018, 96, 30-39.	0.6	6
2504	Evaluation of DNA binding and DNA cleavage of nickel(II) complexes with tridentate $\hat{\pm}$ -N-heterocyclic thiosemicarbazones ligands. <i>Inorganica Chimica Acta</i> , 2018, 471, 194-202.	1.2	25
2505	Theoretical Probing of Weak Anion-Cation Interactions in Certain Pyridinium-Based Ionic Liquid Ion Pairs and the Application of Molecular Electrostatic Potential in Their Ionic Crystal Density Determination: A Comparative Study Using Density Functional Approach. <i>Journal of Physical Chemistry A</i> , 2018, 122, 328-340.	1.1	26
2506	Design of zinc porphyrin- <i>perylene</i> diimide donor-bridge-acceptor chromophores for large second-order nonlinear optical response: A theoretical exploration. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25536.	1.0	10
2507	Quantum chemical analysis of electronic structure and bonding aspects of choline based ionic liquids. <i>Journal of Molecular Liquids</i> , 2018, 249, 637-649.	2.3	19
2508	Adsorption, intercalation and sensing of helium on yttrium functionalized open edge boron nitride: A first principle DFT and TDDFT study. <i>Chemical Physics Letters</i> , 2018, 691, 231-237.	1.2	13

#	ARTICLE	IF	CITATIONS
2509	Mechanistic study on the Rh(III)-catalyzed synthesis of indolines via selective O-atom transfer of aryl nitrones: Origins of the regioselectivity and the improved yield with pivalic acid additive. <i>Journal of Organometallic Chemistry</i> , 2018, 854, 15-26.	0.8	7
2510	Sky-blue thermally activated delayed fluorescence material employing a diphenylethyne acceptor for organic light-emitting diodes. <i>Journal of Materials Chemistry C</i> , 2018, 6, 36-42.	2.7	23
2511	A nanoscopic approach on benzene-toluene-xylenes extraction by sulfolane. <i>Journal of Molecular Liquids</i> , 2018, 249, 1039-1046.	2.3	8
2512	The triel bond: a potential force for tuning anion-π interactions. <i>Molecular Physics</i> , 2018, 116, 388-398.	0.8	26
2513	Silicon carbide nanotubes (SiCNTs) serving for catalytic decomposition of toxic diazomethane (DAZM) gas: a DFT study. <i>Molecular Physics</i> , 2018, 116, 414-422.	0.8	3
2514	Electronic structures of Al ₈ Si ₄ clusters and the magic number structure Al ₈ Si ₄ . <i>Molecular Physics</i> , 2018, 116, 449-459.	0.8	2
2515	HNgBeF ₃ (Ng=Ar, Rn): Superhalogen-supported noble gas insertion compounds. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25499.	1.0	15
2516	Bioinspired water-soluble two-photon fluorophores. <i>Dyes and Pigments</i> , 2018, 150, 105-111.	2.0	27
2517	Selective Separation of Methacrylic Acid and Acetic Acid from Aqueous Solution Using Carboxyl-Functionalized Ionic Liquids. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 1215-1224.	3.2	26
2518	Study on the Geometric and Electronic Structures of Al _n Si _m (n=3, 4, 5; m=1, 2, 3, 4) Clusters. <i>Journal of Cluster Science</i> , 2018, 29, 141-150.	1.7	4
2519	A quantum-chemical DFT study of the mechanism and regioselectivity of the 1,3-dipolar cycloaddition reaction of nitrile oxide with electron-rich ethylenes. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25540.	1.0	17
2520	A comparative view on the potential acting on an electron in a molecule and the electrostatic potential through the typical halogen bonds. <i>Journal of Computational Chemistry</i> , 2018, 39, 573-580.	1.5	33
2521	Dispersion and distortion in heavy group 2 and lanthanide decamethylmetallocenes: The (C ₅ Me ₅) ₂ (Sr,Sm) connection. <i>Journal of Organometallic Chemistry</i> , 2018, 857, 145-151.	0.8	4
2522	Probing the geometries and electronic properties of charged Zr ₂ Si _n q (n=12, q=±1) clusters. <i>Structural Chemistry</i> , 2018, 29, 139-146.	1.0	2
2523	Thermochemical and conformational study of optical active phenylbenzazole derivatives. <i>Journal of Chemical Thermodynamics</i> , 2018, 116, 7-20.	1.0	8
2524	Investigation of carboxylation of carbon nanotube in the adsorption of anti-cancer drug: A theoretical approach. <i>Applied Surface Science</i> , 2018, 427, 112-125.	3.1	21
2525	Space Charge Analysis of Polyethylene with Chemical Defects Based on Density Function Theory. , 2018, ..		0
2526	Trapping of an Heterometallic Unsaturated Hydride: Structure and Properties of the Ammonia Complex [MoMnCp(1/4-H)(1/4-PPh ₂)(CO) ₅ (NH ₃)]. <i>Inorganics</i> , 2018, 6, 125.	1.2	2

#	ARTICLE	IF	CITATIONS
2527	Structural Elucidation of Covalent Organic Polymers (COP) and Their Linker Effect on Gas Adsorption Performance via Density Functional Theory Approach. <i>ChemistrySelect</i> , 2018, 3, 8294-8305.	0.7	6
2528	A theoretical study on lidocaine solubility in deep eutectic solvents. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27464-27473.	1.3	54
2529	Tetracyclo(9-methyl-2,7-carbazole) as a promising nano hoop for gas trapping: a multiscale study. <i>New Journal of Chemistry</i> , 2018, 42, 19101-19112.	1.4	1
2530	Understanding the mechanism and stereoselectivity of NHC-catalyzed [3 + 2] cycloaddition of 3-bromoaldehydes and isatin <i>N</i> -Boc ketimines. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 9251-9258.	1.5	14
2531	Polymer semiconductors incorporating head-to-head linked 4-alkoxy-5-(3-alkylthiophen-2-yl)thiazole. <i>RSC Advances</i> , 2018, 8, 35724-35734.	1.7	6
2532	Assessment of electronic transitions involving intermolecular charge transfer in complexes formed by fullerenes and donor-acceptor nano hoops. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27791-27803.	1.3	5
2533	The role played by ethanol in achieving the successive versus simultaneous mechanism of excited-state double proton transfer in dipyrido[2,3- <i>a</i> :3',2'- <i>b</i>]carbazole. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26259-26265.	1.3	47
2534	Long-lived triplet excited state in a platinum(ii) perylene monoimide complex. <i>Dalton Transactions</i> , 2018, 47, 15071-15081.	1.6	16
2535	The coordination chemistry of lanthanide and actinide metal ions with hydroxypyridinone-based decorporation agents: orbital and density based analyses. <i>Dalton Transactions</i> , 2018, 47, 16603-16615.	1.6	15
2536	Reactions of dicobalt octacarbonyl with dinucleating and mononucleating bis(imino)pyridine ligands. <i>Dalton Transactions</i> , 2018, 47, 15353-15363.	1.6	17
2537	Mechanochemical fabrication and properties of CL-20/RDX nano co/mixed crystals. <i>RSC Advances</i> , 2018, 8, 34126-34135.	1.7	28
2538	Understanding the effects of vicinal carbon substituents and configuration on organofluorine hydrogen-bonding interaction. <i>RSC Advances</i> , 2018, 8, 38980-38986.	1.7	3
2539	Guest-induced reversible crystal-to-amorphous-to-crystal transformation in a Co(II)-based metal-organic framework. <i>CrystEngComm</i> , 2018, 20, 6828-6833.	1.3	9
2540	Unveiling the role of intra and interatomic interactions in the energetics of reaction schemes: a quantum chemical topology analysis. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27558-27570.	1.3	5
2541	Computational investigations of intermolecular interactions between electron-accepting bromo- and iodo-pentafluorobenzene and electron-donating furan and thiophene. <i>New Journal of Chemistry</i> , 2018, 42, 20101-20112.	1.4	5
2542	The regulation of hydroboration of olefins by oriented external electric field. <i>New Journal of Chemistry</i> , 2018, 42, 18402-18408.	1.4	11
2543	Pb(II)-catalyzed transformation of aromatic nitriles to heptanitrogen anions via sodium azide: a combined experimental and theoretical study. <i>RSC Advances</i> , 2018, 8, 39929-39936.	1.7	3
2544	Electronic spectrum and characterization of diabatic potential energy surfaces for thiophenol. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28144-28154.	1.3	14

#	ARTICLE	IF	CITATIONS
2545	Visible colorimetric fluoride and hydroxide sensing by asymmetric tris-urea receptors: combined experimental and theoretical studies. <i>RSC Advances</i> , 2018, 8, 39394-39407.	1.7	12
2546	High-Order harmonic generation of aligned acetylene in elliptically polarized strong laser fields. <i>Chinese Journal of Chemical Physics</i> , 2018, 31, 471-476.	0.6	4
2547	Influence of electron donating ability on reverse intersystem crossing rate for one kind of thermally activated delayed fluorescence molecules. <i>Chinese Journal of Chemical Physics</i> , 2018, 31, 291-299.	0.6	3
2548	Ab Initio Molecular Dynamics Simulation Study on the Stereo Reactions between Atomic Oxygen Anion and Methane. <i>Molecules</i> , 2018, 23, 2495.	1.7	2
2549	Influences of the substituents on the Cr=C bond in [(OC) ₅ Cr=C(OEt)-para-C ₆ H ₄ X] complexes: quantum Theory of Atoms in Molecules, Energy Decomposition Analysis, and Interacting Quantum Atoms. <i>Monatshefte für Chemie</i> , 2018, 149, 2167-2174.	0.9	7
2550	Origin of High Efficiencies for Thermally Activated Delayed Fluorescence Organic Light-Emitting Diodes: Atomistic Insight into Molecular Orientation and Torsional Disorder. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27191-27197.	1.5	48
2551	Density Function Study of the Interaction of a Surface Modifier with the Oxidized Coal Surface Model. <i>ACS Omega</i> , 2018, 3, 14585-14591.	1.6	9
2553	Theoretical Insights into Preorganized Pyridylpyrazole-Based Ligands toward the Separation of Am(III)/Eu(III). <i>Inorganic Chemistry</i> , 2018, 57, 14810-14820.	1.9	48
2554	Analysis of Stability and (Anti)aromaticity of BNâ€¦Dibenzo[<i>a</i> , <i>e</i>]pentalenes. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 6230-6240.	1.2	4
2555	Metal-Rich Oxametallaboranes of Group 5 Metals: Synthesis and Structure of a Face-Fused $\frac{1}{4}$ -Boride Cluster. <i>Inorganic Chemistry</i> , 2018, 57, 14748-14757.	1.9	14
2556	Specificity of Amino Acidâ€“Aluminum Cluster Interaction and Subsequent Oxygen Activation by the above Complex. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28310-28323.	1.5	13
2557	Probing inhibition mechanisms of adenosine deaminase by using molecular dynamics simulations. <i>PLoS ONE</i> , 2018, 13, e0207234.	1.1	7
2558	(2-Pyridyloxy)silanes as Ligands in Transition Metal Coordination Chemistry. <i>Inorganics</i> , 2018, 6, 119.	1.2	16
2559	Aromatic Motifs Dictate Nanohelix Handedness of Tripeptides. <i>ACS Nano</i> , 2018, 12, 12305-12314.	7.3	53
2560	Understanding Adsorption of Violanthrone-79 as a Model Asphaltene Compound on Quartz Surface Using Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28787-28796.	1.5	30
2561	A dynamical model for the generation of H ₂ in microhydrated Al clusters. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 23285-23298.	3.8	3
2562	First report of a planar and a quasi-planar Al ₁₃ ⁺ cluster having localized antiaromatic deltas within an aromatic sea: NICS, ELF, AIM, and AdNDP bonding analysis. <i>Journal of Molecular Modeling</i> , 2018, 24, 344.	0.8	8
2563	Exceptionally Long C~C Single Bonds in Diaminoâ€“carborane as Induced by Negative Hyperconjugation. <i>Angewandte Chemie</i> , 2018, 131, 1411.	1.6	16

#	ARTICLE	IF	CITATIONS
2564	Hybrid Organic–Inorganic Functionalized Dodecaboranes and Their Potential Role in Lithium and Magnesium Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27947-27954.	1.5	7
2565	QTAIM Assessment of the Intra- and Intermolecular Bonding in a Bis(nitramido–oxadiazolate) Energetic Ionic Salt at 20 K. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9676-9687.	1.1	2
2566	In situ monitoring of molecular aggregation using circular dichroism. <i>Nature Communications</i> , 2018, 9, 4961.	5.8	70
2567	Products and Mechanistic Investigations on the Reactions of Hydrazines with Ozone in Gas-Phase. <i>Symmetry</i> , 2018, 10, 394.	1.1	5
2568	Outer electronic shell visualization by NMR chemical shift laplacian of a helium probe. <i>Journal of Computational Chemistry</i> , 2018, 39, 2459-2462.	1.5	8
2569	Synthesis and Characterization of Non-Isolated-Pentagon-Rule Actinide Endohedral Metallofullerenes $U@C_{17418}$ - C_{76} , $U@C_{128324}$ - C_{80} , and $Th@C_{128324}$ - C_{80} : Low-Symmetry Cage Selection Directed by a Tetravalent Ion. <i>Journal of the American Chemical Society</i> , 2018, 140, 18039-18050.	6.6	73
2570	Impact of t-butyl group on the singlet–triplet energy gap via weak orbital overlap of [1,2,5]-thiadiazolo[3,4-C] pyridine-based TADF emitters: Structural modification. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1850048.	1.8	0
2571	Computation Revealed Mechanistic Complexity of Low-Valent Cobalt-Catalyzed Markovnikov Hydrosilylation. <i>Journal of Organic Chemistry</i> , 2018, 83, 14646-14657.	1.7	8
2572	A Computational Study on the Hydride Transfer Mechanism between Nicotinamide and Menadione. <i>ChemistrySelect</i> , 2018, 3, 11977-11985.	0.7	4
2573	Confinement Effects in Protonation Reactions Catalyzed by Zeolites with Large Void Structures. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27350-27359.	1.5	15
2574	Microwave spectrum and non-covalent interactions of the 1, 2, 3, 4-tetrafluorobenzene-water complex. <i>Journal of Chemical Physics</i> , 2018, 149, 164306.	1.2	5
2575	Interplay between Aromaticity and Radicaloid Character in Nitrogen-Doped Oligoacenes Revealed by High-Level Multireference Methods. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9464-9473.	1.1	6
2576	Molecular Design for Electron-Driven Double-Proton Transfer: A New Scenario for Excited-State Proton-Coupled Electron Transfer. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9191-9198.	1.1	11
2577	Structural evolution and bonding properties of $BSn^+/ (n = 4-12)$ clusters: Size-selected anion photoelectron spectroscopy and theoretical calculations. <i>Journal of Chemical Physics</i> , 2018, 149, 174314.	1.2	17
2578	Heterobiaryl synthesis by contractive C–C coupling via P(V) intermediates. <i>Science</i> , 2018, 362, 799-804.	6.0	145
2579	The model of the fullerene C_{60} and its ions C_{60}^+ , C_{60}^{\bullet} pseudopotentials for molecular dynamics purposes. <i>European Physical Journal D</i> , 2018, 72, 1.	0.6	6
2580	Theoretical investigation of auxiliary electronic acceptors in modifying D-D–A sensitizers for dye-sensitized solar cells. <i>Journal of Molecular Modeling</i> , 2018, 24, 339.	0.8	1
2581	Theoretical Insights into the Electron Capture Behavior of $H_2SO_4 \cdot \cdot N_2O$ Complex: A DFT and Molecular Dynamics Study. <i>Molecules</i> , 2018, 23, 2349.	1.7	2

#	ARTICLE	IF	CITATIONS
2582	Quantitative Assessment of Tetrel Bonding Utilizing Vibrational Spectroscopy. <i>Molecules</i> , 2018, 23, 2763.	1.7	84
2583	Assessing the Performance of Cobalt Phthalocyanine Nanoflakes as Molecular Catalysts for Li-Promoted Oxalate Formation in Li ⁺ CO ₂ Oxalate Batteries. <i>Journal of Physical Chemistry C</i> , 2018, 122, 25776-25784.	1.5	22
2584	An ab initio study and the corresponded instructing improvement of the multicomponent reaction consisted of acetone, aniline and 4-hydrocoumarine. <i>Computational and Theoretical Chemistry</i> , 2018, 1145, 22-27.	1.1	1
2585	Theoretical Study of the Arene Ligand Effect on the Structure and Properties of Cr(CO) ₃ (Arene) Complexes (Arene = Benzene, Biphenyl, Triphenyl, Tetraphenyl). <i>Journal of Structural Chemistry</i> , 2018, 59, 1784-1790.	0.3	3
2586	Theoretical study on nonlinear optical properties of <i>N</i> -(6-hydroxyhexyl)-5-nitroazophenyl carbazole. <i>Journal of Nonlinear Optical Physics and Materials</i> , 2018, 27, 1850036.	1.1	0
2587	Activation of Small Molecules (H ₂ , CO ₂ , N ₂ O, CH ₄), Tj ETQq1 1 0.784314 rgBT / Omega, 2018, 3, 17199-17211.	1.6	13
2588	Enhanced Adsorption of SO ₂ Molecule on Al- and Si-Doped Pyridinic Nitrogen Doped Graphene. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 2556-2564.	0.1	1
2589	Toward Understanding the Isomeric Stability of Fullerenes with Density Functional Theory and the Information-Theoretic Approach. <i>ACS Omega</i> , 2018, 3, 17986-17990.	1.6	48
2590	Simulation of Capture and Release Processes of Hydrogen by β -Hydroquinone Clathrate. <i>ACS Omega</i> , 2018, 3, 18771-18782.	1.6	16
2591	Electronic and Optical Properties of Ultrasmall ABX ₃ (A = Cs), Tj ETQq1 1 0.784314 rgBT / Overlock 10 Tf 50 387 Td (CH Omega, 2018, 3, 18917-18924.	1.6	18
2592	Synthesis and Characterization of a Molecularly Imprinted Polymer of Spermidine and the Exploration of Its Molecular Recognition Properties. <i>Polymers</i> , 2018, 10, 1389.	2.0	17
2593	The Structure of 2-Methylphenylcyanamide in the Solid State. <i>Journal of Structural Chemistry</i> , 2018, 59, 1302-1307.	0.3	2
2594	Rational Design of Efficient Environmental Sensors: Ring-Shaped Nanostructures Can Capture Quat Herbicides. <i>ACS Omega</i> , 2018, 3, 16976-16988.	1.6	5
2595	Chemical Bonding in Transition Metal Nitride Os ₃ N ₃ ⁺ Cluster: δ Inorganic Benzene and σ Aromaticity. <i>ACS Omega</i> , 2018, 3, 17083-17091.	1.6	0
2596	Reactivity of the metalloligand [Pt ₂ (μ -S) ₂ (PPh ₃) ₂ (PPh ₃) ₄] toward tellurium(II) thiourea complexes: synthesis and structural characterization of the ditellurium(I) derivative [Pt ₂ (μ -S) ₂ (PPh ₃) ₂ (PPh ₃) ₄] ₂ Te ₂ ²⁺ . <i>Journal of Coordination Chemistry</i> , 2018, 71, 3807-3823.	0.8	1
2597	Baird's Rule in Substituted Fulvene Derivatives: An Information-Theoretic Study on Triplet-State Aromaticity and Antiaromaticity. <i>ACS Omega</i> , 2018, 3, 18370-18379.	1.6	29
2598	Photoelectron Spectroscopy and Theoretical Study of Cr _n Si ₁₅ (n = 1-3): Effects of Doping Cr Atoms on the Structural and Magnetic Properties. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9886-9893.	1.1	38
2599	CA ₃ X (X = B/Al/Ga/In/Tl) with 16 valence electrons: can planar tetracoordinate carbon be stable?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26266-26272.	1.3	22

#	ARTICLE	IF	CITATIONS
2600	A comparative study on the bond features in CO, CS, and PbS. <i>Journal of Chemical Physics</i> , 2018, 149, 224302.	1.2	3
2601	Ethene Protonation Over Silica-Grafted Metal (Cr, Mo, and W) Oxide Catalysts: A Comparative Nanocluster Modeling Study. <i>Russian Journal of Inorganic Chemistry</i> , 2018, 63, 1570-1577.	0.3	33
2602	Rotational spectroscopy of chiral tetrahydro-2-furoic acid: Conformational landscape, conversion, and abundances. <i>Journal of Chemical Physics</i> , 2018, 149, 224306.	1.2	21
2603	A Dft Investigation of the Interaction of B- And Al-Doped C60 Fullerenes with Cyclopropylpiperazine. <i>Journal of Structural Chemistry</i> , 2018, 59, 1271-1275.	0.3	7
2604	Excited-State Switching between Ligand-Centered and Charge Transfer Modulated by Metal-Carbon Bonds in Cyclopentadienyl Iridium Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 15445-15461.	1.9	12
2605	Facially Polarized Molecule for Alkalides and Superalkalides with Considerable Nonlinear Optical Response. <i>ChemistrySelect</i> , 2018, 3, 12782-12790.	0.7	16
2606	A DFT Study of Disperse Yellow 119 Degradation Mechanism by Hydroxyl Radical Attack. <i>ChemistrySelect</i> , 2018, 3, 12988-12997.	0.7	7
2607	Reversible Solubilization of Pyrene by a Gas Switchable Surfactant Investigated by Molecular Dynamics Simulation. <i>Langmuir</i> , 2018, 34, 15445-15454.	1.6	8
2608	Heat Capacity Prediction of Ionic Liquids Based on Quantum Chemistry Descriptors. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 16989-16994.	1.8	13
2609	Frustrated Lewis Pair Oxidation Permits Synthesis of a Fluoroazaphosphatane, [FP(MeNCH ₂ CH ₂) ₃ N] ⁺ . <i>Inorganic Chemistry</i> , 2018, 57, 15299-15304.	1.9	13
2610	Experimental and Theoretical Comparison of Transition-Metal and Actinide Tetravalent Schiff Base Coordination Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 15389-15398.	1.9	36
2611	Polymeric vanadyl species determine the low-temperature activity of V-based catalysts for the SCR of NO _x with NH ₃ . <i>Science Advances</i> , 2018, 4, eaau4637.	4.7	206
2612	Analysis of the Interaction Between the C20 Cage and cis-PtCl ₂ (NH ₃) ₂ : A DFT Investigation of the Solvent Effect, Structures, Properties, and Topologies. <i>Journal of Structural Chemistry</i> , 2018, 59, 1044-1051.	0.3	7
2613	Biosensor Properties of DA-DA Dinucleotide in the Presence of DI-L-Lysine and Single Carbon Nanotubes: Molecular Dynamics Simulation and Density Functional Theory Approach. <i>Journal of Structural Chemistry</i> , 2018, 59, 1228-1235.	0.3	1
2614	Probing Hyperconjugative Aromaticity of Monosubstituted Cyclopentadienes. <i>Asian Journal of Organic Chemistry</i> , 2019, 8, 123-127.	1.3	19
2615	Comparison of halide donators based on π-σ-M (M = Cu, Ag, Au), π-H and π-halogen bonds. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	9
2616	Effects of ortho-Linkages on the Molecular Stability of Organic Light-Emitting Diode Materials. <i>Chemistry of Materials</i> , 2018, 30, 8771-8781.	3.2	36
2617	Pyrenimidazolyl-Benzaldehyde Fluorophores: Synthesis, Properties, and Sensing Function for Fluoride Anions. <i>ACS Omega</i> , 2018, 3, 16387-16397.	1.6	25

#	ARTICLE	IF	CITATIONS
2618	Liquid-Liquid Extraction of Benzene Using Low Transition Temperature Mixtures: COSMO-SAC Predictions and Experiments. <i>Journal of Chemical & Engineering Data</i> , 0, , .	1.0	7
2619	Extraordinary Redox Activities in Ladder-Type Conjugated Molecules Enabled by B-N Coordination-Promoted Delocalization and Hyperconjugation. <i>Journal of the American Chemical Society</i> , 2018, 140, 18173-18182.	6.6	63
2620	Desensitization of the dinitromethyl group: molecular/crystalline factors that affect the sensitivities of energetic materials. <i>Journal of Materials Chemistry A</i> , 2018, 6, 22705-22712.	5.2	57
2621	Can Synthetic All-Metal Cluster Compound Support Multifold (π and σ) Aromaticity and Orbital Aromaticity?. <i>Chinese Journal of Chemistry</i> , 2019, 37, 126-130.	2.6	2
2622	Mechanistic insight on water and substrate catalyzed the synthesis of 3-(1-hydroxyindol-3-yl)-2-(4-methoxybenzyl)isoindolin-1-one: Driving by noncovalent interactions. <i>Journal of Computational Chemistry</i> , 2018, 39, 2316-2323.	1.0	1
2623	On the electron flow sequence driving the hydrometallation of acetylene by lithium hydride. <i>Journal of Molecular Modeling</i> , 2018, 24, 305.	0.8	5
2624	Mechanistic Insights into Manganese (I)-Catalyzed Chemoselective Hydroarylations of Alkynes: A Theoretical Study. <i>ChemCatChem</i> , 2018, 10, 5280-5286.	1.8	12
2625	Quantum mechanical studies of full-shell noble metal nanoclusters in water. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25709.	1.0	0
2626	Energy-Transfer Pathways and Triplet Lifetime Manipulation in a Zinc Porphyrin/F8BT Hybrid Polymer. <i>Journal of Physical Chemistry C</i> , 2018, 122, 23950-23958.	1.5	5
2627	Dimerization of Metallofullerenes to Obtain Materials with Enhanced Nonlinear Optical Properties. <i>ChemPhysChem</i> , 2018, 19, 2995-3000.	1.0	5
2628	Supramolecular Binding of bis-naphthalene Cleft based Molecular Tubes. <i>ChemistrySelect</i> , 2018, 3, 10537-10542.	0.7	1
2629	Density functional theory studies on a non-covalent interaction system: hydrogen-bonded dimers of zoledronate. <i>Journal of Molecular Modeling</i> , 2018, 24, 310.	0.8	0
2630	Odd aromatic Si ₄ ring stabilized by π - σ bond passing through it: May π -bonding form without σ -bonding as precondition?. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25788.	1.0	1
2631	Theoretical investigation into the cooperativity effect between the intermolecular π - π and H-bonding interactions in the curcumin TM cytosine TM H ₂ O system. <i>Journal of Molecular Modeling</i> , 2018, 24, 298.	0.8	3
2632	Strong interaction between 5f-electron atoms (Th-Cm) and point-defect graphene. <i>Solid State Ionics</i> , 2018, 325, 221-227.	1.3	1
2633	Superoctazethrene: An Open-Shell Graphene-like Molecule Possessing Large Diradical Character but Still with Reasonable Stability. <i>Journal of the American Chemical Society</i> , 2018, 140, 14054-14058.	6.6	65
2634	Mechanistic insights into N-Bromosuccinimide-promoted synthesis of imidazo[1,2-a]pyridine in water: Reactivity mediated by substrates and solvent. <i>Journal of Computational Chemistry</i> , 2018, 39, 2324-2332.	1.5	2
2635	Exploration of High-Energy-Density Materials: Computational Insight into Energetic Derivatives Based on 1,2,4,5-tetrahydro-1,2,4,5-tetrazine. <i>ChemistryOpen</i> , 2018, 7, 780-788.	0.9	9

#	ARTICLE	IF	CITATIONS
2636	What kind of neutral halogen bonds can be modulated by solvent effects?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26126-26139.	1.3	21
2637	Molecular insight into the interaction mechanisms of an annulated pyrazole (DB08446) with HIV-1 RT: a QM and QM/QM ² study. <i>Monatshefte für Chemie</i> , 2018, 149, 1919-1929.	0.9	1
2638	Theoretical Investigations on the Structural, Electronic and Spectral Properties of VF _n (n = 1-7) Clusters. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2018, 73, 1091-1104.	0.7	7
2639	Can Combined Electrostatic and Polarization Effects Alone Explain the F ⁻ -F ⁻ Negative-Negative Bonding in Simple Fluoro-Substituted Benzene Derivatives? A First-Principles Perspective. <i>Computation</i> , 2018, 6, 51.	1.0	32
2640	New Insights into the Configurations of Lead(II)-Benzohydroxamic Acid Coordination Compounds in Aqueous Solution: A Combined Experimental and Computational Study. <i>Minerals (Basel, Switzerland)</i> , 2018, 8, 368.	0.8	17
2641	A challenging redox neutral Cp*Co(III)-catalysed alkylation of acetanilides with 3-buten-2-one: synthesis and key insights into the mechanism through DFT calculations. <i>Beilstein Journal of Organic Chemistry</i> , 2018, 14, 2366-2374.	1.3	7
2642	Modeling protic dicationic ionic liquids based on quaternary ammonium, imidazolium or pyrrolidinium cations and bis(trifluoromethanesulfonyl)imide anion: Structure and spectral characteristics. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 85, 304-315.	1.3	9
2643	Structures and Fluorescence Properties for the Crystals, Powders, and Thin Films of Dithienylhexatrienes: Effects of Positional Isomerism. <i>Crystal Growth and Design</i> , 2018, 18, 6477-6487.	1.4	5
2644	Examination of Structure and Bonding in 10-Coordinate Europium and Americium Terpyridyl Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 12969-12975.	1.9	22
2645	Structural Stability and Evolution of Scandium-Doped Silicon Clusters: Evolution of Linked to Encapsulated Structures and Its Influence on the Prediction of Electron Affinities for ScSi _n (n = 4-16) Clusters. <i>Inorganic Chemistry</i> , 2018, 57, 12934-12940.	1.9	39
2646	Insight into the Photocatalytic Mechanism of Tin Dioxide/Polyaniline Nanocomposites for NO Degradation under Solar Light. <i>ACS Applied Nano Materials</i> , 2018, 1, 5786-5794.	2.4	39
2647	On the Nature of Bonding in Synthetic Charged Molecular Alloy [P7ZnP7]4 ⁺ Cluster and Its Relevant [P7]3 ⁺ Zintl Ion. <i>ACS Omega</i> , 2018, 3, 11958-11965.	1.6	3
2648	Unexpected formation of polymeric silver(I) complexes of azine-type ligand via self-assembly of Ag-salts with isatin oxamohydrazide. <i>Royal Society Open Science</i> , 2018, 5, 180434.	1.1	7
2649	Tungsten-Embedded Graphene: Theoretical Study on a Potential High-Activity Catalyst toward CO Oxidation. <i>Materials</i> , 2018, 11, 1848.	1.3	13
2650	Biosynthesis of Grandione: An Example of Tandem Hetero Diels-Alder/Retro-Claisen Rearrangement Reaction?. <i>Molecules</i> , 2018, 23, 2505.	1.7	5
2651	Mechanism of Propylene Epoxidation via O ₂ with Co ^{II} Oxidation of Aldehydes by Metalloporphyrins. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 6557-6565.	1.2	12
2652	Linear polarizabilities and second hyperpolarizabilities of streptocyanines: Results from broken-symmetry DFT and new CCSD(T) benchmarks. <i>Journal of Computational Chemistry</i> , 2018, 39, 2350-2359.	1.5	24
2653	Theoretical design of novel energetic salts derived from bicyclo-HMX. <i>Journal of Molecular Modeling</i> , 2018, 24, 304.	0.8	0

#	ARTICLE	IF	CITATIONS
2654	Role of hydrogen bonding in the conformations of lidocaine, mepivacaine and bupivacaine under aqueous solvation. <i>Computational and Theoretical Chemistry</i> , 2018, 1144, 9-17.	1.1	2
2655	Structural Properties and Reactive Site Selectivity of Some Transition Metal Complexes of 2,2-bis(1E,1E)-(ethane-1,2-diylbis(azan-1-yl-1-ylidene))bis(phenylmethan-1-yl-1-ylidene)dibenzoic Acid: DFT, Conceptual DFT, QTAIM, and MEP Studies. <i>Bioinorganic Chemistry and Applications</i> , 2018, 2018, 1-11.	1.8	10
2656	Behaviors and interactions of H ₂ absorption to CuRn ⁺ . <i>International Journal of Hydrogen Energy</i> , 2018, 43, 20892-20899.	3.8	3
2657	Systematic Study of the Effect of Auxiliary Acceptors in Dye-Sensitizers Used on Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2018, 122, 23890-23898.	1.5	20
2658	Coordination diversity in tin compounds with bis(benzoxazole)phenol as a polydentate ligand: Synthesis and crystal structure studies. <i>Journal of Coordination Chemistry</i> , 2018, 71, 3790-3805.	0.8	2
2659	The effects of aerogen-bonding on the geometries and spectral properties of several small molecular clusters containing XeO ₃ . <i>Journal of Physics Condensed Matter</i> , 2018, 30, 444001.	0.7	7
2660	Building polynitrogen clusters with metal-metal multiple bonds. <i>Polyhedron</i> , 2018, 156, 54-57.	1.0	5
2661	Synthesis and spectroscopic characterization of a photo-stable tetrazinc(II)-Schiff base cluster: A rare case of ligand centric phenoxazinone synthase activity. <i>Polyhedron</i> , 2018, 156, 223-230.	1.0	27
2662	Superhalogen-based composite with strong acidity-a crossing point between two topics. <i>Inorganic Chemistry Frontiers</i> , 2018, 5, 2934-2947.	3.0	17
2663	syn- and anti-H Bonds in Ammonia and Phosphine Complexes with Proton Donors. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 1959-1969.	0.1	1
2664	2,2'-Azobispyridine in Phosphorus Coordination Chemistry: A New Approach to 1,2,4,3-Triazaphosphole Derivatives. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 4245-4254.	1.0	9
2665	Information theoretic approach provides a reliable description for kinetic component of correlation energy density functional. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25791.	1.0	8
2666	DFT study of the catalytic effect of Na on the gasification of carbon-CO ₂ . <i>Combustion and Flame</i> , 2018, 197, 471-486.	2.8	47
2667	Lewis Acidity and Basicity of Mixed Chlorometallate Ionic Liquids: Investigations from Surface Analysis and Fukui Function. <i>Molecules</i> , 2018, 23, 2516.	1.7	9
2668	A Computational Study on the 4-Dimethylaminopyridine (DMAP)-Catalyzed Regioselective [2+4] Cyclization of Allenic Ester with Cyclic Ketimine. <i>ChemistrySelect</i> , 2018, 3, 10553-10558.	0.7	7
2669	DFT and TD-DFT design of small π -conjugated molecules with narrow band gap and high efficiency for organic solar cells. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	5
2670	Constructing soft-conjugated materials from small molecules to polymers: a theoretical study. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	1
2671	The adsorption of bromomethane onto the exterior surface of aluminum nitride, boron nitride, carbon, and silicon carbide nanotubes: A PBC-DFT, NBO, and QTAIM study. <i>Computational and Theoretical Chemistry</i> , 2018, 1144, 26-37.	1.1	56

#	ARTICLE	IF	CITATIONS
2672	Probing the Electron Accepting Orbitals of Ni-Centered Hydrogen Evolution Catalysts with Noninnocent Ligands by Ni L-Edge and S K-Edge X-ray Absorption. <i>Inorganic Chemistry</i> , 2018, 57, 13167-13175.	1.9	13
2673	Quantification of the resonance stabilized C ₄ H ₅ isomers and their reaction with acetylene. <i>Combustion and Flame</i> , 2018, 198, 334-341.	2.8	16
2674	Theoretical Insights on A series of Cyclic Energetic Derivatives. <i>ChemistrySelect</i> , 2018, 3, 11160-11166.	0.7	4
2675	Influence of Charge Distribution on Structural Changes of Aromatic Imide Derivatives upon One-Electron Reduction Revealed by Time-Resolved Resonance Raman Spectroscopy during Pulse Radiolysis. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8738-8744.	1.1	8
2676	Universal Method for Electrostatic Interaction Energies Estimation with Charge Penetration and Easily Attainable Point Charges. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6336-6345.	2.3	10
2677	Mixed Chlorometallate Ionic Liquids as C ₄ Alkylation Catalysts: A Quantitative Study of Acceptor Properties. <i>Catalysts</i> , 2018, 8, 498.	1.6	3
2678	Critical assessment of charge transfer estimates in non-covalent graphene doping. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	7
2679	NO ₂ -NO ₂ Contacts under Compression: Testing the Forces in Soft Donor-Acceptor Interactions. <i>Crystal Growth and Design</i> , 2018, 18, 7579-7589.	1.4	19
2680	Noncovalent Interactions Involving Iodofluorobenzenes: The Interplay of Halogen Bonding and Weak lp(O)-Hole-arene Interactions. <i>Crystal Growth and Design</i> , 2018, 18, 7641-7654.	1.4	62
2681	Design of Zero Oxygen Balance Energetic Materials on the Basis of Diels-Alder Chemistry. <i>Journal of Organic Chemistry</i> , 2018, 83, 14698-14702.	1.7	28
2682	Identifying the Role of Intramolecular Charge Transfer and Excited-State Proton Transfer in Fluorescence Mechanism for an Azido-Based Chemosensor. <i>Journal of Physical Chemistry C</i> , 2018, 122, 26576-26583.	1.5	27
2683	Reaction probability and defluorination mechanisms of a potent greenhouse gas SF ₅ CF ₃ attacked by CH ₃ radical: a theoretical study. <i>Molecular Physics</i> , 2018, 116, 2226-2238.	0.8	1
2684	To Be or Not To Be Protonated: <i>cyclo</i> -N ₅ ⁺ in Crystal and Solvent. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 7137-7145.	2.1	12
2685	Polarizable force field parameterization and theoretical simulations of ThCl ₄ -LiCl molten salts. <i>Journal of Computational Chemistry</i> , 2018, 39, 2432-2438.	1.5	11
2686	Theoretical studies on thermally activated delayed fluorescence mechanism of a series of organic light-emitting diodes emitters comprising 2,7-diphenylamino-9,9-dimethylacridine as electron donor. <i>Journal of Computational Chemistry</i> , 2018, 39, 2601-2606.	1.5	14
2687	Mechanism and Origins of Chemo- and Stereoselectivities of Aryl Iodide-Catalyzed Asymmetric Difluorinations of <i>l</i> ² -Substituted Styrenes. <i>Journal of the American Chemical Society</i> , 2018, 140, 15206-15218.	6.6	89
2688	Study of CD_{5}^{+} Ions and Deuterated Variants() Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 107 Td (C^{H}) of Physical Chemistry A, 2018, 92, 2215-2226.	0.1	0
2689	Theoretical Investigations on the Reactivity of Methylidyne Radical toward 2,3,7,8-Tetrachlorodibenzo-p-Dioxin: A DFT and Molecular Dynamics Study. <i>Molecules</i> , 2018, 23, 2685.	1.7	1

#	ARTICLE	IF	CITATIONS
2690	Spontaneous Substitutions at Phosphorus Trihalides in Imidazolium Halide Ionic Liquids: Grotthuss Diffusion of Anions?. <i>Chemistry - A European Journal</i> , 2018, 24, 16323-16331.	1.7	8
2691	Synthesis of (MeO) ₂ Bn ₂ C ₇₀ : Regiochemistry of 2-fold Additions to C ₇₀ with Addends That Are Preferential for Ortho Addition and Capable of Para Addition. <i>Journal of Organic Chemistry</i> , 2018, 83, 13716-13725.	1.7	6
2692	M ⁺ S Multiple Bond in HMSH, H ₂ MS, and HMS Molecules (M = B, Al, Ga): Matrix Infrared Spectra and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8626-8635.	1.1	3
2693	Molecular orbital composition and its effect on electron-impact ionization cross sections of molecules: A comparative study. <i>Physics of Plasmas</i> , 2018, 25, .	0.7	10
2694	Exploring the structural evolution and electronic properties of medium-sized Nb ₂ Si _n ^{+/0} (n = 13-20) clusters by density functional theory calculations. <i>Chemical Physics Letters</i> , 2018, 713, 58-64.	1.2	15
2696	Structures and magnetic properties of small $\{Co_{n}^{+}\}$ and Co_{n}^{+} clusters. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 474002.		
2697	A dinuclear Cu(⁺)-mediated complex: Theoretical studies of the G ₂ Cu ₂₄ ⁺ cluster ion. <i>Journal of Chemical Physics</i> , 2018, 149, 144308.	1.2	3
2698	Theoretical Study on Unsupported Uranium-Metal Bonding in Uranium-Group 8 Complexes. <i>Organometallics</i> , 2018, 37, 3678-3686.	1.1	24
2699	Methanol to Olefins Reaction over Cavity-type Zeolite: Cavity Controls the Critical Intermediates and Product Selectivity. <i>ACS Catalysis</i> , 2018, 8, 10950-10963.	5.5	59
2700	Diradical Anion of Potassium Aggregate: Reduction of Dimer Boroxide Complex. <i>Inorganic Chemistry</i> , 2018, 57, 13544-13551.	1.9	8
2701	Low Temperature Electrochemical Deposition of Aluminum in Organic Bases/Thiourea-Based Deep Eutectic Solvents. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 15480-15486.	3.2	18
2702	Modulating stability of functionalized fullerene cations [C ₆₀] ⁺ with the nature of R-group. <i>Journal of Computational Chemistry</i> , 2018, 39, 2385-2396.	1.5	3
2703	Quantum chemical study of formation of Cu ⁺ -YIII metallamacrocyclic complexes based on glycinehydroximate ligands. <i>Russian Chemical Bulletin</i> , 2018, 67, 1173-1181.	0.4	7
2704	Noble gas inserted compounds of borazine and its derivative B ₃ N ₃ R ₆ : structures and bonding. <i>Journal of Molecular Modeling</i> , 2018, 24, 326.	0.8	5
2705	Influence of complexing species on the extraction of trivalent actinides from lanthanides with CyMe ₄ -BTBP: a theoretical study. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2018, 318, 1453-1463.	0.7	11
2706	A joint MD/QM study on the possibility of alkaloids detection by cucurbiturils and graphene oxide-cucurbituril composites. <i>Journal of Molecular Liquids</i> , 2018, 272, 963-972.	2.3	12
2707	Influence of one-dimensional TiO ₂ nanotube on interfacial electron transfer in dye-sensitized solar cells: Insights from theoretical investigation. <i>Solar Energy</i> , 2018, 176, 545-555.	2.9	15
2708	Effects of NO ₂ Addition on the NH ₃ -SCR over Small-Pore Cu-SSZ-13 Zeolites with Varying Cu Loadings. <i>Journal of Physical Chemistry C</i> , 2018, 122, 25948-25953.	1.5	58

#	ARTICLE	IF	CITATIONS
2709	Vibrational spectra and electronic structure of 11-vertex boron-containing clusters: a comparative study of [B ₁₁ H ₁₁] ²⁺ , [CB ₁₀ H ₁₁] ⁺ , and C ₂ B ₉ H ₁₁ . Russian Chemical Bulletin, 2018, 67, 1340-1349.	0.4	2
2710	Modeling of the Functionalized Gold Nanoparticle Aggregation in the Presence of Dopamine: A Joint MD/QM Study. Journal of Physical Chemistry C, 2018, 122, 26130-26141.	1.5	15
2711	Mechanistic Study on Complexation-Induced Spring and Hover Dissolution Behavior of Ibuprofen-Nicotinamide Cocrystal. Crystal Growth and Design, 2018, 18, 7343-7355.	1.4	50
2712	Adsorption of Biomass-Derived Products on MoO ₃ : Hydrogen Bonding Interactions under the Spotlight. ACS Omega, 2018, 3, 14165-14172.	1.6	10
2713	Broad-Range Spectral Analysis for Chiral Metal Coordination Compounds: (Chiro)optical Superspectrum of Cobalt(II) Complexes. Inorganic Chemistry, 2018, 57, 13397-13408.	1.9	30
2714	Investigation of nondegenerate two-photon absorption in common fluorescent dyes. Journal of Nonlinear Optical Physics and Materials, 2018, 27, 1850027.	1.1	3
2715	On the theoretical rationalization of intermolecular interactions: insights from DFT energy partitioning schemes. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	2
2716	Halogen bond in the water adduct of chloropentafluoroethane revealed by rotational spectroscopy. Journal of Chemical Physics, 2018, 149, 154307.	1.2	5
2717	Decomposition of d- and f-Shell Contributions to Uranium Bonding from the Quantum Theory of Atoms in Molecules: Application to Uranium and Uranyl Halides. Inorganics, 2018, 6, 88.	1.2	19
2718	Photoactuated Properties of Acetylene-Congeners Non-Metallic Dyes and Molecular Design for Solar Cells. Materials, 2018, 11, 2027.	1.3	0
2719	Strong Tetrel Bonds: Theoretical Aspects and Experimental Evidence. Molecules, 2018, 23, 2642.	1.7	43
2720	Exploring the Aggregation Mechanism of Graphene Oxide in the Presence of Radioactive Elements: Experimental and Theoretical Studies. Environmental Science & Technology, 2018, 52, 12208-12215.	4.6	49
2721	Electronic Effect on the Molecular Motion of Aromatic Amides: Combined Studies Using VT-NMR and Quantum Calculations. Molecules, 2018, 23, 2294.	1.7	7
2722	Theoretical Insights into the Interaction Mechanisms between Nitric Acid and Nitrous Oxide Initiated by an Excess Electron. Journal of Physical Chemistry A, 2018, 122, 7312-7319.	1.1	6
2723	Ammonia and phosphine complexes with proton donors. Hydrogen bonding from the backside of the N(P) lone pair. Computational and Theoretical Chemistry, 2018, 1142, 28-38.	1.1	7
2724	Larger V_H (Hole Distribution Volume)/ V_M (Molecular Volume) Induced Higher Charge Mobility of Group IVA Element-Based Host Materials for Potentially Highly Efficient Blue OLEDs. Journal of Physical Chemistry C, 2018, 122, 22273-22279.	1.5	11
2725	Vertical Tunnel Junction Embedding a Spin Crossover Molecular Film. Advanced Electronic Materials, 2018, 4, 1800204.	2.6	37
2726	Pt/Pd and I/Br Isostructural Exchange Provides Formation of $\text{Pt}^{\text{I}}\text{I}^{\text{I}}\text{Pd}$, $\text{Pt}^{\text{I}}\text{Br}^{\text{I}}\text{Pt}$, and $\text{Pt}^{\text{I}}\text{Br}^{\text{I}}\text{Pd}$ Metal-Involving Halogen Bonding. Crystal Growth and Design, 2018, 18, 5973-5980.	1.4	52

#	ARTICLE	IF	CITATIONS
2727	Infrared Spectra of the SO ₂ F ₂ ⁺ Anion in Solid Argon and Neon. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7723-7729.	1.1	7
2728	Phosphorescent Modulation of Metallophilic Clusters and Recognition of Solvents through a Flexible Host-Guest Assembly: A Theoretical Investigation. <i>Nanomaterials</i> , 2018, 8, 685.	1.9	2
2729	The reason why a kind of diketopyrrolopyrrole analogue can act as acceptors: Theoretical study and characterization. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25782.	1.0	0
2730	Matrix Infrared Spectra and Theoretical Calculations of Fluoroboryl Complexes F ₂ BMF (M = C, Si, Ge, Sn and Pb). <i>Journal of Physical Chemistry A</i> , 2018, 122, 7301-7311.	1.1	4
2731	Insight into the stereoselectivity of TS-1 in epoxidation of <i>cis</i> / <i>trans</i> -2-hexene: a computational study. <i>Catalysis Science and Technology</i> , 2018, 8, 4975-4984.	2.1	8
2732	TD DFT insights into unusual properties of excited sandwich complexes: structural transformations and vibronic interactions in Rydberg-state bis(1,6-benzene)chromium. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23988-23997.	1.3	3
2733	Spectroscopic (FT-IR, FT-Raman) investigation, topology (ESP, ELF, LOL) analyses, charge transfer excitation and molecular docking (dengue, HCV) studies on ribavirin. <i>Chemical Data Collections</i> , 2018, 17-18, 236-250.	1.1	76
2734	Theoretical investigation of gold(I)-catalyzed intramolecular SEAr in isoxazole derivatives: Mechanisms, origin of regioselectivity, and role of hydrogen acceptor. <i>Molecular Catalysis</i> , 2018, 460, 27-35.	1.0	11
2735	Electronic Structure Origins of Surface-Dependent Growth in III-V Quantum Dots. <i>Chemistry of Materials</i> , 2018, 30, 7154-7165.	3.2	25
2736	Theoretical insight into the role of urea in the hydrolysis reaction of NO ₂ as a source of HONO and aerosols. <i>Environmental Chemistry</i> , 2018, 15, 372.	0.7	8
2737	Efficient and stable Ru(III)-choline chloride catalyst system with low Ru content for non-mercury acetylene hydrochlorination. <i>Chinese Journal of Catalysis</i> , 2018, 39, 1770-1781.	6.9	33
2738	Sublimation enthalpy of 1-aminoadamantane: Comparison of theory and experiment. <i>Chemical Physics Letters</i> , 2018, 711, 231-235.	1.2	8
2739	Fluorescence, Phosphorescence, or Delayed Fluorescence? A Theoretical Exploration on the Reason Why a Series of Similar Organic Molecules Exhibit Different Luminescence Types. <i>Journal of Physical Chemistry C</i> , 2018, 122, 23091-23101.	1.5	27
2740	The σ -Hg agostic interactions in the mercury complexes of N-confused porphyrin. <i>Dalton Transactions</i> , 2018, 47, 14774-14784.	1.6	7
2741	Periodic DFT study of structural transformations of cocrystal NTO/TZTN under high pressure. <i>RSC Advances</i> , 2018, 8, 32241-32251.	1.7	7
2742	Triel-Bonded Complexes between TrR ₃ (Tr=B, Al, Ga; R=H, F, Cl, Br, CH ₃) and Pyrazine. <i>ChemPhysChem</i> , 2018, 19, 3122-3133.	1.0	25
2743	Metallophilic Mercuriazamacrocycles Derived from Bis{6-formyl-(2,3,4-trimethoxy)phenyl}mercury: Reactivity with d ¹⁰ and d ⁸ Metal Ions. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 4093-4105.	1.0	5
2744	Oriented-External Electric Fields Create Absolute Enantioselectivity in Diels-Alder Reactions: Importance of the Molecular Dipole Moment. <i>Journal of the American Chemical Society</i> , 2018, 140, 13350-13359.	6.6	113

#	ARTICLE	IF	CITATIONS
2745	Concyclic CH ₃ arrays for single-axis rotations of a bowl in a tube. <i>Nature Communications</i> , 2018, 9, 3779.	5.8	59
2746	On the consequences of the stereochemical activity of the Bi(<i>iii</i>) 6s ² lone pair in cyclen-based complexes. The [Bi(DO3A)] case. <i>Dalton Transactions</i> , 2018, 47, 13830-13842.	1.6	19
2747	Probing the Strongest Aromatic Cyclopentadiene Ring by Hyperconjugation. <i>Organometallics</i> , 2018, 37, 3219-3224.	1.1	20
2748	C ₈ N ₁₂ O ₈ : A Promising Insensitive High-Energy-Density Material. <i>Crystal Growth and Design</i> , 2018, 18, 6150-6154.	1.4	44
2749	Degradation of PFOA Substitute: GenX (HFPO-DA Ammonium Salt): Oxidation with UV/Persulfate or Reduction with UV/Sulfite?. <i>Environmental Science & Technology</i> , 2018, 52, 11728-11734.	4.6	59
2750	Quantum Tunneling Tautomer of <i>N,N</i> -Dimethyl- <i>p</i> -toluidine Dehydrogenates Identified by Deep-UV Laser Ionization Mass Spectroscopy. <i>ACS Omega</i> , 2018, 3, 10743-10747.	1.6	2
2751	Transition State Structure and Mechanism of the Reaction of Hydroxybenzenes with N-Centered Radical in Non-Ionizing Media. <i>Russian Journal of General Chemistry</i> , 2018, 88, 1351-1362.	0.3	4
2752	Clarification of the Molecular Doping Mechanism in Organic Single-Crystalline Semiconductors and their Application in Color-Tunable Light-Emitting Devices. <i>Advanced Materials</i> , 2018, 30, e1801078.	11.1	53
2753	Temperature-responsive self-separation ionic liquid system of zwitterionic-type quaternary ammonium-KI for CO ₂ fixation. <i>Chinese Journal of Catalysis</i> , 2018, 39, 1854-1860.	6.9	25
2754	Exciton Binding Energies of Nonfullerene Small Molecule Acceptors: Implication for Exciton Dissociation Driving Forces in Organic Solar Cells. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22309-22316.	1.5	93
2755	DFT, QTAIM and NBO Investigation of the Interaction of Rare Gases with Pristine and Decorated Boron Nitride Nanotube. <i>ChemistrySelect</i> , 2018, 3, 9833-9840.	0.7	25
2756	Intramolecular interactions Sn ^{IV} in organotin heterocyclic compounds [<i>D</i> (C ₆ H ₄ CH ₂)] ₂ SnBr ₂ . <i>Inorganic Chemistry Communication</i> , 2018, 97, 44-48.	1.8	4
2757	Global Aromaticity in Macrocyclic Cyclopenta-Fused Tetraphenanthrenylene Tetradicaloid and Its Charged Species. <i>Angewandte Chemie</i> , 2018, 130, 13236-13240.	1.6	17
2758	Hierarchically Porous Single Nanocrystals of Bimetallic Metal-Organic Framework for Nanoreactors with Enhanced Conversion. <i>Chemistry of Materials</i> , 2018, 30, 6458-6468.	3.2	24
2759	Why the lowest electronic excitations of rhodamines are overestimated by time-dependent density functional theory. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25780.	1.0	31
2760	Spectroscopic profiling (FT-IR, FT-Raman, NMR and UV-Vis), autoxidation mechanism (H-BDE) and molecular docking investigation of 3-(4-chlorophenyl)- <i>N,N</i> -dimethyl-3-pyridin-2-ylpropan-1-amine by DFT/TD-DFT and molecular dynamics: A potential SSRI drug. <i>Computational Biology and Chemistry</i> , 2018, 77, 131-145.	1.1	29
2761	Theoretical research on the effect of Eosin Y adsorption action on Ru ₄ and Pt ₄ clusters on the hydrogen evolution performance. <i>Computational and Theoretical Chemistry</i> , 2018, 1142, 15-20.	1.1	3
2762	A dipotassium 1,2,4-diazaphospholide dianion radical as an organometallic building block: the first 1,2-diaza-4-phosphine ruthenocene. <i>Dalton Transactions</i> , 2018, 47, 13332-13336.	1.6	3

#	ARTICLE	IF	CITATIONS
2763	A simulation study of water property changes using geometrical alteration in SPC/E. Chinese Physics B, 2018, 27, 083103.	0.7	6
2764	Initiation of heterogeneous Schrock-type Mo and W oxide metathesis catalysts: A quantum thermochemical study. Computational Materials Science, 2018, 155, 197-208.	1.4	31
2765	An Orbital-Overlap Complement to Ligand and Binding Site Electrostatic Potential Maps. Journal of Chemical Information and Modeling, 2018, 58, 1836-1846.	2.5	22
2766	Molecular Controlling the Transport Properties for Benzothiadiazole-Based Hole Transport Materials. Applied Sciences (Switzerland), 2018, 8, 1461.	1.3	2
2767	Al doped boron clusters: Planar B ₁₉ Al. Chemical Physics Letters, 2018, 710, 26-30.	1.2	4
2768	How Do Secondary Phosphine Oxides Interact with Silver Nanoclusters? Insights from Computation. Journal of Physical Chemistry C, 2018, 122, 21449-21461.	1.5	5
2769	Multiscale Simulation Approach on Sub-10 nm Extreme Ultraviolet Photoresist Patterning: Insights from Nanoscale Heterogeneity of Polymer. Macromolecules, 2018, 51, 6922-6935.	2.2	18
2770	Ingenious modification of molecular structure effectively regulates excited-state intramolecular proton and charge transfer: a theoretical study based on 3-hydroxyflavone. RSC Advances, 2018, 8, 29589-29597.	1.7	42
2771	In Situ Doping Boron Atoms into Porous Carbon Nanoparticles with Increased Oxygen Graft Enhances both Affinity and Durability toward Electrolyte for Greatly Improved Supercapacitive Performance. Advanced Functional Materials, 2018, 28, 1804190.	7.8	149
2772	Competitive Routes for Electrochemical Oxidation of Substituted Diarylamines: the Guidelines. ChemElectroChem, 2018, 5, 3391-3410.	1.7	11
2773	Analyzing torquoselectivity in a series of unusual ring-opening reactions through bond reactivity indices and the adaptive natural density partitioning method. International Journal of Quantum Chemistry, 2018, 118, e25778.	1.0	5
2774	Cycloaddition reactions of pristine and endohedral fullerene molecules: possible anticancer activity. Journal of Molecular Modeling, 2018, 24, 268.	0.8	4
2775	Is π -hole an electronic exchange channel in YX \cdots CO interactions?. Chemical Physics Letters, 2018, 710, 113-117.	1.2	3
2776	Electrochemical oxidation of pyrrole, pyrazole and tetrazole using a TiO ₂ nanotubes based SnO ₂ -Sb/3D highly ordered macro-porous PbO ₂ electrode. Journal of Electroanalytical Chemistry, 2018, 826, 181-190.	1.9	39
2777	Pentafluoroethane Dehydration with Ionic Liquids. Industrial & Engineering Chemistry Research, 2018, 57, 12225-12234.	1.8	12
2778	Counter-Intuitive Stability in Actinide-Encapsulated Metalloid Clusters with Broken Aromaticity. Journal of Physical Chemistry C, 2018, 122, 22469-22479.	1.5	1
2779	Selective Adsorption and Separation of Xylene Isomers and Benzene/Cyclohexane with Microporous Organic Polymers POP-1. ACS Applied Materials & Interfaces, 2018, 10, 32717-32725.	4.0	47
2780	Computational Mechanistic Analysis of Intramolecular Cycloadditions of the 1,3-Dithiolium Cation with Adjacent Alkene and Allene Functional Groups. ACS Omega, 2018, 3, 9770-9780.	1.6	4

#	ARTICLE	IF	CITATIONS
2781	Substituent effect of the stacking interaction between carbon monoxide and benzene. <i>Journal of Molecular Modeling</i> , 2018, 24, 136.	0.8	4
2782	Gas separation by ionic liquids: A theoretical study. <i>Chemical Engineering Science</i> , 2018, 189, 43-55.	1.9	38
2783	Monodisperse π - π Stacking Anthracene Dimer under Pressure: Unique Fluorescence Behaviors and Experimental Determination of Interplanar Distance at Excimer Equilibrium Geometry. <i>Advanced Optical Materials</i> , 2018, 6, 1800085.	3.6	63
2784	Theoretical insights into the structural and fluorescence properties of DNA containing fluorescent nucleobases. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16641-16649.	1.3	1
2785	Complexes between neutral oxyacid beryllium salts and dihydrogen: a possible way for hydrogen storage?. <i>Dalton Transactions</i> , 2018, 47, 12516-12520.	1.6	7
2786	Zinc(II)-N ₂ O ₂ ligation complex-based DNA/protein binder and cleaver having enhanced cytotoxic and phosphatase activity. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4400.	1.7	4
2787	Structures and bonding properties of Pd _n C ₂₀ (n = 1-7) clusters. <i>Chemical Physics Letters</i> , 2018, 705, 65-70.	1.2	1
2788	Aqueous solutions of NMA, Na ₂ HPO ₄ , and NaH ₂ PO ₄ as models for interaction studies in phosphate-protein systems. <i>Journal of Molecular Liquids</i> , 2018, 265, 361-371.	2.3	16
2789	Th-Based Endohedral Metallofullerenes: Anomalous Metal Position and Significant Metal-Cage Covalent Interactions with the Involvement of Th 5f Orbitals. <i>Inorganic Chemistry</i> , 2018, 57, 7142-7150.	1.9	21
2790	Cluster-model DFT simulations of the infrared spectra of triazine-based molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20779-20784.	1.3	14
2791	Diisopropyl fluorophosphate (DFP) degradation activity using transition metal-dipicolylamine complexes. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4383.	1.7	4
2792	A DFT assessment of some physical properties of iodine-centered halogen bonding and other non-covalent interactions in some experimentally reported crystal geometries. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 15316-15329.	1.3	23
2793	C ₂ N-supported single metal ion catalysts for HCOOH dehydrogenation. <i>Journal of Materials Chemistry A</i> , 2018, 6, 11105-11112.	5.2	40
2794	Hole Mobility Modulation in Single-Crystal Metal Phthalocyanines by Changing the Metal- π - π Interactions. <i>Angewandte Chemie</i> , 2018, 130, 10269-10274.	1.6	10
2795	Crystal structure and theoretical charge density studies of dilantin molecule. <i>Journal of Molecular Structure</i> , 2018, 1170, 105-118.	1.8	8
2796	Most favorable cumulenic structures in iron-capped linear carbon chains are short singlet odd-carbon dications: a theoretical view. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 15496-15506.	1.3	6
2797	Effect of side chain edge functionalization in pristine and defected graphene-DFT study. <i>Computational and Theoretical Chemistry</i> , 2018, 1135, 34-47.	1.1	6
2798	Investigations based on non-covalent interactions in 1-(4-chloromethylbenzoyl)-3-(4, 6-di-substituted) Tj ETQq1 1 0.784314 rgBT /Overd Molecular Structure, 2018, 1169, 85-95.	1.8	12

#	ARTICLE	IF	CITATIONS
2799	Macrocyclic Receptor for Precious Gold, Platinum, or Palladium Coordination Complexes. <i>Journal of the American Chemical Society</i> , 2018, 140, 6810-6813.	6.6	47
2800	A theoretical investigation on Cu/Ag/Au bonding in $XH_2P\hat{c}MY$ ($X = H, CH_3, F, CN, NO_2$; $M = Cu, Ag, Au$; $Y = F$) $Tj ETQq1 1 0.784314$	1.2	27
2801	A Computational Mechanistic Study of the Chemo- and Enantioselectivity in the 1,4-Addition Reaction Catalyzed by a Rh Complex of Sulfinyl-Phosphine. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 3426-3431.	1.2	2
2802	Spatio-temporal profiling of abscisic acid, indoleacetic acid and jasmonic acid in single rice seed during seed germination. <i>Analytica Chimica Acta</i> , 2018, 1031, 119-127.	2.6	44
2803	Improving the NLO response of bis-cyclometalated iridium(\hat{c}) complexes by modifying ligands: A DFT study. <i>Journal of Organometallic Chemistry</i> , 2018, 869, 18-25.	0.8	23
2804	Lewis acidity of benzene in half-sandwich ruthenium arene complex. A computational study. <i>Computational and Theoretical Chemistry</i> , 2018, 1136-1137, 34-48.	1.1	7
2805	Zwitterions of the excited 4-([2,2'-bipyridine]-4-yl) phenol photoacid molecules: Formation and fluorescence. <i>Journal of Molecular Liquids</i> , 2018, 264, 48-53.	2.3	24
2806	Ligation-Enhanced \hat{c} -Hole- \hat{c} Interactions Involving Isocyanides: Effect of \hat{c} -Hole- \hat{c} Noncovalent Bonding on Conformational Stabilization of Acyclic Diaminocarbene Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 6722-6733.	1.9	50
2807	Mechanistic insights into the catalytic role of various acid sites on ZSM-5 zeolite in the carbonylation of methanol and dimethyl ether. <i>Catalysis Science and Technology</i> , 2018, 8, 3193-3204.	2.1	29
2808	X-ray structures, spectroscopic, electrochemical, thermal, antibacterial, and DFT studies of two nickel(II) and cobalt(III) complexes constructed from a new quinazoline-type ligand. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4426.	1.7	30
2809	Temperature dependent chiroptical response of sigmoidal gold clusters: probing the stability of chiral metal clusters. <i>Chemical Science</i> , 2018, 9, 5614-5622.	3.7	14
2810	Structural evolution and properties of small-size thiol-protected gold nanoclusters. <i>Molecular Physics</i> , 2018, 116, 1804-1811.	0.8	3
2811	Revisiting electronic nature and geometric parameters of cyclophanes and their relation with stability \hat{c} DFT, QTAIM and NCI study. <i>Computational and Theoretical Chemistry</i> , 2018, 1135, 18-27.	1.1	4
2812	An insight into the relationship between morphology and open circuit voltage/electronic absorption spectrum at donor-acceptor interface in boron subphthalocyanine chloride/C70 solar cell: A DFT/TDDFT exploration. <i>Organic Electronics</i> , 2018, 59, 279-287.	1.4	22
2813	S \hat{c} -S and S \hat{c} -P chalcogen bonding in solution: a cryospectroscopic study of the complexes of 2,2,4,4-tetrafluoro-1,3-dithietane with dimethyl sulfide and trimethylphosphine. <i>New Journal of Chemistry</i> , 2018, 42, 10563-10571.	1.4	8
2814	A detailed DFT/TDDFT study on excited-state intramolecular hydrogen bonding dynamics and proton-transfer mechanism of 2-phenanthro[9,10-d]oxazol-2-yl-phenol. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3857.	0.9	17
2815	Thorium Cubanes \hat{c} Synthesis, Solid-State and Solution Structures, Thermolysis, and Chalcogen Exchange Reactions. <i>Inorganic Chemistry</i> , 2018, 57, 7129-7141.	1.9	10
2816	Unmasking the Optimal Isomers of $Ti_{2}C_{84}$: $Ti_{2}C_{82}$ Instead of $Ti_{2}C_{84}$. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13148-13155.	1.5	10

#	ARTICLE	IF	CITATIONS
2817	Computational studies on the doped graphene quantum dots as potential carriers in drug delivery systems for isoniazid drug. <i>Structural Chemistry</i> , 2018, 29, 1427-1448.	1.0	63
2818	The influence of aggregation on the third-order nonlinear optical property of π -conjugated chromophores: the case of cyanine dyes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16777-16785.	1.3	8
2819	Towards the low-sensitive and high-energetic co-crystal explosive CL-20/TNT: from intermolecular interactions to structures and properties. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17253-17261.	1.3	24
2820	The role of nitric acid in atmospheric new particle formation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17406-17414.	1.3	47
2821	Formation and Extractive Desulfurization Mechanisms of Aromatic Acid Based Deep Eutectic Solvents: An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2018, 24, 11021-11032.	1.7	59
2822	Van der Waals interaction between perhalogenated ethylene and rare gas: A rotational study of chlorotrifluorethylene-argon. <i>Journal of Chemical Physics</i> , 2018, 148, 154302.	1.2	1
2823	Insights into the luminescent properties of anionic cyclometalated iridium(III) complexes with ligands derived from natural products. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25664.	1.0	6
2824	Experimental and computational study on mechanism of dichromate adsorption by ionic liquid-bonded silica gel. <i>Separation and Purification Technology</i> , 2018, 205, 84-93.	3.9	23
2825	Structure-Directing Weak Interactions with 1,4-Diodotetrafluorobenzene Convert One-Dimensional Arrays of $[M^{II}(acac)_2]$ Species into Three-Dimensional Networks. <i>Crystal Growth and Design</i> , 2018, 18, 3626-3636.	1.4	50
2826	Rigidity and Polarity Effects on the Electronic Properties of Two Deep Blue Delayed Fluorescence Emitters. <i>Journal of Physical Chemistry C</i> , 2018, 122, 11961-11972.	1.5	13
2827	Mechanistic understanding of $[Rh(NHC)]$ -catalyzed intramolecular $[5 + 2]$ cycloadditions of vinylxiranes and vinylcyclopropanes with alkynes. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 4295-4303.	1.5	8
2828	Cooperative effects between $F\cdots Ag$ bonded and $X\cdots Br$ (Cl) halogen-bonded interaction in $BrF(ClF)\cdots AgX\cdots BrF(ClF)$ ($X = F, Cl, Br$) complexes: a theoretical study. <i>Molecular Physics</i> , 2018, 116, 1834-1843.	1.1	1
2829	Vibrational spectra of alkylamino substituted phthalocyanine compounds: Density functional theory calculations. <i>Journal of Porphyrins and Phthalocyanines</i> , 2018, 22, 771-776.	0.4	4
2830	Density functional study of adsorption and desorption dynamics of hydrogen in zirconium doped aluminium clusters. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 21724-21731.	3.8	11
2831	New shape-selectivity discovered on graphene-based materials in catching tobacco specific nitrosamines. <i>Journal of Hazardous Materials</i> , 2018, 358, 234-242.	6.5	16
2832	A theoretical design of performant chlorinated benzothiadiazole-based polymers as donor for organic photovoltaic devices. <i>Organic Electronics</i> , 2018, 61, 46-55.	1.4	5
2833	Reproduction of the UV-vis spectra of boron subphthalocyanine chloride in different solvents using time-dependent generalized Kohn-Sham density functionals with first solvation shell. <i>Journal of Porphyrins and Phthalocyanines</i> , 2018, 22, 670-678.	0.4	8
2834	Structure and stability of propellane-like $E_2E_2\hat{E}^2$. <i>Journal of Molecular Modeling</i> , 2018, 24, 190.	0.8	1

#	ARTICLE	IF	CITATIONS
2835	Theoretical models to predict the inhibitory effect of ligands of sphingosine kinase 1 using QTAIM calculations and hydrogen bond dynamic propensity analysis. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 781-791.	1.3	9
2836	Serine adsorption through different functionalities on the B12N12 and Pt-B12N12 nanocages. <i>Materials Science and Engineering C</i> , 2018, 92, 216-227.	3.8	45
2837	Krypton-methanol spectroscopic study: Assessment of the complexation dynamics and the role of the van der Waals interaction. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 205, 179-185.	2.0	4
2838	Rational Design of Mono- and Dianions as Superacids Through π -Hole Interaction: Implications for Lithium and Magnesium Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16464-16472.	1.5	3
2839	Density functional theory study on the adsorption of valproic acid to doped fullerenes. <i>Main Group Metal Chemistry</i> , 2018, 41, 67-71.	0.6	5
2840	A Peri-tetracene Diradicaloid: Synthesis and Properties. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 9697-9701.	7.2	92
2841	Boron-Substituted Coronene: Intriguing Geometric and Electronic Properties, and Large Nonlinear Optical Response. <i>ChemPhysChem</i> , 2018, 19, 2518-2524.	1.0	11
2842	First-Principles Study on the Adsorption of HF on Reduced Graphene Oxide. <i>ChemistrySelect</i> , 2018, 3, 6979-6984.	0.7	8
2843	Wrinkle- and Edge-Adsorption of Aromatic Compounds on Graphene Oxide as Revealed by Atomic Force Microscopy, Molecular Dynamics Simulation, and Density Functional Theory. <i>Environmental Science & Technology</i> , 2018, 52, 7689-7697.	4.6	84
2844	Strategic design of thiophene-fused nickel dithiolene derivatives for efficient NLO response. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19007-19016.	1.3	13
2845	Mono BN-substituted analogues of naphthalene: a theoretical analysis of the effect of BN position on stability, aromaticity and frontier orbital energies. <i>New Journal of Chemistry</i> , 2018, 42, 12968-12976.	1.4	15
2846	An Algorithm for Evaluation of Potential Hazards in Research and Development of New Energetic Materials in Terms of their Detonation and Ballistic Profiles. <i>Propellants, Explosives, Pyrotechnics</i> , 2018, 43, 818-824.	1.0	11
2847	Enantioseparation of fluorinated 3-arylthio-4,4'-bipyridines: Insights into chalcogen and π -hole bonds in high-performance liquid chromatography. <i>Journal of Chromatography A</i> , 2018, 1567, 119-129.	1.8	22
2848	A Peri-tetracene Diradicaloid: Synthesis and Properties. <i>Angewandte Chemie</i> , 2018, 130, 9845-9849.	1.6	40
2849	Conformational analysis of ticagrelor: effect of noncovalent interaction on conformational population. <i>Structural Chemistry</i> , 2018, 29, 1663-1670.	1.0	3
2850	Molecular dynamics investigation of structures and the potentials of para tellurite (TeO_2) and europium oxide (Eu_2O_3) materials by aiming the effect of Eu^{3+} low doping in TeO_2 on the mechanical and structural properties. <i>Indian Journal of Physics</i> , 2018, 92, 1373-1384.	0.9	0
2851	Theoretical study of a series of 4,4'-azo-1,2,4-triazol-5-one based nitrogen-rich salts as potential energetic compounds. <i>RSC Advances</i> , 2018, 8, 23805-23816.	1.7	7
2852	Preparation and reactivity of half-sandwich dioxygen complexes of ruthenium. <i>Dalton Transactions</i> , 2018, 47, 9173-9184.	1.6	6

#	ARTICLE	IF	CITATIONS
2853	Synthesis, structure, and photophysical and electrochemical properties of Ru(II) complexes of arylenevinylene terpyridyl conjugates. <i>Dalton Transactions</i> , 2018, 47, 9877-9888.	1.6	3
2854	Theoretical study on the acidities of pyrrole, indole, carbazole and their hydrocarbon analogues in DMSO. <i>Canadian Journal of Chemistry</i> , 2018, 96, 1001-1009.	0.6	4
2855	A mechanistic MEDT study of the competitive catalysed [4+2] and [2+2] cycloaddition reactions between 1-methyl-1-phenylallene and methyl acrylate: the role of Lewis acid on the mechanism and selectivity. <i>Structural Chemistry</i> , 2018, 29, 1709-1721.	1.0	15
2856	ONIOM DFT study of the adsorption of cytosine on the Au/Ag and Ag/Au bimetallic nanosurfaces: The effect of sublayer. <i>Applied Surface Science</i> , 2018, 457, 712-725.	3.1	12
2857	Computational screening and molecular design of anthracene-based semiconductors. <i>Organic Electronics</i> , 2018, 61, 87-95.	1.4	5
2858	Theoretical exploitation of acceptors based on benzobis(thiadiazole) and derivatives for organic NIR-II fluorophores. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19759-19767.	1.3	24
2859	Structural evolution and bonding properties of Au ₂ Sin ^{+/0} (n = 1-7) clusters: Anion photoelectron spectroscopy and theoretical calculations. <i>Journal of Chemical Physics</i> , 2018, 148, 244306.	1.2	33
2860	Quantum mechanical studies on dioxin-imprinted polymer precursor composites: Fundamental insights to enhance the binding strength and selectivity of biomarkers. <i>Journal of Molecular Recognition</i> , 2018, 31, e2736.	1.1	12
2861	Insertion of 1-t-butylpropyne into singly tucked-in permethyltitanocene. Synthesis, crystal structure of product and transition-state geometry. <i>Journal of Molecular Structure</i> , 2018, 1167, 180-186.	1.8	4
2862	Physical Insight on Mechanism of Photoinduced Charge Transfer in Multipolar Photoactive Molecules. <i>Scientific Reports</i> , 2018, 8, 10089.	1.6	14
2863	Theoretical insight into the mechanism, regioselectivity, and substituent group effect of Rh-catalyzed synthesis of 1,2-benzothiazines from NH-sulfoximines and diazo compounds. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 5321-5331.	1.5	4
2864	Excited state intramolecular proton transfer mechanism of o-hydroxynaphthyl phenanthroimidazole. <i>Chinese Physics B</i> , 2018, 27, 023103.	0.7	19
2865	Choice of a spin singlet or triplet: electronic properties of Bis-Co(II), Bis-Ni(II), Bis-Cu(II) and Bis-Zn(II) oxygen doubly N-confused hexaphyrin (1.1.1.1.1.1). <i>Journal of Molecular Modeling</i> , 2018, 24, 185.	0.8	0
2866	A good balance between the energy density and sensitivity from assembly of bis(dinitromethyl) and bis(fluorodinitromethyl) with a single furazan ring. <i>Journal of Analytical and Applied Pyrolysis</i> , 2018, 134, 218-230.	2.6	15
2867	Conformational sensitivity of surface selection rules for quantitative Raman identification of small molecules in biofluids. <i>Nanoscale</i> , 2018, 10, 14342-14351.	2.8	13
2868	Achieving Efficient and Low Content Ru-Based Catalyst for Acetylene Hydrochlorination Based on N,N'-Dimethylpropyleneurea. <i>ChemCatChem</i> , 2018, 10, 4090-4099.	1.8	29
2869	Synthesis, structural characterization, DFT calculations and Hirshfeld surface analysis of (R)-2-((S)-2((S)-hydroxy(ferrocenyl)methyl)aziridin-1-yl)butan-1-ol. <i>Journal of Molecular Structure</i> , 2018, 1173, 33-41.	1.8	2
2870	Anion photoelectron spectroscopy and chemical bonding of ThO ₂ ⁺ and ThO ₃ ⁺ . <i>Journal of Chemical Physics</i> , 2018, 148, 244304.	1.2	6

#	ARTICLE	IF	CITATIONS
2871	Study of the Deformation/Interaction Model: How Interactions Increase the Reaction Barrier. <i>Journal of Chemistry</i> , 2018, 2018, 1-8.	0.9	5
2872	Conjugation in multi-tetrazole derivatives: a new design direction for energetic materials. <i>Journal of Molecular Modeling</i> , 2018, 24, 173.	0.8	4
2873	Synthesis, crystal structure, magnetic properties and DFT calculations of a mononuclear copper(II) complex: Relevance of halogen bonding for magnetic interaction. <i>Inorganica Chimica Acta</i> , 2018, 482, 395-401.	1.2	8
2874	Insights into the N-Heterocyclic Carbene (NHC)-Catalyzed Oxidative \hat{I}^3 -C(sp ³)â€“H Deprotonation of Alkylalens and Cascade [4 + 2] Cycloaddition with Alkenylisoxazoles. <i>Journal of Organic Chemistry</i> , 2018, 83, 8543-8555.	1.7	61
2875	Exploring the mechanisms of aqueous methanol dehydrogenation catalyzed by defined PNP Mn and Re pincer complexes under base-free as well as strong base conditions. <i>Catalysis Science and Technology</i> , 2018, 8, 3649-3665.	2.1	32
2876	Frozen-density embedding as a quasi-diabatization tool: Charge-localized states for spin-density calculations. <i>Journal of Chemical Physics</i> , 2018, 148, 214104.	1.2	13
2877	Evaluation of Nâ€“H...S and Nâ€“H...Ï€ interactions in <i>O</i>, <i>O</i>â€“diethyl<i>N</i>-(2,4,6-trimethylphenyl)thiophosphate: a combination of X-ray crystallographic and theoretical studies. <i>Acta Crystallographica Section C, Structural Chemistry</i>, 2018, 74, 847-855.</i>	0.2	11
2878	A theoretical prediction about harnessing ESPT process for HBO derivatives. <i>Structural Chemistry</i> , 2018, 29, 1655-1661.	1.0	11
2879	The role of chlorine substituents in lichexanthones properties: the ionic and halogen bond interactions. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	0
2880	Computational assessment of energetic salts containing 7H-[1,2,4]triazolo[4,3-b][1,2,4]triazole. <i>Journal of Chemical Sciences</i> , 2018, 130, 1.	0.7	0
2881	Ultrafast Deep-Ultraviolet Laser Ionization Mass Spectrometry Applicable To Identify Phenylenediamine Isomers. <i>Analytical Chemistry</i> , 2018, 90, 10635-10640.	3.2	19
2882	Effect of Cosolvents DMSO and Glycerol on the Self-Assembly Behavior of SDBS and CPC: An Experimental and Theoretical Approach. <i>Journal of Chemical & Engineering Data</i> , 2018, 63, 3083-3096.	1.0	27
2883	Cooperative effects between Ï€-hole triel and Ï€-hole chalcogen bonds. <i>RSC Advances</i> , 2018, 8, 26580-26588.	1.7	33
2884	Theoretical investigations on azole-fused tricyclic 1,2,3,4-tetrazine-2-oxides. <i>RSC Advances</i> , 2018, 8, 27235-27245.	1.7	9
2885	Mechanistic investigation in the [1,4] and [1,2] Wittig rearrangement reactions: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21457-21473.	1.3	3
2886	Chiral bisoxazoline catalyzed decarboxylative aldol reactions between \hat{I}^2 -carbonyl acids and trifluoroacetaldehyde hemiacetals as well as trifluoroacetaldehyde: the mechanism, the origin of enantioselectivity and the role of a catalyst. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2692-2709.	2.3	18
2887	Influence of an exciton-delocalizing ligand on the structural, electronic, and spectral features of the Cd ₃₃ S ₃₃ quantum dot: insights from computational studies. <i>Journal of Materials Chemistry C</i> , 2018, 6, 8751-8761.	2.7	7
2888	Enantioselective permeations of amino acids through l-proline-modified gold nanochannel membrane: an experimental and theoretical study. <i>Amino Acids</i> , 2018, 50, 1549-1556.	1.2	17

#	ARTICLE	IF	CITATIONS
2889	Assessment of solvent effects on the inclusion behavior of pyrazinamide drug into cyclic peptide based nanotubes as novel drug delivery vehicles. <i>Journal of Molecular Liquids</i> , 2018, 268, 326-334.	2.3	28
2890	Origin and Structural Characteristics of Tri-coordinated Extra-framework Aluminum Species in Dealuminated Zeolites. <i>Journal of the American Chemical Society</i> , 2018, 140, 10764-10774.	6.6	113
2891	Synthesis, X-ray structure, DFT and antimicrobial studies of Ag(I) complexes with nicotinic acid derivatives. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2018, 187, 48-53.	1.7	14
2892	Understanding of Structure and Thermodynamics of Melamine Association in Aqueous Solution from a Unified Theoretical and Experimental Approach. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1610-1624.	2.5	11
2893	Conformational dynamics of 1-phenyl-2,2,2-trifluoroethanol by rotational spectroscopy and ab initio calculations. <i>Journal of Molecular Spectroscopy</i> , 2018, 351, 62-67.	0.4	31
2894	Tetrel bonds between $\text{PhSiF}_3/\text{PhTH}_3$ ($\text{T} = \text{Si, Ge, Sn}$) and H_3ZO ($\text{Z} = \text{N, Tj ET O}$) e25660.	1.0	4
2895	Strong metallophilic interactions in nickel coordination compounds. <i>Inorganica Chimica Acta</i> , 2018, 483, 21-25.	1.2	12
2896	Exciton Self-Trapping in sp^2 Carbon Nanostructures Induced by Edge Ether Groups. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4857-4864.	2.1	55
2897	Supramolecular structures of rhenium(I) complexes mediated by ligand planarity <i>via</i> the interplay of substituents. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 997-1006.	0.2	12
2898	Modeling the Self-Assembly of 5-Hydroxy-6-methyluracil within Electrostatic Potential Approach. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 1523-1529.	0.1	1
2899	Hydrogen migration in Coulomb explosion of cyclohexane to C_2H_4^+ and C_4H_8^+ : Theoretical and experimental studies. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25764.	1.0	2
2900	Structural and bonding properties of Cu_3O_3^+ and Cu_3O_4^+ clusters: anion photoelectron spectroscopy and density functional calculations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20622-20628.	1.3	6
2901	Hierarchical tandem assembly of planar $[3\text{Å}-3]$ building units into $\{3\text{Å}-[3\text{Å}-3]\}$ oligomers: mixed-valency, electrical conductivity and magnetism. <i>Chemical Science</i> , 2018, 9, 7498-7504.	3.7	23
2902	Hybrid DFT study on non-covalent interactions and their influence on pKa's of magnesium-carboxylate complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 85, 13-24.	1.3	5
2903	Toward Electron Correlation and Electronic Properties from the Perspective of Information Functional Theory. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6424-6437.	1.1	12
2904	Effective Impact of Dielectric Constant on Thermally Activated Delayed Fluorescence and Nonlinear Optical Properties: Through-Bond/Space Charge Transfer Architectures. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18850-18859.	1.5	27
2905	Interaction between doped C_{60} fullerenes and piperazine-2,3,5,6-tetraone: DFT simulation. <i>Main Group Metal Chemistry</i> , 2018, 41, 63-66.	0.6	8
2906	Computational study on the interaction of nucleobases with boron-rich boron nitride nanotubes. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25757.	1.0	4

#	ARTICLE	IF	CITATIONS
2907	Flap-site Fragment Restores Back Wild-type Behaviour in Resistant Form of HIV Protease. <i>Molecular Informatics</i> , 2018, 37, 1800053.	1.4	2
2908	Tautomerism of protonated imidazoles: A perspective from ab initio valence bond theory. <i>Tetrahedron</i> , 2018, 74, 4791-4798.	1.0	7
2909	Co-synthesis of atomically precise nickel nanoclusters and the pseudo-optical gap of Ni ₄ (SR) ₈ . <i>Dalton Transactions</i> , 2018, 47, 11097-11103.	1.6	10
2910	Unexpected diverseness on electronic density and bonding behaviours for Sc ₂ X@C ₂ (63751)-C ₈₆ and Sc ₂ X@C ₁ (63755)-C ₈₆ (X = S and O). <i>Chemical Physics Letters</i> , 2018, 707, 93-100.	1.2	3
2911	Combined Experimental and Theoretical Investigations of Group 6 Dimetallaboranes [(Cp* <i>M</i>) ₂ B ₄ H ₁₀] (M = Mo and W). <i>Organometallics</i> , 2018, 37, 2419-2428.	1.1	12
2912	Observation of Olefin/Paraffin Selectivity in Azo Compound and Its Application into a Metal-Organic Framework. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 27521-27530.	4.0	26
2913	High efficiency green OLEDs based on homoleptic iridium complexes with steric phenylpyridazine ligands. <i>Dalton Transactions</i> , 2018, 47, 12243-12252.	1.6	23
2914	Porphyrin-Coumarin Dyads: Investigation of Photophysical Properties and DNA Interactions. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7797-7810.	1.2	9
2915	Theoretical Investigations on Molecular Packing Motifs and Charge Transport Properties of a Family of Trialkylsilylethynyl-Modified Pentacenes/Anthradithiophenes. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18880-18894.	1.5	15
2916	The Dual Role of Gold(I) Complexes in Photosensitizer-Free Visible-Light-Mediated Gold-Catalyzed 1,2-Difunctionalization of Alkynes: A DFT Study. <i>Chemistry - A European Journal</i> , 2018, 24, 14119-14126.	1.7	29
2917	Quantum-mechanical investigation of tetrel bond characteristics based on the point-of-charge (PoC) approach. <i>Journal of Molecular Modeling</i> , 2018, 24, 219.	0.8	22
2918	Chiral recognition of propranolol enantiomers by chiral ionic liquid: A quantum chemical calculation analysis. <i>Computational and Theoretical Chemistry</i> , 2018, 1140, 38-48.	1.1	12
2919	A Molecular Electron Density Theory Study of the Role of the Copper Metalation of Azomethine Ylides in [3 + 2] Cycloaddition Reactions. <i>Journal of Organic Chemistry</i> , 2018, 83, 10959-10973.	1.7	41
2920	Global Aromaticity in Macrocyclic Cyclopenta-Fused Tetraphenanthrenylene Tetraradicaloid and Its Charged Species. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 13052-13056.	7.2	54
2921	DFT study of single-walled carbon hollows as media for hydrogen storage. <i>Computational and Theoretical Chemistry</i> , 2018, 1140, 80-85.	1.1	20
2922	A high-rate and ultrastable anode enabled by boron-doped nanoporous carbon spheres for high-power and long life lithium ion capacitors. <i>Materials Today Energy</i> , 2018, 9, 428-439.	2.5	19
2923	Using phosphorescent PtAu ₃ clusters for superior solution-processable organic light emitting diodes with very small efficiency roll-off. <i>Journal of Materials Chemistry C</i> , 2018, 6, 8966-8976.	2.7	24
2924	Density functional theory studies on PVDF/ionic liquid composite systems. <i>Journal of Chemical Sciences</i> , 2018, 130, 1.	0.7	36

#	ARTICLE	IF	CITATIONS
2925	Synergy between Cu and Brønsted acid sites in carbonylation of dimethyl ether over Cu/H-MOR. <i>Journal of Catalysis</i> , 2018, 365, 440-449.	3.1	36
2926	First-principles and Molecular Dynamics simulation studies of functionalization of Au ₃₂ golden fullerene with amino acids. <i>Scientific Reports</i> , 2018, 8, 11400.	1.6	24
2927	Nonlinear optical properties of aluminum nitride nanotubes doped by excess electron: a first principle study. <i>Journal of Molecular Modeling</i> , 2018, 24, 205.	0.8	7
2928	Computational Evidence for the Enzymatic Transformation of 2-Hydroxypropylphosphonate to Methylphosphonate. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 888-894.	1.2	8
2929	Substituted troponimines: when aromatization of the conjugate acid leads to very strong neutral organic superbases. <i>New Journal of Chemistry</i> , 2018, 42, 14568-14575.	1.4	7
2930	Intra-/Intermolecular Bifurcated Chalcogen Bonding in Crystal Structure of Thiazole/Thiadiazole Derived Binuclear (Diaminocarbene)PdII Complexes. <i>Crystals</i> , 2018, 8, 112.	1.0	46
2931	Theoretical study of Sn adsorbed on the MgO(100) surface with defects. <i>Comptes Rendus Chimie</i> , 2018, 21, 669-675.	0.2	5
2932	Recent theoretical progress in the organic/metal-organic sensitizers as the free dyes, dye/TiO ₂ and dye/electrolyte systems; Structural modifications and solvent effects on their performance. <i>Renewable and Sustainable Energy Reviews</i> , 2018, 94, 609-655.	8.2	26
2933	Strategy Used for Controlling the Photostability of Tridentate Pt(II) Complexes To Enhance the Device Lifetimes of Blue Phosphorescent Organic Light-Emitting Diodes: The Role of the Pt-C*(NHC) Bond and Auxiliary Ligand. <i>Journal of Physical Chemistry C</i> , 2018, 122, 16872-16878.	1.5	6
2934	Novel molecular descriptors for prediction of H ₂ S solubility in ionic liquids. <i>Journal of Molecular Liquids</i> , 2018, 265, 756-764.	2.3	25
2935	Rhodamine 6G-Labeled Pyridyl Aroylhydrazone Fe(II) Complex Exhibiting Synergetic Spin Crossover and Fluorescence. <i>Journal of the American Chemical Society</i> , 2018, 140, 9426-9433.	6.6	93
2936	Geometrical Structures and Electronic Properties of Ga ₆ and Ga ₅ X (X = B, C, N, O, F, Al, Si, P, S, Cl) Clusters. <i>Materials</i> , 2018, 11, 552.	1.3	0
2937	Synthesis, Crystal Structure and DFT Studies of a New Dinuclear Ag(I)-Malonamide Complex. <i>Molecules</i> , 2018, 23, 888.	1.7	7
2938	Highly Efficient Luminescent Polycarboxylate Lanthanide Complexes Incorporated into Di-Ureasils by an In-Situ Sol-Gel Process. <i>Polymers</i> , 2018, 10, 434.	2.0	8
2939	A novel hydrogen storage medium of Ca-coated B40: First principles study. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 15338-15347.	3.8	30
2940	Deciphering the binding behavior of flavonoids to the cyclin dependent kinase 6/cyclin D complex. <i>PLoS ONE</i> , 2018, 13, e0196651.	1.1	15
2941	Excited state properties of two unusual thermally activated delayed fluorescence molecules: A theoretical investigation. <i>Journal of Luminescence</i> , 2018, 204, 312-318.	1.5	10
2942	Probing the oxidation state of transition metal complexes: a case study on how charge and spin densities determine Mn L-edge X-ray absorption energies. <i>Chemical Science</i> , 2018, 9, 6813-6829.	3.7	60

#	ARTICLE	IF	CITATIONS
2943	Bridgeâ€Caging Strategy in Phosphorusâ€CSubstituted Rhodamine for Modular Development of Nearâ€CInfrared Fluorescent Probes. Chemistry - A European Journal, 2018, 24, 14506-14512.	1.7	26
2944	Computational study of the NO, SO ₂ , and NH ₃ adsorptions on fragments of 3N-graphene and Al/3N graphene. Journal of Molecular Modeling, 2018, 24, 210.	0.8	6
2945	Bifunctional Separator Coated with Hexachlorocyclotriphosphazene/Reduced Graphene Oxide for Enhanced Performance of Lithiumâ€CSulfur Batteries. Chemistry - A European Journal, 2018, 24, 13582-13588.	1.7	12
2946	Halogen Bonding in Ring-Substituted Group 10 POCOP Iodido Complexes with Iodine and Its Possible Role in Oxidative Addition. European Journal of Inorganic Chemistry, 2018, 2018, 3913-3921.	1.0	5
2947	Improvement of Interfacial Stability for LiNi _{0.5} Mn _{1.5} O ₄ Cathode: Insight into the Effect and Mechanism of Additive with Special Structure. Energy Technology, 2018, 6, 2450-2460.	1.8	6
2948	The electronic structures and excitation properties of three meso-pentafluorophenyl substituted zinc porphyrinâ€Cfullerene dyad. Journal of Molecular Structure, 2018, 1173, 398-405.	1.8	13
2949	Unveiling Noncovalent Interactions in Imidazolium, Pyrrolidinium, or Quaternary Ammonium Cation and Acetate Anion Based Protic Ionic Liquids: Structure and Spectral Characteristics. Journal of Physical Chemistry A, 2018, 122, 6225-6235.	1.1	14
2950	Theoretical insight into the structure and bonding characteristics of Bisphenol-A. QTAIM and NBO analyses. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850034.	1.8	1
2951	Investigation on 1-Acetyl-4-(4-hydroxyphenyl) piperazine an anti-fungal drug by spectroscopic, quantum chemical computations and molecular docking studies. Journal of Molecular Structure, 2018, 1173, 583-595.	1.8	28
2952	Unified Mechanistic Understandings of Pictet-Spengler Reactions. Chem, 2018, 4, 1952-1966.	5.8	65
2953	Theoretical Insights into D-Dâ€CA Sensitizers Employing <i>N</i>-Annulated Perylene for Dye-Sensitized Solar Cells. Journal of Physical Chemistry A, 2018, 122, 6328-6342.	1.1	21
2954	Photoelectron spectroscopic and computational studies of [EDTAâ€CM(ⁱⁱⁱ)] ^{â€C} complexes (M = H ₃ , Al, Sc, Vâ€C-Co). Physical Chemistry Chemical Physics, 2018, 20, 19458-19469.	1.3	9
2955	[1,3]Thiazolo[3,2- <i>b</i>][1,2,4]triazol-7-ium salts: synthesis, properties and structural studies. Heterocyclic Communications, 2018, 24, 197-203.</i>	0.6	15
2956	Inferring the molecular arrangements of boron subphthalocyanine chloride in thin film from a DFT/TDDFT study of molecular clusters and experimental electronic absorption spectra. Organic Electronics, 2018, 62, 667-675.	1.4	16
2957	Noble gas hydrides in the triplet state: HNgCCO ⁺ (Ng = He, Ne, Ar, Kr, and Xe). Physical Chemistry Chemical Physics, 2018, 20, 20270-20279.	1.3	11
2958	Periodic and non-periodic DFT modeling of CO reduction on the surface of Ni-doped graphene nanosheet. Molecular Catalysis, 2018, 455, 239-249.	1.0	8
2959	Structural evolution and magnetic properties of anionic clusters Cr ₂ Ge _{n</sub> (<i>n</i>=14): photoelectron spectroscopy and density functional theory computation. Journal of Physics Condensed Matter, 2018, 30, 335501.}		20
2960	Synthesis and structural characterization of a diruthenium pentalene complex, $\{Cp\}^*Ru\{Cp\}^*Ru\}_2\{B\}_6\{H\}_{14}$. <i>Journal of Organometallic Chemistry</i> , 2018, 850, 1-10. DOI: 10.1016/j.jorganchem.2018.08.011	0.784314	0

#	ARTICLE	IF	CITATIONS
2961	Theoretical Mechanistic Study of Nickel(0)/Lewis Acid Catalyzed Polyfluoroarylcyanation of Alkynes: Origin of Selectivity for C≡CN Bond Activation. <i>Organometallics</i> , 2018, 37, 2594-2601.	1.1	12
2962	Theoretical evaluation of symmetrical 1,1,1,1-tetramethyl cucurbit[6]uril for haloalkane 1-(3-chlorophenyl)-4-(3-chloropropyl)-piperazinium and chloroform encapsulation. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2018, 92, 103-114.	0.9	2
2963	Insight into the optoelectronic properties of designed solar cells efficient tetrahydroquinoline dye-sensitizers on TiO ₂ (101) surface: first principles approach. <i>Scientific Reports</i> , 2018, 8, 10997.	1.6	44
2964	SCI: a robust and reliable density-based descriptor to determine multiple covalent bond orders. <i>Journal of Molecular Modeling</i> , 2018, 24, 213.	0.8	15
2965	Optical anti-counterfeiting of a single molecule by two solvents based on intra- and intermolecular excited state proton transfer mechanisms. <i>Dyes and Pigments</i> , 2018, 159, 506-512.	2.0	47
2966	The influence of the structural variations of the fused electron rich-electron deficient unit in the A-D-π-D-A organic dyes on the efficiency of dye-sensitized solar cells: A computational study. <i>Organic Electronics</i> , 2018, 62, 43-55.	1.4	13
2967	Rotational Spectrum and Conformational Analysis of N-Methyl-2-Aminoethanol: Insights into the Shape of Adrenergic Neurotransmitters. <i>Frontiers in Chemistry</i> , 2018, 6, 25.	1.8	6
2968	A density functional theory study on the interaction between UO ₂ ²⁺ and the carbamoylphosphoramidic acid ligand for uranium extraction from seawater. <i>Nuclear Science and Techniques/Hewuli</i> , 2018, 29, 1.	1.3	1
2969	Theoretical Exploration of Halogen Bonding Interactions in the Complexes of Novel Nitroxide Radical Probes and Comparison with Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5058-5068.	1.1	13
2971	Theoretical study on reaction mechanism of thermal decomposition of dialkyl peroxides. <i>Computational and Theoretical Chemistry</i> , 2018, 1135, 11-17.	1.1	10
2972	Selective extraction of plutonium(IV) over uranium(VI), americium(III), europium(III) and zirconium(IV) with bidentate O-phenoxydiamide ligands: experimental and theoretical study. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2018, 317, 103-110.	0.7	6
2973	Theoretical investigation on cyclohexane dehydrogenation catalyzed by V ²⁺ in gas-phase. <i>Structural Chemistry</i> , 2018, 29, 1129-1137.	1.0	2
2974	Theoretical study on the effective dehydrochlorination of 1,2-dichloroethane catalyzed by tetraalkylphosphonium chlorides: electrostatically controlled reactivity. <i>New Journal of Chemistry</i> , 2018, 42, 10084-10091.	1.4	2
2975	Cellulose nanofiber induced self-assembly of zinc oxide nanoparticles: Theoretical and experimental study on interfacial interaction. <i>Carbohydrate Polymers</i> , 2018, 195, 525-533.	5.1	45
2976	The order of multiple excited state proton transfer in ternary complex of norharmane and acetic acids. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 202, 30-35.	2.0	20
2977	Carbon-doped boron-nitride fullerenes as efficient metal-free catalysts for oxidation of SO ₂ : a DFT study. <i>Structural Chemistry</i> , 2018, 29, 275-283.	1.0	12
2978	Benchmark study of ionization potentials and electron affinities of armchair single-walled carbon nanotubes using density functional theory. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 215501.	0.7	10
2979	Hole Mobility Modulation in Single-Crystal Metal Phthalocyanines by Changing the Metal-π/π Interactions. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 10112-10117.	7.2	54

#	ARTICLE	IF	CITATIONS
2980	Theoretical investigation on the excited state intramolecular proton coupled charge transfer phenomenon for a novel fluorophore. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3856.	0.9	11
2981	Computational Approach to Unravel the Role of Hydrogen Bonding in the Interaction of NAMI-A with DNA Nucleobases and Nucleotides. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8397-8411.	1.1	4
2982	Noble Gas Inserted Metal Acetylides (Metal = Cu, Ag, Au). <i>Journal of Physical Chemistry A</i> , 2018, 122, 7391-7401.	1.1	25
2983	Synthesis, structures and characterization of complexes containing a 2,6-bis(guanidinyl)pyridine ligand on iron(II), cobalt(II), nickel(II), copper(I), copper(II) and zinc(II). <i>Polyhedron</i> , 2018, 155, 77-84.	1.0	4
2984	Insight into the nature of M=C bonding in the lanthanide/actinide-biscarbene complexes: a theoretical perspective. <i>Dalton Transactions</i> , 2018, 47, 12718-12725.	1.6	25
2985	Synthesis and characterization of N,N=C-bound organotellurium(IV) and organomercury(II) derivatives. <i>Inorganica Chimica Acta</i> , 2018, 483, 218-228.	1.2	4
2986	Designing an asymmetrical isomer to promote the LUMO energy level and molecular packing of a non-fullerene acceptor for polymer solar cells with 12.6% efficiency. <i>Chemical Science</i> , 2018, 9, 8142-8149.	3.7	67
2987	Confinement induced catalytic activity in a Diels-Alder reaction: comparison among various CB[n], n=6-8, cavitands. <i>Journal of Molecular Modeling</i> , 2018, 24, 228.	0.8	7
2988	Effect of a molecule of imidazolium bromide ionic liquid on the structure and properties of cytosine by density functional theory. <i>Chemical Physics Letters</i> , 2018, 708, 109-116.	1.2	7
2989	Exploring and elaborating the novel excited state dynamical behavior of a bisflavonol system. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2710-2718.	2.3	126
2990	A spectroscopic and <i>ab initio</i> study of the hydrogen peroxide-formic acid complex: hindering the internal motion of H ₂ O ₂ . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21345-21351.	1.3	10
2991	Chalcogenolato-bridged dinuclear half sandwich complexes of ruthenium and iridium. <i>Inorganica Chimica Acta</i> , 2018, 483, 106-110.	1.2	4
2992	Effects of oxygen functional complexes on arsenic adsorption over carbonaceous surface. <i>Journal of Hazardous Materials</i> , 2018, 360, 436-444.	6.5	66
2993	Theoretical study on crystal morphologies of 1,1-diamino-2,2-dinitroethene in solvents: Modified attachment energy model and occupancy model. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 85, 262-269.	1.3	16
2994	Insulation property analysis of cross-linked polyethylene based on density functional theory. , 2018, , .		2
2995	Investigating the Thermal Stability of Organic Thin-Film Transistors and Phototransistors Based on [1-Benzo-thieno[3,2-b]thiophene Dimeric Derivatives. <i>Chemistry - A European Journal</i> , 2018, 24, 16595-16602.	1.7	13
2996	Effects on the aromatic character of DNA/RNA nucleobases due to its adsorption onto graphene. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25699.	1.0	6
2997	Gas phase transformation from organic acid to organic sulfuric anhydride: Possibility and atmospheric fate in the initial new particle formation. <i>Chemosphere</i> , 2018, 212, 504-512.	4.2	29

#	ARTICLE	IF	CITATIONS
2998	Probing the geometric structures and bonding properties in Nb ₂ Si ₂₀ O clusters by density functional theory calculations. <i>Chemical Physics Letters</i> , 2018, 709, 60-64.	1.2	15
2999	Stabilities and electronic properties of nanowires made of single atomic sulfur chains encapsulated in zigzag carbon nanotubes. <i>Nanotechnology</i> , 2018, 29, 415703.	1.3	14
3000	Probing the structural and electronic properties of zirconium doped boron clusters: Zr distorted B ₁₂ ligand framework. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23740-23746.	1.3	43
3001	Structure, Conformational Equilibria, and Weak Hydrogen Bonding in the CH ₂ F ₂ CF ₃ CH ₂ F Dimer. <i>ChemPhysChem</i> , 2018, 19, 2655-2661.	1.0	4
3002	Charge transfer interactions of pyrazine with Ag ₁₂ clusters towards precise SERS chemical mechanism. <i>Nanoscale</i> , 2018, 10, 16787-16794.	2.8	12
3003	The Effect of Dyes with Different Ĥ-Linkers on the Overall Performance of P-DSSCs: Lessons from Theory. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7491-7496.	1.1	11
3004	Ab initio investigation of structure, stability, thermal behavior and infrared spectra of (BN) ₄ cluster. <i>Computational and Theoretical Chemistry</i> , 2018, 1141, 1-6.	1.1	5
3005	Solvation effect on the ESIPT mechanism of 2-(4- <i>o</i> -amino-2-hydroxyphenyl)-1H-imidazo-[4,5-c]pyridine. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 367, 261-269.	2.0	38
3006	Influence of Alkyne and Azide Substituents on the Choice of the Reaction Mechanism of the Cu ⁺ -Catalyzed Addition of Azides to Iodoalkynes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7497-7507.	1.1	12
3007	<i>N</i> -Fluoro functionalization of heterocyclic azoles: a new strategy towards insensitive high energy density materials. <i>New Journal of Chemistry</i> , 2018, 42, 16244-16257.	1.4	6
3008	Terahertz spectroscopy and vibrational analysis of sulfur mustard by quantum chemical calculations. <i>Computational and Theoretical Chemistry</i> , 2018, 1142, 21-27.	1.1	1
3009	Extended First Hyperpolarizability of Quasi-Octupolar Molecules by Halogenated Methylation: Whether the Iodine Atom is the Best Choice. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21548-21556.	1.5	30
3010	Theoretical investigations of the Ir-catalyzed direct borylation of B(3,6)-H of <i>o</i> -carborane: the actual catalyst, mechanism, and origin of regioselectivity. <i>Catalysis Science and Technology</i> , 2018, 8, 5165-5177.	2.1	22
3011	3D Porous Tin Created by Tuning the Redox Potential Acts as an Advanced Electrode for Sodium-Ion Batteries. <i>ChemSusChem</i> , 2018, 11, 3376-3381.	3.6	35
3012	Explicit Aqueous Solvation Treatment of Epinephrine from Car Parrinello Molecular Dynamics: Effect of Hydrogen Bonding on the Electronic Absorption Spectrum. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8439-8450.	1.2	7
3013	Regium bonds between M _n clusters (M = Cu, Ag, Au and <i>n</i> = 2-6) and nucleophiles NH ₃ and HCN. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22498-22509.	1.3	46
3014	Hydrogen storage on volleyballene. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21251-21256.	1.3	4
3015	Experimental and Theoretical Investigation of the Photoelectrical Properties of Tetrabromophenol Blue- and Bromoxylene Blue-Based Solar Cells. <i>Journal of Nanomaterials</i> , 2018, 2018, 1-13.	1.5	4

#	ARTICLE	IF	CITATIONS
3016	Theoretical insights into the magneto-structural correlation: Comparison between series of copper(I) and silver(I) metal complexes with nitronyl nitroxide radicals. <i>Computational and Theoretical Chemistry</i> , 2018, 1141, 53-65.	1.1	3
3017	Toward a Predictive Understanding of Phosphine-Catalyzed [3 + 2] Annulation of Allenolates with Acrylate or Imine. <i>Journal of Organic Chemistry</i> , 2018, 83, 9729-9740.	1.7	22
3018	Insights into N-heterocyclic carbene-catalyzed [3 + 4] annulation reactions of 2-bromoaldehydes with N-Ts hydrazones. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2739-2748.	2.3	49
3019	A Molecular Electron Density Theory Study of the Competitiveness of Polar Diels-Alder and Polar Alder-ene Reactions. <i>Molecules</i> , 2018, 23, 1913.	1.7	13
3020	Why Do B ^{III} -P and Al ^{III} -P Polymers Differ? Structures, Stability, and Electronic Properties of Chain and Ring [H ₂ PEH ₂] _n Oligomers (E=B, Al; n = 1-15). <i>Chemistry - A European Journal</i> , 2018, 24, 17046-17054.	1.7	7
3021	Replacement of an Azide Group with Carbonyl-Azide in Nitrogen-Rich Energetic Materials: Searching for Possible Alternatives with a Computational Approach. <i>ChemistrySelect</i> , 2018, 3, 8651-8655.	0.7	2
3022	Self-Catalytic Reaction of SO ₃ and NH ₃ To Produce Sulfamic Acid and Its Implication to Atmospheric Particle Formation. <i>Journal of the American Chemical Society</i> , 2018, 140, 11020-11028.	6.6	86
3023	Theoretical (density functional theory) studies on the structural, electronic and catalytic properties of the ionic liquid 4-amino-1H-1,2,4-triazolium nitrate. <i>Journal of Molecular Liquids</i> , 2018, 269, 529-539.	2.3	21
3024	Theoretical investigation of the effects of various substituents on the large energy gap between triplet excited-states of anthracene. <i>RSC Advances</i> , 2018, 8, 27979-27987.	1.7	10
3025	Thermally activated delayed fluorescence processes for Cu(I) complexes in solid-state: a computational study using quantitative prediction. <i>RSC Advances</i> , 2018, 8, 28421-28432.	1.7	8
3026	Probing the Structural Evolution and Stabilities of Medium-Sized MoB _n Clusters. <i>Journal of Physical Chemistry C</i> , 2018, 122, 20000-20005.	1.5	47
3027	Theoretical insight into the adsorption of aromatic compounds on graphene oxide. <i>Environmental Science: Nano</i> , 2018, 5, 2357-2367.	2.2	76
3028	Probing the geometric structures and bonding mechanisms of Cu I hybrid clusters: Cu ₄ I ₄ . <i>Computational and Theoretical Chemistry</i> , 2018, 1139, 102-105.	1.1	11
3029	Capturing Condensable Gases with Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 12202-12214.	1.8	43
3030	M-Learning: Atomic Orbitals of Elements in Periodic Table using SPATO. <i>Journal of Physics: Conference Series</i> , 2018, 1049, 012016.	0.3	0
3031	Theoretical modeling of argentophilic interactions in [Ag(CN) ₂] ₃ trimer found in a copper(II) complex of cis-1,2-diaminocyclohexane (Dach), [Cu(Dach) ₂ -Ag(CN) ₂ -Cu(Dach) ₂][Ag(CN) ₂] ₃ . <i>Chemical Physics Letters</i> , 2018, 709, 11-15.	1.2	4
3032	Beryllium-beryllium double- π bonds in the octahedral cluster of Be ₂ ($\frac{1}{4}$ Be ₂ -X) ₄ (X = Li, Cu, BeF). <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23898-23902.	1.3	38
3033	A combined molecular dynamics simulation and quantum mechanics study on the physisorption of biodegradable CBNAILs on h-BN nanosheets. <i>Journal of Chemical Physics</i> , 2018, 149, 074704.	1.2	11

#	ARTICLE	IF	CITATIONS
3034	Characterizing the sensitivity of bonds to the curvature of carbon nanotubes. <i>Journal of Molecular Modeling</i> , 2018, 24, 249.	0.8	25
3035	High-Energy Nitramine Explosives: A Design Strategy from Linear to Cyclic to Caged Molecules. <i>ACS Omega</i> , 2018, 3, 9739-9745.	1.6	32
3036	Ring-Closing Synthesis of Dibenzothiophene Sulfonium Salts and Their Use as Leaving Groups for Aromatic ¹⁸ F-Fluorination. <i>Journal of the American Chemical Society</i> , 2018, 140, 11125-11132.	6.6	63
3037	Synthesis and photophysical properties of ruthenium(^{II}) polyimine complexes decorated with flavin. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17504-17516.	1.3	16
3038	Solvent-regulated preparation of well-intercalated Ti ₃ C ₂ T _x MXene nanosheets and application for highly effective electromagnetic wave absorption. <i>Nanotechnology</i> , 2018, 29, 355201.	1.3	62
3039	Sulfadiazine oxidation by permanganate: Kinetics, mechanistic investigation and toxicity evaluation. <i>Chemical Engineering Journal</i> , 2018, 349, 56-65.	6.6	79
3040	Reaction Mechanism of Photodeamination Induced by Excited-State Intramolecular Proton Transfer of the Anthrol Molecule. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5409-5417.	1.1	18
3041	The surrounding environments on the structure and antioxidative activity of luteolin. <i>Journal of Molecular Modeling</i> , 2018, 24, 149.	0.8	11
3042	Electrostatic Polarization Energies of Charge Carriers in Organic Molecular Crystals: A Comparative Study with Explicit State-Specific Atomic Polarizability Based AMOEBA Force Field and Implicit Solvent Method. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3728-3739.	2.3	20
3043	Quantum-Chemical Study of the Oxidative Ability of Nitro Compounds Using Decomposition of Some Simple Amines in the Presence of Triplet Nitromethane as an Example. <i>High Energy Chemistry</i> , 2018, 52, 217-221.	0.2	3
3044	Structure and Reactivity of Pd Complexes in Various Oxidation States in Identical Ligand Environments with Reference to C-C and C-Cl Coupling Reactions: Insights from Density Functional Theory. <i>Inorganic Chemistry</i> , 2018, 57, 6833-6846.	1.9	13
3045	Hydrogen Storage on Volleyballene: Prediction of the Sc ₂₀ C ₆₀ H ₇₀ Cluster. <i>Journal of Physical Chemistry C</i> , 2018, 122, 14971-14978.	1.5	7
3046	Halogen bonding driven crystal engineering of iodophthalonitrile derivatives. <i>CrystEngComm</i> , 2018, 20, 3858-3867.	1.3	18
3047	Roles of different amino-acid residues towards binding and selective transport of K ⁺ through KcsA K ⁺ -ion channel. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17517-17529.	1.3	10
3048	Cyanide [−] isocyanide isomerization: stability and bonding in noble gas inserted metal cyanides (metal =) Tj ETQq0,0,0 rgBT /Qverlock 1	1.3	32
3049	Donor [−] Acceptor Complexes between 1,2,5-Chalcogenadiazoles (Te, Se, S) and the Pseudohalides CN [−] and XCN [−] (X=O, S, Se, Te). <i>Chemistry - A European Journal</i> , 2018, 24, 12983-12991.	1.7	41
3050	Active Mechanism of the Interphase Film-Forming Process for an Electrolyte Based on a Sulfolane Solvent and a Chelato-Borate Complex. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 25744-25753.	4.0	21
3051	Theoretical insights into the reaction mechanisms between 2,3,7,8-tetrachlorodibenzofuran and the methylidyne radical. <i>RSC Advances</i> , 2018, 8, 21150-21163.	1.7	6

#	ARTICLE	IF	CITATIONS
3052	Adsorption sensitivity of Fe decorated different graphene supports toward toxic gas molecules (CO) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	9.1	58
3053	Enhanced electro-optic activity and thermal stability by introducing rigid steric hindrance groups into double-donor chromophore. <i>Dyes and Pigments</i> , 2018, 159, 222-229.	2.0	4
3054	Designing High-Performance Composite Electrodes for Vanadium Redox Flow Batteries: Experimental and Computational Investigation. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 22381-22388.	4.0	42
3055	New Insights into Adsorption Behaviour of NH ₃ Molecules on Small (SiO ₂) _n (n=2-7) Clusters Through Systematic Analysis of Structural and Topological Properties. <i>Australian Journal of Chemistry</i> , 2018, 71, 482.	0.5	2
3056	A combined experimental and computational study of a ruthenium(II) polypyridyl complex: Synthesis, characterization, electronic structures and spectral properties. <i>Polyhedron</i> , 2018, 151, 441-445.	1.0	2
3057	Study of the effects of methanol, ethanol and propanol alcohols as Co-solvents on the interaction of methimazole, propranolol and phenazopyridine with carbon dioxide in supercritical conditions by molecular dynamics. <i>Journal of Supercritical Fluids</i> , 2018, 140, 91-100.	1.6	6
3058	Heteroleptic Cu(<i>scp</i>) complexes bearing methoxycarbonyl-imidoylindazole and POP ligands – an experimental and theoretical study of their photophysical properties. <i>New Journal of Chemistry</i> , 2018, 42, 12576-12586.	1.4	12
3059	Theoretical Study of Oil Desulfuration by Ammonium-Based Deep Eutectic Solvents. <i>Energy & Fuels</i> , 2018, 32, 7497-7507.	2.5	20
3060	The effects of different heterocycles and solvents on the ESIPT mechanisms of three novel photoactive mono-formylated benzoxazole derivatives. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2234-2243.	2.3	14
3061	Origin of Different Photovoltaic Activities in Regioisomeric Small Organic Molecule Solar Cells: The Intrinsic Role of Charge Transfer Processes. <i>Journal of Physical Chemistry C</i> , 2018, 122, 14296-14303.	1.5	18
3062	Clustering mechanism of oxocarboxylic acids involving hydration reaction: Implications for the atmospheric models. <i>Journal of Chemical Physics</i> , 2018, 148, 214303.	1.2	22
3063	Catalytic mechanism of sulfuric acid in cellulose pyrolysis: A combined experimental and computational investigation. <i>Journal of Analytical and Applied Pyrolysis</i> , 2018, 134, 183-194.	2.6	44
3064	Modulation of an Anagostic Interaction in SiPSi-Type Pincer Platinum Complexes. <i>Organometallics</i> , 2018, 37, 3581-3587.	1.1	8
3065	Diruthenium(ii)-capped oligothiénylethynyl bridged highly soluble organometallic wires exhibiting long-range electronic coupling. <i>Dalton Transactions</i> , 2018, 47, 14304-14317.	1.6	10
3066	Determination of antibiotics in feedstuff samples by microemulsion electrokinetic chromatography using fullerene as additive. <i>Electrophoresis</i> , 2018, 39, 2228-2235.	1.3	5
3067	Carbon Dioxide Absorption by the Imidazolium-Amino Acid Ionic Liquids, Kinetics, and Mechanism Approach. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5721-5729.	1.1	13
3068	Theoretical investigation of (tetrazine-3,6-diyl) dihydrazinecarboxamide-based high-nitrogen-containing energetic macromolecules. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1850028.	1.8	1
3069	Topology and Equilibrium Analysis of the Monovalent Aluminum Compound Al ₄ Cp*Ph ₄ . <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2018, 644, 454-464.	0.6	0

#	ARTICLE	IF	CITATIONS
3070	Diimidazolium Halobismuthates [Dim] ₂ [BiX ₁₀] (X =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 747 Photoluminescent Materials. Inorganic Chemistry, 2018, 57, 7655-7664.	1.9	56
3071	Molecular Insights into Benzimidazole-Linked Polymer Interactions with Carbon Dioxide and Nitrogen. ChemistrySelect, 2018, 3, 3691-3701.	0.7	10
3072	Covalent character and electric field dependence of H ₂ -AgX (X = F, I). Journal of Molecular Modeling, 2018, 24, 163.	0.8	1
3073	The ion pair mechanism in the thermal deamination of primary amines catalyzed by HBr in the gas phase: DFT and AIM analysis. Chemical Physics Letters, 2018, 703, 117-123.	1.2	4
3074	The effects of cation-π and anion-π interactions on halogen bonds in the [N ⁻ X ⁻ N] ⁺ complexes: A comprehensive theoretical study. Journal of Molecular Graphics and Modelling, 2018, 84, 134-144.	1.3	12
3075	UV and Resonance Raman Spectroscopic and Theoretical Studies on the Solvent-Dependent Ground and Excited-State Thione ↔ Thiol Tautomerization of 4,6-Dimethyl-2-mercaptopyrimidine (DMMP). Journal of Physical Chemistry A, 2018, 122, 5710-5720.	1.1	13
3076	Theoretical study on photophysical properties of three high water solubility polypyridyl complexes for two-photon photodynamic therapy. Physical Chemistry Chemical Physics, 2018, 20, 18074-18081.	1.3	12
3077	Quantification and origin of cooperativity: insights from density functional reactivity theory. Physical Chemistry Chemical Physics, 2018, 20, 17990-17998.	1.3	39
3078	E ₅ M ₇ (E = Ca, Pb, M = Li, Cs): A Source of Viable Star-Shaped Clusters. Chemistry - an Asian Journal, 2018, 13, 1751-1755.	1.7	15
3079	Increasing the open-circuit voltage and adsorption stability of squaraine dye binding onto the TiO ₂ anatase (101) surface via heterocyclic anchoring groups used for DSSC. Applied Surface Science, 2018, 455, 1095-1105.	3.1	30
3080	Structure effect on transition mechanism of UV-visible absorption spectrum in polyimides: A density functional theory study. Polymer, 2018, 148, 356-369.	1.8	22
3081	Effects of Structural Modification on the Photoelectrical Properties of the Dye-Sensitized Type Dyes in DSSCs: A Computational Investigation. ChemistrySelect, 2018, 3, 6622-6637.	0.7	8
3082	How does the presence of an oxyradical influence the behavior of polyphenolic antioxidant? A case study on gallic acid. Journal of Molecular Modeling, 2018, 24, 165.	0.8	7
3083	Synthesis, structural characterization, spectroscopic, and DFT studies of two penta-coordinated zinc(II) complexes containing quinazoline and 1, 10-phenanthroline as mixed ligands. Journal of Luminescence, 2018, 203, 234-246.	1.5	42
3084	Stereoelectronic Effects: The ³ -Gauche Effect in Sulfoxides. Journal of Physical Chemistry A, 2018, 122, 5764-5772.	1.1	11
3085	Ballistic molecular transport through two-dimensional channels. Nature, 2018, 558, 420-424.	13.7	139
3086	Molecular design towards suppressing electron recombination and enhancing the light-absorbing ability of dyes for use in sensitized solar cells: a theoretical investigation. New Journal of Chemistry, 2018, 42, 12891-12899.	1.4	10
3087	The mechanistic study of reaction between N-benzoyl carbamates and aliphatic/aromatic amines for synthesis of substituted N-benzoyl urea derivatives: a DFT approach. Structural Chemistry, 2019, 30, 37-51.	1.0	2

#	ARTICLE	IF	CITATIONS
3088	Radical Anions, Radical Anion Salts, and Anionic Complexes of 2,1,3-Benzochalcogenadiazoles. <i>Chemistry - A European Journal</i> , 2019, 25, 806-816.	1.7	24
3089	Efficiency of electrostatic and steric forces in theoretical appreciating chemical reactivity-related phenomena. <i>Molecular Physics</i> , 2019, 117, 136-142.	0.8	5
3090	Synthesis, molecular structure, quantum chemical analysis, spectroscopic and molecular docking studies of N-(Morpholinomethyl) succinimide using DFT method. <i>Journal of Molecular Structure</i> , 2019, 1175, 609-623.	1.8	10
3091	Experimental and DFT analysis of structural and spectroscopic features of nitroterephthalic acid, and computational insights into its molecular interactions with hER-1 α via molecular docking. <i>Journal of Molecular Structure</i> , 2019, 1175, 458-470.	1.8	9
3092	Assessment of the chitosan-functionalized graphene oxide as a carrier for loading thioguanine, an antitumor drug and effect of urea on adsorption process: Combination of DFT computational and molecular dynamics simulation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 2487-2497.	2.0	31
3093	Noncovalent interactions between O ₆ -corona[6]arene nanorings and fullerenes C ₆₀ and C ₇₀ : atypical ring ball-shaped host-guest systems. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3892.	0.9	4
3094	The influence of Cu ⁺ binding to hypoxanthine on stabilization of mismatches involving hypoxanthine and DNA bases: a DFT study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 1923-1934.	2.0	3
3095	Tuning of pnictogen and chalcogen bonds by an aerogen-bonding interaction: a comparative <i>ab initio</i> study. <i>Molecular Physics</i> , 2019, 117, 58-66.	0.8	25
3096	Optical properties of bilayer quantum dot models based on coronene and its BN analogues with a BODIPY dye: Theoretical TD-CAM-B3LYP-D3 investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 206, 498-505.	2.0	13
3097	Why do A-T and G-C self-sort? Hückel aromaticity as a driving force for electronic complementarity in base pairing. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 1881-1885.	1.5	7
3098	Synthesis and characterization of azathiaethers macrocyclic rings decorated with one or two 2-pyridylmethyl fragments. <i>Journal of Molecular Structure</i> , 2019, 1176, 54-65.	1.8	1
3099	Semiexperimental equilibrium molecular structures of the maleimide and phthalimide. <i>Molecular Physics</i> , 2019, 117, 1097-1103.	0.8	3
3100	A computational study on the tunability of woven covalent organic frameworks for photocatalysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 546-553.	1.3	14
3101	Adsorption of toxic mercury, lead, cadmium, and arsenic ions on black phosphorous nanosheet: first-principles calculations. <i>Structural Chemistry</i> , 2019, 30, 85-96.	1.0	31
3102	Case study of 2-vinylpyridine: Quantitative assessment of the intramolecular C-H \cdots N hydrogen bond energy and its contribution to the one-bond ¹³ C- ¹ H coupling constant. <i>Journal of Molecular Structure</i> , 2019, 1176, 73-85.	1.8	9
3103	Effect of substituent and π -stacking interaction on the metal chelation ability of 7-substituted 2-oxyisoquinoline-1,3(2H,4H)-diones as an HIV integrase inhibitor: A DFT study. <i>Journal of Molecular Structure</i> , 2019, 1175, 734-744.	1.8	1
3104	Shape and non-bonding interactions in the formic acid-difluoromethane complex by rotational spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 206, 185-189.	2.0	8
3105	Self-assembled energetic coordination polymers based on multidentate pentazole cyclo-N ₅ . <i>Science China Materials</i> , 2019, 62, 122-129.	3.5	46

#	ARTICLE	IF	CITATIONS
3106	Mechanism and Substituent Effects of Benzene Arylation via a Phenyl Cation Strategy: A Density Functional Theory Study. <i>ChemCatChem</i> , 2019, 11, 5068-5076.	1.8	5
3107	Topological analysis of the electron localisation function (ELF) applied to the electronic structure of oxaziridine: the nature of N-O bond. <i>Structural Chemistry</i> , 2019, 30, 2181-2189.	1.0	27
3108	Influence of Br substituent position at the carbazole on spin-orbit coupling element matrix. <i>Chemical Physics</i> , 2019, 527, 110500.	0.9	3
3109	A DFT study of polyaniline/ZnO nanocomposite as a photocatalyst for the reduction of methylene blue dye. <i>Journal of Molecular Liquids</i> , 2019, 293, 111528.	2.3	31
3110	Polyaromatic Systems Combining Increasing Optical Gaps and Amplified Nonlinear Optical Properties. A Comprehensive Theoretical Study on B ₃ N ₃ Doped Nanographenes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 21135-21149.	1.5	11
3111	The enzyme-like catalytic hydrogen abstraction reaction mechanisms of cyclic hydrocarbons with magnesium-diluted Fe-MOF-74. <i>RSC Advances</i> , 2019, 9, 23622-23632.	1.7	4
3112	Theoretical insights into the hydrogen bonding interaction in the complexation of epinephrine with uracil. <i>Journal of Molecular Modeling</i> , 2019, 25, 252.	0.8	10
3113	Computational study on C1- versus C3-regioselectivity in Pd(II)-catalyzed olefination/dearomatization of 2-naphthyl ureas. <i>Molecular Catalysis</i> , 2019, 477, 110540.	1.0	0
3114	Encapsulation of Monometal Uranium into Fullerenes C _{2<i>n</i>} (2 <i>n</i> = 70-74): Important Ionic U ⁴⁺ C _{2<i>n</i>} ⁴⁻ Characters and Covalent U-Cage Bonding Interactions. <i>Inorganic Chemistry</i> , 2019, 58, 10629-10636.	1.9	8
3115	New lithium-electride design: material properties of Li _n @porphyrin. <i>Materials Research Express</i> , 2019, 6, 105516.	0.8	4
3116	Ferrocenyl hetaryl thioketones: A computational study of their conformational stability. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e26033.	1.0	2
3117	Adsorption mechanism of As(III) on polytetrafluoroethylene particles of different size. <i>Environmental Pollution</i> , 2019, 254, 112950.	3.7	92
3118	Competitive adsorption on single-atom catalysts: Mechanistic insights into the aerobic oxidation of alcohols over Co N C. <i>Journal of Catalysis</i> , 2019, 377, 283-292.	3.1	48
3119	Does Involving Additional Linker Always Increase the Efficiency of an Organic Dye for <i>p</i> -Type Dye-Sensitized Solar Cells?. <i>ACS Applied Energy Materials</i> , 2019, 2, 6341-6347.	2.5	33
3120	Mechanistic insights and origin of chemoselectivity for S=O bond cleavage in dinitrobenzenesulfonic carbamates. <i>New Journal of Chemistry</i> , 2019, 43, 14594-14602.	1.4	1
3121	Can Hammett indicators accurately measure the acidity of zeolite catalysts with confined space? Insights into the mechanism of coloration. <i>Catalysis Science and Technology</i> , 2019, 9, 5045-5057.	2.1	11
3122	Theoretical Study of the Mechanisms of Two Copper Water Oxidation Electrocatalysts with Bipyridine Ligands. <i>ACS Catalysis</i> , 2019, 9, 8798-8809.	5.5	9
3123	The chalcogen bond: can it be formed by oxygen?. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19969-19986.	1.3	32

#	ARTICLE	IF	CITATIONS
3124	Vacuum ultraviolet absorbance of alkanes: an experimental and theoretical investigation. Structural Chemistry, 2019, 30, 2217-2224.	1.0	17
3125	Reaction Mechanisms on Unusual 1,2-Migrations of N-Heterocyclic Carbene-Ligated Transition Metal Complexes. Chemistry - an Asian Journal, 2019, 14, 3313-3319.	1.7	7
3126	Mechanism of Glucose-Fructose Isomerization over Aluminum-Based Catalysts in Methanol Media. ACS Sustainable Chemistry and Engineering, 2019, 7, 14962-14972.	3.2	18
3127	A facile method to synthesize water-soluble Pd ₈ nanoclusters unraveling the catalytic mechanism of p-nitrophenol to p-aminophenol. Nano Research, 2019, 12, 2589-2596.	5.8	17
3128	Modeling of Si-N Sheets and Derivatives as a Potential Sorbent Material for the Adsorption of Li ⁺ Ion and CO ₂ Gas Molecule. ACS Omega, 2019, 4, 13808-13823.	1.6	14
3129	Theoretical investigation on interactions of H ₂ absorption to CuXe cations I and II. European Physical Journal D, 2019, 73, 1.	0.6	0
3130	Effect of Paramagnetic Open-Shell Gadolinium(III) Texaphyrin on Its Kinetics and Electronic Structures in Fluorescence and Phosphorescence Emission States. Journal of Physical Chemistry C, 2019, 123, 28327-28335.	1.5	6
3131	Theoretical Study on Asymmetric [2 + 2] Cycloaddition of an Alkynone with a Cyclic Enol Silyl Ether Catalyzed by a Chiral N ₂ -Dioxide-Zn(II) Complex. Organometallics, 2019, 38, 3111-3123.	1.1	5
3132	Unraveling the marked differences of the phosphorescence efficiencies of blue-emitting iridium complexes with isomerized phenyltriazole ligands. Inorganic Chemistry Frontiers, 2019, 6, 2776-2787.	3.0	5
3133	Structural evolution and electronic properties of medium-sized boron clusters doped with scandium. Journal of Physics Condensed Matter, 2019, 31, 485302.	0.7	18
3134	Quantum Chemistry Insight into the Interactions Between Deep Eutectic Solvents and SO ₂ . Molecules, 2019, 24, 2963.	1.7	36
3135	Electronic structure and spectral characteristics of alkyl substituted imidazolium based dication-X ₂ (X ⁻ = Br, BF ₄ , PF ₆ and CF ₃ SO ₃) complexes from theory. Journal of Molecular Liquids, 2019, 293, 111548.	2.3	5
3136	Quantum chemical calculations, Hirshfeld surface analysis, and molecular docking studies of antibacterial E-N ₂ -((1H-Indol-3-yl)methylene)-4-bromobenzohydrazide. Spectroscopy Letters, 2019, 52, 398-412.	0.5	1
3137	Developing Dual-Graphite Batteries with Pure 1-Ethyl-3-methylimidazolium Trifluoromethanesulfonate Ionic Liquid as the Electrolyte. ChemElectroChem, 2019, 6, 4681-4688.	1.7	23
3138	The reaction pathway analysis of phosphoric acid with the active radicals: a new insight of the fire-extinguishing mechanism of ABC dry powder. Journal of Molecular Modeling, 2019, 25, 255.	0.8	18
3139	Alkylation of 2-oxo(thioxo)-thieno[2,3-d]pyrimidine-4-ones: Experimental and theoretical study. Journal of Molecular Structure, 2019, 1198, 126858.	1.8	16
3140	Synthesis, characterization, DFT calculations, electric and dielectric properties of (C ₆ H ₁₀ (NH ₃) ₂)CdCl ₄ H ₂ O organic-inorganic hybrid compound. Journal of Molecular Structure, 2019, 1198, 126887.	1.8	7
3141	Photosensitization mechanism of algogenic extracellular organic matters (EOMs) in the photo-transformation of chlortetracycline: Role of chemical constituents and structure. Water Research, 2019, 164, 114940.	5.3	40

#	ARTICLE	IF	CITATIONS
3142	A comprehensive DFT study on the sensing abilities of cyclic oligothiophenes (C _n CTs). <i>New Journal of Chemistry</i> , 2019, 43, 14120-14133.	1.4	45
3143	Effect of Natural Organic Matter Model Compounds on the Structure Memory Effect of Different Layered Double Hydroxides. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 2175-2189.	1.2	20
3144	Violation of Electrostatic Rules: Shifting the Balance between Pnictogen Bonds and Lone Pair-π Interactions Tuned by Substituents. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7288-7295.	1.1	11
3145	Exploring the structure, bonding and stability of noble gas compounds promoted by superhalogens. A case study on HNgMX ₃ (Ng = Ar-Rn, M = Be-Ca, X = F-Br) via combined high-level ab initio and DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19104-19114.	1.3	11
3146	A QTAIM and DFT study of the dizinc bond in non-symmetric [CpZn ₂ Ln] complexes. <i>Journal of Organometallic Chemistry</i> , 2019, 898, 120878.	0.8	8
3147	Excited-State Modulation for Controlling Fluorescence and Phosphorescence Pathways toward White-Light Emission. <i>Advanced Optical Materials</i> , 2019, 7, 1900767.	3.6	34
3148	Rational design non-fullerene acceptor-based high efficiency BHJ polymer solar cells through theoretical investigations. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 383, 111985.	2.0	6
3149	Second-Order Nonlinear Optical Switch Manipulation of Photosensitive Layer by an External Electric Field Coupled with Graphene Quantum Dots. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7401-7407.	1.1	11
3150	Multimolecular Complexes of CL-20 with Nitropyrazole Derivatives: Geometric, Electronic Structure, and Stability. <i>ACS Omega</i> , 2019, 4, 13408-13417.	1.6	15
3151	Alternative trajectories of electron density to plot the atomic connectivity graph in the region of nondirectional interactions. <i>Russian Chemical Bulletin</i> , 2019, 68, 1343-1349.	0.4	1
3152	Rapid, repeatable, highly sensitive and semi-quantitative colorimetric detection of elemental sulfur with a colored clathrate. <i>Sensors and Actuators B: Chemical</i> , 2019, 299, 126948.	4.0	5
3153	Experiments, Modeling, and Simulation of CO ₂ Dehydration by Ionic Liquid, Triethylene Glycol, and Their Binary Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 15588-15597.	1.8	18
3154	Oenin/Syringic Acid Copigmentation: Insights From a Theoretical Study. <i>Frontiers in Chemistry</i> , 2019, 7, 579.	1.8	9
3155	Enzymatic degradation of extracellular DNA exposed to chlorpyrifos and chlorpyrifos-methyl in an aqueous system. <i>Environment International</i> , 2019, 132, 105087.	4.8	20
3156	B(C ₆ F ₅) ₃ -catalyzed divergent cyanosilylations of chromones dependent on temperature. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 8354-8357.	1.5	7
3157	Tuning of the conformation of asymmetric nonfullerene acceptors for efficient organic solar cells. <i>Journal of Materials Chemistry A</i> , 2019, 7, 22279-22286.	5.2	67
3158	Facile preparation of a cationic COF functionalized magnetic nanoparticle and its use for the determination of nine hydroxylated polycyclic aromatic hydrocarbons in smokers' urine. <i>Analyst</i> , 2019, 144, 5829-5841.	1.7	36
3159	Photocatalyst with a metal-free electron-hole pair double transfer mechanism for pharmaceutical and personal care product degradation. <i>Environmental Science: Nano</i> , 2019, 6, 3292-3306.	2.2	14

#	ARTICLE	IF	CITATIONS
3160	Degradation of propranolol by UV-activated persulfate oxidation: Reaction kinetics, mechanisms, reactive sites, transformation pathways and Gaussian calculation. <i>Science of the Total Environment</i> , 2019, 690, 878-890.	3.9	72
3161	Global Aromaticity in Macrocyclic Polyradicaloids: Hückel's Rule or Baird's Rule?. <i>Accounts of Chemical Research</i> , 2019, 52, 2309-2321.	7.6	139
3162	Dinitrogen Fixation and Reduction by Ta ₃ N ₃ H _{0,1} ⁺ Cluster Anions at Room Temperature: Hydrogen-Assisted Enhancement of Reactivity. <i>Journal of the American Chemical Society</i> , 2019, 141, 12592-12600.	6.6	65
3163	Revealing the switching mechanisms of an off-on-off fluorescent logic gate system. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16798-16803.	1.3	23
3164	Theoretical investigations of the substituent effect on the electronic and charge transport properties of butterfly molecules. <i>New Journal of Chemistry</i> , 2019, 43, 12440-12452.	1.4	8
3165	Trisulfide-Bond Acenes for Organic Batteries. <i>Angewandte Chemie</i> , 2019, 131, 13647-13655.	1.6	7
3166	Trisulfide-Bond Acenes for Organic Batteries. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 13513-13521.	7.2	28
3167	Aromaticity analysis of fused heterometallacycles containing M ₂ (M = Cr, Mo and W) quintuple bond. <i>Chemical Physics Letters</i> , 2019, 731, 136600.	1.2	7
3168	Harnessing fluoroacetate dehalogenase for defluorination of fluorocarboxylic acids: in silico and in vitro approach. <i>Environment International</i> , 2019, 131, 104999.	4.8	16
3169	Coordination of Eu(III) with 1,10-Phenanthroline-2,9-dicarboxamide Derivatives: A Combined Study by MS, TRLIF, and DFT. <i>Inorganic Chemistry</i> , 2019, 58, 10239-10247.	1.9	41
3170	Made From Henna! A Fast-Charging, High-Capacity, and Recyclable Tetraakislawsonone Cathode Material for Lithium Ion Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 13836-13844.	3.2	36
3171	A new strategy to generate super and hyper acids with simple organic molecules exploiting σ -hole interaction. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17772-17778.	1.3	2
3172	Effect of heteroatom doping on the hydrogenation of volleyballene. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 1519-1526.	1.2	2
3173	Complexes of Diiodine with Heteroaromatic N-Oxides: Effects of Halogen-Bond Acceptors in Halogen Bonding. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7113-7123.	1.1	21
3174	Importance of Conformational Change in Excited States for Efficient Thermally Activated Delayed Fluorescence. <i>Journal of Physical Chemistry C</i> , 2019, 123, 19322-19332.	1.5	26
3175	Mechanistic studies on the N-heterocyclic carbene-catalyzed reaction of isatin-derived enals with hydrazones. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 7442-7447.	1.5	25
3176	Frequency Shifts in Surface-Enhanced Raman Spectroscopy-Based Immunoassays: Mechanistic Insights and Application in Protein Carbonylation Detection. <i>Analytical Chemistry</i> , 2019, 91, 9376-9381.	3.2	27
3177	Electronic Properties of Electron-Deficient Zn(II) Porphyrins for HBr Splitting. <i>Applied Sciences (Switzerland)</i> , 2019, 9, 2739.	1.3	6

#	ARTICLE	IF	CITATIONS
3178	Searching new structural scaffolds for BRAF inhibitors. An integrative study using theoretical and experimental techniques. <i>Bioorganic Chemistry</i> , 2019, 91, 103125.	2.0	9
3179	Inverse Trans Influence in Low-Valence Actinide "Group 10 Metal Complexes of Phosphinoaryl Oxides: A Theoretical Study via Tuning Metals and Donor Ligands. <i>Inorganic Chemistry</i> , 2019, 58, 10028-10037.	1.9	6
3180	Bromine Substituent Position Triggered Halogen versus Hydrogen Bond in 2D Self-Assembly of Fluorenone Derivatives. <i>Journal of Physical Chemistry C</i> , 2019, 123, 26191-26200.	1.5	17
3181	Dynamic π -Bonding of Imidazolyl Substituent in a Formally 16-Electron $Cp^*Ru(\eta^2-PN)_2$ Catalyst Allows Dramatic Rate Increases in E -Selective Monoisomerization of Alkenes. <i>ACS Catalysis</i> , 2019, 9, 7217-7231.	5.5	24
3182	Correlation of the partial charge-transfer and covalent nature of halogen bonding with the THz and IR spectral changes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17118-17125.	1.3	10
3183	A theoretical study of the ESIPT mechanism of 3-hydroxyflavone derivatives: solvation effect and the importance of TICT for its dual fluorescence properties. <i>Organic Chemistry Frontiers</i> , 2019, 6, 3136-3143.	2.3	43
3184	A new insight into the role of coal adsorbed water in low-temperature oxidation: Enhanced $\cdot OH$ radical generation. <i>Combustion and Flame</i> , 2019, 208, 27-36.	2.8	42
3185	Adsorption of actinide ion complexes on C60O: An all-electron ZORA-DFT-D3 study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 223, 117375.	2.0	7
3186	Dissociative ionization dynamics of dielectric gas C_3F_7CN . <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16451-16458.	1.3	21
3187	A cationic tetrahedral $Zn(\text{scp})_4$ cluster based on a new salicylamide imine multidentate ligand: synthesis, structure and fluorescence sensing study. <i>Dalton Transactions</i> , 2019, 48, 12326-12335.	1.6	14
3188	Revealing resonance effects and intramolecular dipole interactions in the positional isomers of benzonitrile-core thermally activated delayed fluorescence materials. <i>Journal of Materials Chemistry C</i> , 2019, 7, 9184-9194.	2.7	42
3189	Effect of the Si, Al and B doping on the sensing behaviour of carbon nanotubes toward ethylene oxide: a computational study. <i>Molecular Simulation</i> , 2019, 45, 1384-1394.	0.9	8
3190	Interaction between succinic acid and sulfuric acid "base clusters. <i>Atmospheric Chemistry and Physics</i> , 2019, 19, 8003-8019.	1.9	33
3191	Purely Organic Crystals Exhibit Bright Thermally Activated Delayed Fluorescence. <i>Angewandte Chemie</i> , 2019, 131, 13656-13665.	1.6	24
3192	A DFT study on graphene-based surface-enhanced Raman spectroscopy of Benzenedithiol adsorbed on gold/graphene. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 1510-1518.	1.2	14
3193	Is It Possible To Determine Oxidation States for Atoms in Molecules Using Density-Based Quantities? An Information-Theoretic Approach and Conceptual Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6751-6760.	1.1	43
3194	Triterpenoids from <i>Ganoderma gibbosum</i> : A Class of Sensitizers of FLC-Resistant <i>Candida albicans</i> to Fluconazole. <i>Journal of Natural Products</i> , 2019, 82, 2067-2077.	1.5	18
3195	Nonfullerene Acceptors for Organic Photovoltaics: From Conformation Effect to Power Conversion Efficiencies Prediction. <i>Solar Rrl</i> , 2019, 3, 1900258.	3.1	22

#	ARTICLE	IF	CITATIONS
3196	Is it Always Chemical When Amino Groups Come Across CO ₂ ? Anion-Induced Anion-Interaction-Induced Inhibition of Chemical Adsorption. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6536-6542.	1.2	17
3197	Modulation of Conformational Preferences of Heteroaromatic Ethers and Amides through Protonation and Ionization: Charge Effect. <i>ChemistryOpen</i> , 2019, 8, 840-851.	0.9	3
3198	Ammonium fluoride-induced stabilization for anion attachment mass spectrometry: Facilitating the pseudotargeted profiling of bile acids submetabolome. <i>Analytica Chimica Acta</i> , 2019, 1081, 120-130.	2.6	14
3199	A multicomponent synthesis of stereodefined olefins via nickel catalysis and single electron/triplet energy transfer. <i>Nature Catalysis</i> , 2019, 2, 678-687.	16.1	123
3200	Electron transfer and intersystem crossing triggered fluorescence quenching detection of mercury ions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16676-16685.	1.3	7
3201	Regular tuning of the ESIPT reaction of 3-hydroxychromone-based derivatives by substitution of functional groups. <i>Organic Chemistry Frontiers</i> , 2019, 6, 3093-3100.	2.3	32
3202	Syntheses of Energetic <i>cyclopentazole</i> Salts. <i>Chemistry - an Asian Journal</i> , 2019, 14, 2877-2882.	1.7	32
3203	Enhancing the interaction between CO and single layer black phosphorous via transition metals impurities and external electric field: a theoretical study. <i>Research on Chemical Intermediates</i> , 2019, 45, 5577-5593.	1.3	4
3204	Theoretical Insights into the Selective Extraction of Americium(III) over Europium(III) with Dithioamide-Based Ligands. <i>Inorganic Chemistry</i> , 2019, 58, 10047-10056.	1.9	48
3205	Theoretical investigation on the reaction mechanism and kinetics of a Criegee intermediate with ethylene and acetylene. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16583-16590.	1.3	9
3206	Crystallographic and Theoretical Investigations of Er ₂ @C ₂ (n=82, 84, 86): Indication of Distance-Dependent Metal-Metal Bonding Nature. <i>Chemistry - A European Journal</i> , 2019, 25, 11538-11544.	1.7	29
3207	On a chlorophyll-carotenoid coupling in LHCII. <i>Chemical Physics</i> , 2019, 526, 110439.	0.9	24
3208	DL-3-Aminoisobutyric acid: vibrational, NBO and AIM analysis of N-H...O bonded-zwitterionic dimer model. <i>Heliyon</i> , 2019, 5, e01933.	1.4	11
3209	Strong fluorescence of a complex based on 2,2-dipyridyl derivative—An experimental and theoretical investigation. <i>Journal of Luminescence</i> , 2019, 215, 116611.	1.5	2
3210	Loading and release of anticancer drug from phosphorene as a template material with high efficient carrier: From vacuum to cell membrane. <i>Journal of Molecular Liquids</i> , 2019, 291, 111346.	2.3	26
3211	Theoretical design and characterization of NIR porphyrin-based sensitizers for applications in dye-sensitized solar cells. <i>Solar Energy</i> , 2019, 188, 1031-1040.	2.9	15
3212	Aromaticity of Hückel and Möbius Topologies Involved in Conformation Conversion of Macrocyclic [32]Octaphyrin(1.0.1.0.1.0.1.0): Refined Evidence from Multiple Visual Criteria. <i>Journal of Physical Chemistry C</i> , 2019, 123, 18593-18599.	1.5	26
3213	Intramolecular charge transfer and solvation dynamics of push-pull dyes with different π -conjugated linkers. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17323-17331.	1.3	30

#	ARTICLE	IF	CITATIONS
3214	Effects of Electronic Structure of Adjacent Carbon on the Strength of C-H Organofluorine Hydrogen Bonds. <i>Journal of Computational Chemistry</i> , 2019, 40, 2473-2481.	1.5	0
3215	The nature of the T=T double bond (T=B, Al, Ga, In) in dialumene and its derivatives: topological study of the electron localization function (ELF). <i>Journal of Molecular Modeling</i> , 2019, 25, 211.	0.8	5
3216	Mechanistic Study on the Dominant Promotion Effect of Al-/Ti-/Zr-modifications over the VOx/SiO2 UHMWPE Catalysts. <i>Chinese Journal of Polymer Science (English Edition)</i> , 2019, 37, 995-1004.	2.0	4
3217	The role of hydrogen bonding in π - π stacking interactions in Ni(II) complex derived from triethanolamine: synthesis, crystal structure, antimicrobial, and DFT studies. <i>Research on Chemical Intermediates</i> , 2019, 45, 5649-5664.	1.3	11
3218	Exploration of the basic reactant in CO2 photoreduction: New insights from photophysics and photochemistry. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 382, 111959.	2.0	2
3219	Linkage dependence of charge separated lifetime in small donor-acceptor dyads system. <i>Journal of Molecular Structure</i> , 2019, 1196, 604-610.	1.8	4
3220	Investigation on 4-amino-5-substituent-1,2,4-triazole-3-thione Schiff bases an antifungal drug by characterization (spectroscopic, XRD), biological activities, molecular docking studies and electrostatic potential (ESP). <i>Journal of Molecular Structure</i> , 2019, 1197, 171-182.	1.8	22
3221	Reconsider the fluorescence properties of 5-ASA and its sensing mechanism for iodide ion. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 223, 117369.	2.0	3
3222	Hydrogen physisorption on nitrogen-doped graphene and graphene-like boron nitride-carbon heterostructures: a DFT study. <i>Surfaces and Interfaces</i> , 2019, 17, 100355.	1.5	19
3223	What Is the Nature of Interactions of BF ₄ ⁻ , NO ₃ ⁻ , and ClO ₄ ⁻ to Cu(II) Complexes with Girard TM s T Hydrazine? When Can Binuclear Complexes Be Formed?. <i>Crystal Growth and Design</i> , 2019, 19, 4810-4821.	1.4	13
3224	Exploring the effects of axial halogen substitutions of boron subphthalocyanines on the performance of BsubPC/C60 organic solar cells: a DFT/TDDFT-based computational study. <i>New Journal of Chemistry</i> , 2019, 43, 12719-12726.	1.4	10
3225	A new insight into SO ₂ low-temperature catalytic oxidation in porous carbon materials: non-dissociated O ₂ molecule as oxidant. <i>Catalysis Science and Technology</i> , 2019, 9, 4327-4338.	2.1	20
3226	Synthesis, characterization, spectral property, Hirshfeld surface analysis and TD/DFT calculations of 2, 6-disubstituted benzobisoxazoles. <i>Journal of Molecular Structure</i> , 2019, 1197, 508-518.	1.8	23
3227	Theoretical Insight into Configurational Selectivity of Functionalized Single-Walled Carbon Nanotubes Based on the Clar Sextet Theory. <i>Journal of Physical Chemistry C</i> , 2019, 123, 18629-18637.	1.5	7
3228	Five-Membered Ruthenacycles: Ligand-Assisted Alkyne Insertion into 1,3- η -S ₂ -Chelated Ruthenium Borate Species. <i>Chemistry - A European Journal</i> , 2019, 25, 13537-13546.	1.7	18
3229	Organometallic complexes of carbon nanotori. <i>Journal of Molecular Modeling</i> , 2019, 25, 239.	0.8	2
3230	The effect of sulfur and nitrogen/sulfur co-doping in graphene surface on the adsorption of toxic heavy metals (Cd, Hg, Pb). <i>Journal of Materials Science</i> , 2019, 54, 13175-13189.	1.7	14
3231	Ligands and Bases Mediate Switching between Aminocarbonylations and Alkoxy carbonylations in Coupling of Aminophenols with Iodoarenes. <i>Inorganic Chemistry</i> , 2019, 58, 10217-10226.	1.9	8

#	ARTICLE	IF	CITATIONS
3232	C70 Fullerene Cage as a Novel Catalyst for Efficient Proton Transfer Reactions between Small Molecules: A Theoretical study. <i>Scientific Reports</i> , 2019, 9, 10650.	1.6	8
3233	Polypyrrole derivatives for optoelectronic applications: a DFT study on the influence of side groups. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17729-17739.	1.3	23
3234	Effect of solvent environment on excited state intramolecular proton transfer in 2-(4-(dimethylamino)phenyl)-3-hydroxy-6,7-dimethoxy-4 <i>h</i> -chromen-4-one. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17711-17719.	1.3	23
3235	Removal of Fâ€“53B as PFOS alternative in chrome plating wastewater by UV/Sulfite reduction. <i>Water Research</i> , 2019, 163, 114907.	5.3	66
3236	Determinant of ESIPT Mechanism by the Structure Designed for Symmetrical and Unsymmetrical Molecules. <i>ACS Applied Bio Materials</i> , 2019, 2, 3622-3629.	2.3	7
3237	Extraction and stripping of platinum (IV) from acidic chloride media using guanidinium ionic liquid. <i>Journal of Molecular Liquids</i> , 2019, 293, 111040.	2.3	20
3238	Tautomerism in folic acid: Combined molecular modelling and NMR study. <i>Journal of Molecular Liquids</i> , 2019, 292, 111392.	2.3	10
3239	Intramolecular hydrogen bonding, ĨĤ stacking interactions, and substituent effects of 8-hydroxyquinoline derivative supermolecular structures: a theoretical study. <i>Journal of Molecular Modeling</i> , 2019, 25, 241.	0.8	7
3240	Enhancing Actinide(III) over Lanthanide(III) Selectivity through Hard-by-Soft Donor Substitution: Exploitation and Implication of Near-Degeneracy-Driven Covalency. <i>Inorganic Chemistry</i> , 2019, 58, 9738-9748.	1.9	34
3241	Pd(II) Complexes with Chelating Phosphinoferrrocene Diaminocarbene Ligands: Synthesis, Characterization, and Catalytic Use in Pd-Catalyzed Borylation of Aryl Bromides. <i>Organometallics</i> , 2019, 38, 3060-3073.	1.1	13
3242	Competition between dispersion interactions and conventional hydrogen bonding: insights from a theoretical study on Z-Arg-OH. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17893-17900.	1.3	2
3243	Toward simple model for the production of lithium phthalocyanine (LiPc) nanoflake through hydrogen transfer processes. <i>Computational and Theoretical Chemistry</i> , 2019, 1164, 112549.	1.1	0
3244	Elucidation of key factors in nickel-diphosphines catalyzed isomerization of 2-methyl-3-butenitrile. <i>Journal of Catalysis</i> , 2019, 377, 13-19.	3.1	6
3245	U2C Unit in Fullerenes: Robust Multicenter Bonds with a Cluster Shape Controlled by Cage Size and Charge Transfer. <i>Inorganic Chemistry</i> , 2019, 58, 10648-10655.	1.9	10
3246	Enhanced intramolecular charge transfer of organic dyes containing hydantoin donor: A DFT study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 383, 111979.	2.0	11
3247	A molecular approach on the ability of functionalized gold nanoparticles for selective sensing of Hg ²⁺ . <i>Journal of Molecular Liquids</i> , 2019, 292, 111461.	2.3	3
3248	External Electric Field Induced Second-Order Nonlinear Optical Effects in Hexagonal Graphene Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20020-20025.	1.5	12
3249	Global and local aromaticity of acenes from the information-theoretic approach in density functional reactivity theory. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18195-18210.	1.3	41

#	ARTICLE	IF	CITATIONS
3250	The Unexplored World of Cycloalkeneâ€“Water Complexes: Primary and Assisting Interactions Unraveled by Experimental and Computational Spectroscopy. <i>Angewandte Chemie</i> , 2019, 131, 14073-14079.	1.6	6
3251	The Unexplored World of Cycloalkeneâ€“Water Complexes: Primary and Assisting Interactions Unraveled by Experimental and Computational Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 13935-13941.	7.2	22
3252	Preparation, characterization, inÂvitro and inÂvivo evaluation of metronidazoleâ€“gallic acid cocrystal: A combined experimental and theoretical investigation. <i>Journal of Molecular Structure</i> , 2019, 1197, 727-735.	1.8	17
3253	Clusterâ”Œ Interactions Cause Size-Selective Reactivity of Cationic Silver Clusters with Acetylene: The Distinctive Ag ₇ ⁺ [C ₂ H ₂]. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6921-6926.	1.1	17
3254	Charge Transfer and Delocalization in Ladder-Type Fused Bithiophene Imide Oligomers. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20093-20104.	1.5	7
3255	Formation of S-alkyl thiophenium ionic liquids: mechanistic rationale and structural relationships. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 7772-7781.	1.5	3
3256	Resonance Raman study of the J-type aggregation process of a water soluble perylene bisimide. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18300-18309.	1.3	2
3257	The substituent effect on the excited state intramolecular proton transfer of 3-hydroxychromone*. <i>Chinese Physics B</i> , 2019, 28, 093102.	0.7	13
3258	Quantum interference of multi-orbital effects in high-harmonic spectra from aligned carbon dioxide and nitrous oxide. <i>Chinese Physics B</i> , 2019, 28, 094207.	0.7	4
3259	Resolving multi-orbital effects on high harmonic generation from aligned N ₂ molecules in linearly and elliptically polarized intense laser fields. <i>Chinese Physics B</i> , 2019, 28, 094211.	0.7	4
3260	Sensor application of doped C60 fullerenes in detection of 1-(3-trifluoromethylphenyl)piperazine as an alternative to ecstasy. <i>Main Group Metal Chemistry</i> , 2019, 42, 23-27.	0.6	3
3261	Competition Between Intra- and Intermolecular Hydrogen Bonding: Anisic Acidâ€“Formic Acid Heterodimer. <i>Chemistry - A European Journal</i> , 2019, 25, 12325-12331.	1.7	19
3262	A DFT/TDDFT investigation on structureâ€“photophysical properties relationship of phenothiazine derivatives with substitutions on C-3/N-10 sites. <i>Computational and Theoretical Chemistry</i> , 2019, 1163, 112512.	1.1	4
3263	Noncovalent Close Contacts in Fluorinated Thiopheneâ€“Phenyleneâ€“Thiophene Conjugated Units: Understanding the Nature and Dominance of Oâ€“H versus Sâ€“F and Oâ€“F Interactions with Respect to the Control of Polymer Conformation. <i>Chemistry of Materials</i> , 2019, 31, 7070-7079.	3.2	23
3264	Noncovalent Complexes of the Noble Gas Atoms: Analyzing the Transition from Physical to Chemical Interactions. <i>Journal of Computational Chemistry</i> , 2019, 40, 2318-2328.	1.5	19
3265	Theoretical study of metal ion impact on geometric and electronic properties of terbutaline compounds. <i>Monatshefte f�r Chemie</i> , 2019, 150, 1355-1364.	0.9	27
3266	Theoretical study on design of novel superalkalis doped graphdiyne: A new donorâ€“acceptor (Dâ€“A) strategy for enhancing NLO response. <i>Applied Surface Science</i> , 2019, 492, 255-263.	3.1	66
3267	Untangling Hydrogen Bond Networks with Ion Mobility Spectrometry and Quantum Chemical Calculations: A Case Study on H ₂ XPGG. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5730-5741.	1.2	2

#	ARTICLE	IF	CITATIONS
3268	Optical band gap of cross-linked, curved, and radical polyaromatic hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16240-16251.	1.3	45
3269	Light Harvesting and Optical-Electronic Properties of Two Quercetin and Rutin Natural Dyes. <i>Applied Sciences (Switzerland)</i> , 2019, 9, 2567.	1.3	29
3270	Organobase triggered controlled supramolecular ring opening polymerization and 2D assembly. <i>Chemical Science</i> , 2019, 10, 7345-7351.	3.7	39
3271	Purely Organic Crystals Exhibit Bright Thermally Activated Delayed Fluorescence. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 13522-13531.	7.2	72
3272	Regulating PdC3/PtC3- π -thiophene interaction by small molecule doping (AgOTf, CuBr, CuI, CuBr ₂). <i>Tj ETQq0 0 0 rgBT /Overlock 10 T</i>	1.0	1
3273	Structural, spectroscopic, Hirshfeld surface and charge distribution analysis of 3-(1H-imidazole-1-yl)-1-phenylpropan-1-ol complemented by molecular docking predictions: An integrated experimental and computational approach. <i>Journal of Molecular Structure</i> , 2019, 1196, 578-591.	1.8	5
3274	Hemilabile bonding of 1-oxa-4,7-dithiacyclononane in cyclometallated palladium(ii) complexes. <i>Dalton Transactions</i> , 2019, 48, 11520-11535.	1.6	2
3275	Experimental and molecular modeling study of a novel arylsulfonamide chalcone. <i>Journal of Molecular Modeling</i> , 2019, 25, 208.	0.8	4
3276	Elucidating the origin of selectivity of [3+2]-cycloaddition reactions between thioketone and carbohydrate-derived nitrones by the DFT. <i>Journal of Molecular Modeling</i> , 2019, 25, 209.	0.8	8
3277	1,3,5-Triiodo-2,4,6-trinitrobenzene (TITNB) from benzene: Balancing performance and high thermal stability of functional energetic materials. <i>Chemical Engineering Journal</i> , 2019, 378, 122119.	6.6	18
3278	In-situ N/S Co-doping three-dimensional succulent-like hierarchical carbon assisted by supramolecular polymerization for high-performance supercapacitors. <i>Electrochimica Acta</i> , 2019, 319, 410-422.	2.6	40
3279	Customization of the molecular structure to modulate the crystal packing style of energetic materials. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 1032-1038.	1.7	1
3280	A sterically hindered asymmetric D π A π D π thermally activated delayed fluorescence emitter for highly efficient non-doped organic light-emitting diodes. <i>Chemical Science</i> , 2019, 10, 8129-8134.	3.7	102
3281	Towards boosting the exciton lifetime and efficiency of near-infrared aggregation induced emitters with hybridized local and charge transfer excited states: a multiscale study. <i>Journal of Materials Chemistry C</i> , 2019, 7, 8874-8887.	2.7	35
3282	Deep-Red/Near-Infrared Electroluminescence from Single-Component Charge-Transfer Complex via Thermally Activated Delayed Fluorescence Channel. <i>Advanced Functional Materials</i> , 2019, 29, 1903112.	7.8	59
3283	Terahertz spectroscopic investigation of D- and DL-tartaric acid. <i>Chemical Physics Letters</i> , 2019, 731, 136579.	1.2	7
3284	Understanding the Mechanisms of White Light Emission of a Tetradentate Pt Complex in Various Surrounding Environments. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17968-17975.	1.5	20
3285	The folding equilibria of enterobactin enantiomers and their interaction with actinides. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16017-16031.	1.3	3

#	ARTICLE	IF	CITATIONS
3286	A modern approach for the sensing of aqueous Al(III) ion by Ni(II) Salen-type Schiff base complexes. <i>Applied Organometallic Chemistry</i> , 2019, 33, e5064.	1.7	6
3287	Theoretical studies of perfluorochemicals (PFCs) adsorption mechanism on the carbonaceous surface. <i>Chemosphere</i> , 2019, 235, 606-615.	4.2	23
3288	Theoretical design of porphyrin dyes with electron-deficit heterocycles towards near-IR light sensitization in dye-sensitized solar cells. <i>Solar Energy</i> , 2019, 188, 742-749.	2.9	9
3289	Atomic and Electronic Properties of a 155 H ₂ S Cluster under Pressure. <i>ACS Omega</i> , 2019, 4, 10524-10533.	1.6	5
3290	Antimicrobial activities of self-assembled copper(II), nickel(II), and cobalt(III) complexes combined with crystallographic, spectroscopic, DFT calculations and Hirshfeld surfaces analyses. <i>New Journal of Chemistry</i> , 2019, 43, 12417-12430.	1.4	39
3291	Methyl Trifluoroacetate as a Methylation Reagent for N ^H , O ^H , and S ^H Functionalities under Mild Conditions. <i>Asian Journal of Organic Chemistry</i> , 2019, 8, 1325-1331.	1.3	5
3292	The formation mechanism of uranium and thorium hydride phosphorus: a systematically theoretical study. <i>RSC Advances</i> , 2019, 9, 17119-17128.	1.7	3
3293	Theoretical Studies on Novel Gridspiroarenes: Structures, Noncovalent Interactions and Reorganization Energies. <i>Chinese Journal of Chemistry</i> , 2019, 37, 915-921.	2.6	10
3294	New Insight into U@C ₈₀ : Missing U@D ₃ (31921)-C ₈₀ and Nuanced Enantiomers of U@C ₁ (28324)-C ₈₀ . <i>Inorganic Chemistry</i> , 2019, 58, 14159-14166.	1.9	15
3295	Pushing 3c-4e Bonds to the Limit: A Coupled Cluster Study of Stepwise Fluorination of First-Row Atoms. <i>Inorganic Chemistry</i> , 2019, 58, 14777-14789.	1.9	16
3296	Application of Multifunctional X-Doped Sumanene (X= Si, Ge, O, S and Se) for Concave-Convex Supramolecular Assembly with C ₆₀ and Their Nonlinear Optical Properties. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27811-27822.	1.5	9
3297	Aggregation Promotes Excited-State Intramolecular Proton Transfer for Benzothiazole-Substituted Tetraphenylethylene Compound. <i>ACS Applied Bio Materials</i> , 2019, 2, 5182-5189.	2.3	47
3298	Computational Exploration of Chiral Iron Porphyrin-Catalyzed Asymmetric Hydroxylation of Ethylbenzene Where Stereoselectivity Arises from π-π Stacking Interaction. <i>Journal of Organic Chemistry</i> , 2019, 84, 13755-13763.	1.7	10
3299	DFT Studies on the Al-Speciation and Its Structure in Aqueous Aluminum Sol Formed by Aluminum Formoacetate. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9167-9179.	1.2	3
3300	Theoretical design and experimental study on the gold nanoparticles based colorimetric aptasensors for detection of neomycin B. <i>Sensors and Actuators B: Chemical</i> , 2019, 300, 126947.	4.0	19
3301	Molecular-Level Understanding of Hydroxyl Groups Boosted the Catalytic Activity of the CuZnAl Catalyst in the Conversion of Syngas to Ethanol. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 19421-19433.	1.8	1
3302	Vibrational and computational analysis for molecular structure properties of N-(2-(trifluoromethyl)phenyl)acetamide: Density functional theory approach. <i>Spectroscopy Letters</i> , 2019, 52, 563-576.	0.5	11
3303	Multiple π-Conjugated Molecules with Selectively Enhanced Electrical Performance for Efficient Solution-Processed Blue Electrophosphorescence. <i>Advanced Optical Materials</i> , 2019, 7, 1901124.	3.6	7

#	ARTICLE	IF	CITATIONS
3304	Versatile Host Materials for Highly Efficient Green, Red Phosphorescent and White Organic Light-Emitting Diodes. <i>ChemElectroChem</i> , 2019, 6, 5810-5818.	1.7	15
3305	Hydrogen-Bonding-Driven Ion-Pair Formation in Protic Ionic Liquid Aqueous Solution. <i>ChemPhysChem</i> , 2019, 20, 3259-3268.	1.0	7
3306	Theoretical Investigation of Cyano-Chalcogen Dimers and Their Importance in Molecular Recognition. <i>ChemPhysChem</i> , 2019, 20, 3186-3194.	1.0	11
3307	Uncovering the action of ethanol controlled crystallization of 3,4-bis(3-nitrofurazan-4-yl)furoxan crystal: A molecular dynamics study. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 92, 303-312.	1.3	8
3308	A 3D Analogue of Phenyllithium: Solution-Phase, Solid-State, and Computational Study of the Lithiacarborane [Li ⁺ CB ₁₁ H ₁₁] ⁻ . <i>Angewandte Chemie - International Edition</i> , 2019, 58, 19007-19013.	7.2	12
3309	Thermally Activated Delayed Fluorescent Properties of Ortho-Carbazole-Appended Triazine Compounds. <i>Bulletin of the Korean Chemical Society</i> , 2019, 40, 1112-1116.	1.0	1
3310	1,2,4-Oxadiazole-Bridged Polynitropyrazole Energetic Materials with Enhanced Thermal Stability and Low Sensitivity. <i>ChemPlusChem</i> , 2019, 84, 1567-1577.	1.3	38
3311	pH-Responsive Switching Properties of a Water-Soluble Metallamacrocyclic Phenylalaninehydroximate La(III)-Cu(II) Complex: Insight into Tuning Protonation Ligand States. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 4328-4335.	1.0	8
3312	Rapid relaxation pathway of the excited state of linear merocyanines in solutions. <i>Journal of the Chinese Chemical Society</i> , 2019, 66, 1105-1118.	0.8	0
3313	Unravelling the Weak Interactions in Binary Clusters of Serotonin and Amino Acid Residues. <i>ChemistrySelect</i> , 2019, 4, 9978-9986.	0.7	4
3314	Mechanism of H ₂ generation on the unsaturated Mo and S of Mo-Edge in 2H-MoS ₂ from density functional theory. <i>Computational and Theoretical Chemistry</i> , 2019, 1168, 112623.	1.1	4
3315	Quantum computational, spectroscopic investigations on 6-aminobenzimidazole by DFT/TD-DFT with different solvents and molecular docking studies. <i>Journal of Molecular Liquids</i> , 2019, 296, 111787.	2.3	25
3316	Zinc complexes with 1,2-disubstituted benzimidazole ligands: Experimental and theoretical studies in the catalytic cycloaddition of CO ₂ with epoxides. <i>Polyhedron</i> , 2019, 173, 114134.	1.0	23
3317	Insights into the Electrochemical Behavior of Mercury on Graphene/SiC Electrodes. <i>Journal of Carbon Research</i> , 2019, 5, 51.	1.4	9
3318	Deep eutectic solvents based highly efficient extractive desulfurization of fuels – Eco-friendly approach. <i>Journal of Molecular Liquids</i> , 2019, 296, 111916.	2.3	98
3319	Site-selective remote C(sp ³)-H heteroarylation of amides via organic photoredox catalysis. <i>Nature Communications</i> , 2019, 10, 4743.	5.8	69
3320	Structural and Computational Insights into Cocrystal Interactions: A Case on Cocrystals of Antipyrine and Aminophenazone. <i>Crystal Growth and Design</i> , 2019, 19, 6175-6183.	1.4	31
3321	Probing the structure and electronic properties of beryllium doped boron clusters: A planar BeB ₁₆ cluster motif for metallo-borophene. <i>Scientific Reports</i> , 2019, 9, 14367.	1.6	29

#	ARTICLE	IF	CITATIONS
3322	Water-Soluble Chiral Y(III)–Cu(II) Metallamacrocyclic Phenylalaninehydroximate Complex. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2019, 45, 721-727.	0.3	7
3323	Aromaticity and Induced Current Study of C ₈ H _(n+2) (n = 6, 4, 2, 0): In the Viewpoint of Huckel's Rule. Journal of Structural Chemistry, 2019, 60, 1361-1374.	0.3	2
3325	Are Inorganic Single-Molecule Magnets a Possibility? A Theoretical Insight into Dysprosium Double-Deckers with Inorganic Ring Systems. Inorganic Chemistry, 2019, 58, 14046-14057.	1.9	20
3326	Water Transport through Ultrathin Nanopores with Highly Polar Rims. Journal of Physical Chemistry C, 2019, 123, 27690-27696.	1.5	14
3327	Double-Helicene-Based Hole-Transporter for Perovskite Solar Cells with 22% Efficiency and Operation Durability. ACS Energy Letters, 2019, 4, 2683-2688.	8.8	56
3328	Lipase and Metal Chloride Hydrate-Natural Deep Eutectic Solvents Synergistically Catalyze Amidation Reaction via Multiple Noncovalent Bond Interactions. ACS Sustainable Chemistry and Engineering, 2019, 7, 18174-18184.	3.2	16
3329	M(C ₆ H ₆ R) ₂ (R = BH, Be; M = Cr, Mo, W): Transition-metal sandwich complexes with 7-coordination borepin and beryllepin: A DFT study. Computational and Theoretical Chemistry, 2019, 1165, 112562.	1.1	0
3330	Hydrogen bonding in the complexes formed by arsine and H-X molecules: A theoretical study. Chemical Physics Letters, 2019, 735, 136767.	1.2	6
3331	Effective Virtual Screening Strategy toward heme-containing proteins: Identification of novel IDO1 inhibitors. European Journal of Medicinal Chemistry, 2019, 184, 111750.	2.6	15
3332	Effect of N-doping on NO ₂ adsorption and reduction over activated carbon: An experimental and computational study. Fuel, 2019, 258, 116109.	3.4	39
3333	Theoretical studies on the bond strength and electron density characteristics in multiple hydrogen bonded arrays. Journal of Molecular Graphics and Modelling, 2019, 93, 107439.	1.3	10
3334	Silver-based monomer and coordination polymer with organic thiocyanate ligand: Structural, computational and antiproliferative activity study. Polyhedron, 2019, 173, 114132.	1.0	4
3335	Strong Solid-State Fluorescence Induced by Restriction of the Coordinate Bond Bending in Two-Coordinate Copper(I)–Carbene Complexes. Inorganic Chemistry, 2019, 58, 14403-14409.	1.9	35
3336	Bidentate SO ₂ Complexes of Zirconium and Hafnium Difluorides with Highly Activated S=O Bonds. Journal of Physical Chemistry A, 2019, 123, 9567-9572.	1.1	4
3337	Mechanism of the Iron(0)-Catalyzed Hydrosilylation of Aldehydes: A Combined DFT and Experimental Investigation. Organometallics, 2019, 38, 4105-4114.	1.1	13
3338	DFT/QTAIM analysis of favipiravir adsorption on pristine and silicon doped C ₂₀ fullerenes. Main Group Metal Chemistry, 2019, 42, 143-149.	0.6	29
3339	QCT analysis of molecules containing the first and second period elements based on the PAEM. Electronic Structure, 2019, 1, 044004.	1.0	1
3340	Unexpected Cascade Reactions of Ortho-Hydroxyenaminones and Unsaturated Ketoesters to Access Hydrogenated Benzoxazolepolycycles and Pyrrole-Phenol Atropisomers. Advanced Synthesis and Catalysis, 2019, 361, 4893-4901.	2.1	9

#	ARTICLE	IF	CITATIONS
3341	Insight into Isothiourea-Catalyzed Enantioselective Addition of Saturated Esters to Iminium Ions. <i>Chemistry - an Asian Journal</i> , 2019, 14, 4322-4327.	1.7	6
3342	Predicting an Antiaromatic Benzene Ring in the Ground State Caused by Hyperconjugation. <i>Chemistry - an Asian Journal</i> , 2019, 14, 4309-4314.	1.7	5
3343	Adsorption of diatomic molecules on graphene, h-BN and their BNC heterostructures: DFT study. <i>Diamond and Related Materials</i> , 2019, 100, 107575.	1.8	19
3344	Impact of precipitate characteristics and precipitation conditions on the settling performance of a sulfide precipitation process: An exhaustive characterization of the aggregation behavior. <i>Hydrometallurgy</i> , 2019, 189, 105150.	1.8	13
3345	Synthesis, spectroscopic and DFT studies of copper(I) complexes inserting the electron-donating groups into pyridine-imidazole ligands via an acetylide linker. <i>Inorganica Chimica Acta</i> , 2019, 498, 119155.	1.2	4
3346	Small substituent groups as geometric controllers for tridentate platinum($\text{Pt}(\text{II})$) complexes to effectively suppress non-radiative decay processes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2764-2770.	1.3	14
3347	Interaction Mechanism of Flavonoids and α -Glucosidase: Experimental and Molecular Modelling Studies. <i>Foods</i> , 2019, 8, 355.	1.9	34
3348	Oxygen Functional Group Modification of Cellulose-Derived Hard Carbon for Enhanced Sodium Ion Storage. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 18554-18565.	3.2	72
3349	Wavelength-Tunable Organic Microring Laser Arrays from Thermally Activated Delayed Fluorescent Emitters. <i>ACS Photonics</i> , 2019, 6, 3208-3214.	3.2	42
3350	Luminescent AgI Complexes with 2,2'-Bipyridine Derivatives Featuring $[\text{Ag}(\text{CF}_3)_2\text{Pyrazolate}]_4$ Units. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 4855-4861.	1.0	12
3351	How do halogen atoms affect Xe-Mo double bond? A theoretical study of X_2XeMoY_2 ($\text{X} = \text{F}, \text{Cl}, \text{Br}; \text{Y} = \text{F}, \text{I}$). <i>ETQqO, O rgBT /</i>		
3352	Intramolecular Nonvalent Interactions in the $\text{Eu}(\text{I}^4\text{-ORF})_2(\text{I}^2\text{-ORF})_3(\text{I}^3\text{-ORF})_2(\text{DME})_2$ Complex. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2019, 45, 767-775.	0.3	3
3353	Spectroscopic, Hirshfeld surface, charge transfer excitation, condensed Fukui function and molecular docking investigations of 1-(3-Bromo-2-thienyl)-3-(4-butoxyphenyl)prop-2-en-1-one. <i>Chemical Data Collections</i> , 2019, 24, 100309.	1.1	7
3354	Side-On $\text{OMoF}_2(\text{I}^2\text{-SO})$ and $\text{OWF}_2(\text{I}^2\text{-SO})$ Complexes Featuring Peroxo-Like Sulfur Monoxide Ligand. <i>Inorganic Chemistry</i> , 2019, 58, 15652-15658.	1.9	6
3355	Composites of Platinum-Iridium Alloy Nanoparticles and Graphene Oxide for the Dimethyl Amine Borane (DMAB) dehydrogenation at ambient conditions: An Experimental and Density Functional Theory Study. <i>Scientific Reports</i> , 2019, 9, 15543.	1.6	7
3356	Molecular Structures and Spectral Properties of Natural Indigo and Indirubin: Experimental and DFT Studies. <i>Molecules</i> , 2019, 24, 3831.	1.7	38
3357	Structure of Diferrocenyl Thioketone: From Molecule to Crystal. <i>Molecules</i> , 2019, 24, 3950.	1.7	4
3358	Convolutional Neural Networks for the Design and Analysis of Non-Fullerene Acceptors. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4993-5001.	2.5	29

#	ARTICLE	IF	CITATIONS
3359	Persulfurated Coronene and Its Chalcogenide Analogues: Insight into Effects of Peripheral Substitution. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10273-10280.	1.1	5
3360	Theoretical Insight into Multiple Charge-Transfer Mechanisms at the P3HT/Nonfullerenes Interface in Organic Solar Cells. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 19699-19707.	3.2	27
3361	Novel Angiotensin-Converting Enzyme-Inhibitory Peptides From Fermented Bovine Milk Started by <i>Lactobacillus helveticus</i> KLDS.31 and <i>Lactobacillus casei</i> KLDS.105: Purification, Identification, and Interaction Mechanisms. <i>Frontiers in Microbiology</i> , 2019, 10, 2643.	1.5	35
3362	Theoretical design of novel high energy metal complexes based on two complementary oxygen-rich mixed ligands of 4-amino-4H-1,2,4-triazole-3,5-diol and 1,1-dinitramino-5,5-bistetrazole. <i>Journal of Molecular Modeling</i> , 2019, 25, 340.	0.8	3
3363	Effect of Lysyllysine on non-covalent hybridization of single walled carbon nanotube by single-stranded DNA homodimer: in silico approach. <i>Journal of Nanostructure in Chemistry</i> , 2019, 9, 315-321.	5.3	1
3364	Achieving Enhanced Thermally Activated Delayed Fluorescence Rates and Shortened Exciton Lifetimes by Constructing Intramolecular Hydrogen Bonding Channels. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 45999-46007.	4.0	43
3365	Synthesis of Thermally Stable and Insensitive Energetic Materials by Incorporating the Tetrazole Functionality into a Fused-Ring 3,6-Dinitropyrazolo-[4,3- <i>c</i>]Pyrazole Framework. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 45914-45921.	4.0	58
3366	Combining Charge Density Analysis with Machine Learning Tools To Investigate the Cruzain Inhibition Mechanism. <i>ACS Omega</i> , 2019, 4, 19582-19594.	1.6	13
3367	Understanding the Stability Trend Along Light Lanthanide Complexes with an Ehtylenediamine-Type Ligand: A Quantum Chemical Study. <i>ChemistrySelect</i> , 2019, 4, 12368-12374.	0.7	8
3368	Probing the Structural and Electronic Properties of Neutral and Anionic Lanthanum-Doped Silicon Clusters. <i>Journal of Physical Chemistry C</i> , 2019, 123, 28561-28568.	1.5	82
3369	Photoswitchable Boronic Acid Derived Salicylidenehydrazone Enabled by Photochromic Spirooxazine and Fulgide Moieties: Multiple Responses of Optical Absorption, Fluorescence Emission, and Quadratic Nonlinear Optics. <i>Journal of Physical Chemistry C</i> , 2019, 123, 29838-29855.	1.5	38
3370	Picosecond to Nanosecond Manipulation of Excited-State Lifetimes in Complexes with an Fe ^{II} to Ti ^{IV} Metal-to-Metal Charge Transfer: The Role of Ferrocene Centered Excited States. <i>Inorganic Chemistry</i> , 2019, 58, 15320-15329.	1.9	7
3371	Redetermination of the Structure of a Water-Soluble Hypervalent Iodine(V) Reagent AIBX and Its Synthetic Utility in the Oxidation of Alcohols and Synthesis of IsoxazolineN-Oxides. <i>Journal of Organic Chemistry</i> , 2019, 84, 14381-14393.	1.7	12
3372	A theoretical investigation on the complexes of B ₃ O ₃ H ₃ with acetylene and its substituted derivatives. <i>Journal of Molecular Modeling</i> , 2019, 25, 332.	0.8	2
3373	The role of hydration effects in 5-fluorouridine binding to SOD1: insight from a new 3D-RISM-KH based protocol for including structural water in docking simulations. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 913-926.	1.3	4
3374	Enhancement of the Catalytic Activities of Heteronuclear Bimetallic Cations for the C-H Bond Activation of Cyclohexane. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10397-10405.	1.1	1
3375	Non-covalent Interactions and Charge Transfer between Propene and Neutral Yttrium-Doped and Pure Gold Clusters. <i>Chemistry - A European Journal</i> , 2019, 25, 15795-15804.	1.7	8
3376	Advances in molecular engineering of organic-inorganic/inorganic halide perovskites: Photochemical properties behind the energy conversion ability. <i>Solar Energy</i> , 2019, 194, 51-60.	2.9	14

#	ARTICLE	IF	CITATIONS
3377	Molecular structure and non-covalent interaction of 2-thiophenecarboxaldehyde and its monohydrated complex. <i>Journal of Chemical Physics</i> , 2019, 151, 164307.	1.2	10
3378	Theoretical Studies of IR and NMR Spectral Changes Induced by Sigma-Hole Hydrogen, Halogen, Chalcogen, Pnicogen, and Tetrel Bonds in a Model Protein Environment. <i>Molecules</i> , 2019, 24, 3329.	1.7	35
3379	Interaction of Graphene Quantum Dots with Oligothiophene: A Comprehensive Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 29556-29570.	1.5	22
3380	A 3D Analogue of Phenyllithium: Solution-Phase, Solid-State, and Computational Study of the Lithiacarborane [Li ⁺ CB ₁₁ H ₁₁] ⁻ . <i>Angewandte Chemie</i> , 2019, 131, 19183-19189.	1.6	1
3381	Application of Molecular Electrostatic Potential Surface to Predict Supramolecular Synthons for RDX/Solvent Cocrystals. <i>Crystal Research and Technology</i> , 2019, 54, 1900171.	0.6	6
3382	A Rare Type of Rhenium(I) Diimine Complexes with Unsupported Coordinated Phosphine Oxide Ligands: Synthesis, Structural Characterization, Photophysical and Theoretical Study. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 4350-4357.	1.0	12
3383	clusters (C ₆₀) _n . <i>Journal of Computational Chemistry</i> , 2019, 40, 2858-2867.	1.5	11
3384	Silicon photosensitizers in cancer therapy: Theoretical studies on novel 5-methoxypsoralens. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e4007.	0.9	5
3385	The effect of CO on the transformation of arsenic species: A quantum chemistry study. <i>Energy</i> , 2019, 187, 116024.	4.5	14
3386	Aliphatic Amines: A Critical Analysis of the Experimental Enthalpies of Formation by Comparison with Theoretical Calculations. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 5630-5647.	1.0	7
3387	Reduction Reaction of Nitric Oxide on the Rh ₅ V ⁺ Cluster: A Density Functional Theory Mechanistic Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 24495-24500.	1.5	4
3388	Oxidative Addition Promoted C-C Bond Cleavage in Rh-Mediated Cyclopropanone Activation: A DFT Study. <i>ACS Catalysis</i> , 2019, 9, 10876-10886.	5.5	40
3389	Hydrocarbon Pool Mechanism of the Zeolite-Catalyzed Conversion of Ethene to Propene. <i>ACS Catalysis</i> , 2019, 9, 10640-10648.	5.5	24
3390	Infrared Spectroscopy of Hydrogen-Bonding Interactions in Neutral Dimethylamine-Methanol Complexes. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10109-10115.	1.1	13
3391	Spectroscopic Signature of Proton Location in Proton Bound HSO ₄ ⁻ ·H ⁺ ·X ⁺ (X = F, Cl, Br, and I) Clusters. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6714-6719.	2.1	17
3392	Structural modification as the pioneer strategy in competition of the porphyrin dye and perovskite solar cells: From dynamics to kinetics of the photovoltaic processes. <i>Applied Physics Letters</i> , 2019, 115, .	1.5	14
3393	Towards deep-blue phosphorescence: molecular design and property prediction of iridium complexes with pyridinylphosphinate ancillary ligand. <i>Applied Organometallic Chemistry</i> , 2019, 33, e5167.	1.7	5
3394	Elucidating Solvent Effects on Strong Intramolecular Hydrogen Bond: DFT-MD Study of Dibenzoylmethane in Methanol Solution. <i>ChemPhysChem</i> , 2019, 20, 2852-2859.	1.0	2

#	ARTICLE	IF	CITATIONS
3395	Exploring Nature and Predicting Strength of Hydrogen Bonds: A Correlation Analysis Between Atomsâ€”Molecules Descriptors, Binding Energies, and Energy Components of Symmetry-Adapted Perturbation Theory. <i>Journal of Computational Chemistry</i> , 2019, 40, 2868-2881.	1.5	678
3396	Major Depressive Disorder and Oxidative Stress: In Silico Investigation of Fluoxetine Activity against ROS. <i>Applied Sciences (Switzerland)</i> , 2019, 9, 3631.	1.3	27
3397	Does Oxygen Feature Chalcogen Bonding?. <i>Molecules</i> , 2019, 24, 3166.	1.7	27
3398	A Sublimable Dinuclear Cuprous Complex Showing Selective Luminescence Vapochromism in the Crystalline State. <i>Inorganic Chemistry</i> , 2019, 58, 14478-14489.	1.9	26
3399	Luminescent Platinum(II) Complexes of N^{N} -Amido Ligands with Benzannulated N -Heterocyclic Donor Arms: Quinolines Offer Unexpectedly Deeper Red Phosphorescence than Phenanthridines. <i>Inorganic Chemistry</i> , 2019, 58, 14808-14817.	1.9	34
3400	The adsorption of small size Pd clusters on a $\text{g-C}_{3\text{N}_4}$ quantum dot: DFT and TD-DFT study. <i>Materials Research Express</i> , 2019, 6, 105079.	0.8	10
3401	Self-Assembly of Ferrocene Peptides: A Nonheme Strategy to Construct a Peroxidase Mimic. <i>Advanced Materials Interfaces</i> , 2019, 6, 1901082.	1.9	10
3402	Theoretical insight into the single-atom catalytic mechanism of CeO_2 -supported Ag catalysts in CO oxidation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20346-20353.	1.3	5
3403	Hydrogen Bonding versus $\text{H}\cdots\text{H}$ Interactions in Pillar[n]arenes. <i>ChemistrySelect</i> , 2019, 4, 9354-9359.	0.7	3
3404	Analyses on Molecular Properties of the Diamidinate Cr^{I} Complex by Multireference and DFT Approaches. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7803-7813.	1.1	5
3405	Visualizations of Electric and Magnetic Interactions in Electronic Circular Dichroism and Raman Optical Activity. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8071-8081.	1.1	43
3406	Noble gas insertion compounds of hydrogenated and lithiated hyperhalogens. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20156-20165.	1.3	4
3407	Fluorescence-phosphorescence dual emissive carbon nitride quantum dots show 25% white emission efficiency enabling single-component WLEDs. <i>Chemical Science</i> , 2019, 10, 9801-9806.	3.7	115
3408	Hydrogen-bonding-induced bathochromic effect of Si-coumarin and its use in monitoring adipogenic differentiation. <i>Chemical Communications</i> , 2019, 55, 11802-11805.	2.2	15
3409	BN-Doped Graphene and Single-Walled Carbon Nanotubes for the Catalysis of $\text{S}_{\text{N}}2$ Reactions: Insights from Density Functional Theory Modeling. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8188-8199.	1.1	8
3410	Theoretical screening of bistriazole-derived energetic salts with high energetic properties and low sensitivity. <i>RSC Advances</i> , 2019, 9, 26442-26449.	1.7	4
3411	Unraveling the binding nature of hexane with quinone functionalized pillar[5]quinone: a computational study. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2019, 95, 307-319.	0.9	11
3412	Cationic Iridium Complexes with 5-Phenyl-1H-1,2,4-triazole Type Cyclometalating Ligands: Toward Blue-Shifted Emission. <i>Inorganic Chemistry</i> , 2019, 58, 12132-12145.	1.9	29

#	ARTICLE	IF	CITATIONS
3413	Structure of Butyl Carbamate and of Its Water Complex in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7983-7990.	1.1	3
3414	Reaction Mechanism of Histone Demethylation in Fe^{2+} -dependent Non-Heme Iron Enzymes. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7801-7811.	1.2	8
3415	Coinage metal dimers as the noncovalent interaction acceptors: study of the M^2 -lump interactions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21152-21161.	1.3	11
3416	HgO oxidation and SO_3 , PbO, PbO, PbCl_2 and As_2O_3 adsorption by graphene-based bimetallic catalyst ((Fe,Co)@N-GN): A DFT study. <i>Applied Surface Science</i> , 2019, 496, 143686.	3.1	38
3417	Redox Property of Enamines. <i>Journal of Organic Chemistry</i> , 2019, 84, 12071-12090.	1.7	34
3418	Synthesis and Cyclization-Induced Charge Transfer of Rectangular Bisterthiophenesiloxanes. <i>Chemistry - A European Journal</i> , 2019, 25, 13701-13704.	1.7	1
3419	Electronic effect of N^2 -diketonato ligands on the redox potential of fac and mer tris(N^2 -diketonato) iron(III) complexes: A density functional theory study and molecular electrostatic potential analysis. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e26036.	1.0	7
3420	Theoretical study of gallium nitride nanocage as a carrier for 5-fluorouracil anticancer drug. <i>Journal of Molecular Modeling</i> , 2019, 25, 265.	0.8	17
3421	Characterization of a MnII complex of Alizarin suggests attributes explaining a superior anticancer activity: A comparison with anthracycline drugs. <i>Polyhedron</i> , 2019, 173, 114104.	1.0	3
3422	$\text{C}=\text{H} \cdots \text{Pd}$ interactions in palladium complexes derived from tetrasulfur-difluorinated ligands. Experimental, computational and catalytic studies. <i>Polyhedron</i> , 2019, 173, 114115.	1.0	1
3423	End-On Oxygen-Bound Sulfur Monoxide Complex of Titanium Oxyfluoride. <i>Inorganic Chemistry</i> , 2019, 58, 11801-11806.	1.9	4
3424	$\text{Er}_2\text{C}_2@C_2(43)\text{-C}_{90}$, $\text{Er}_2\text{C}_2@C_2(40)\text{-C}_{90}$, $\text{Er}_2\text{C}_2@C_2(44)\text{-C}_{90}$, and $\text{Er}_2\text{C}_2@C_1(21)\text{-C}_{90}$; the role of cage-shape on Er_2C_2 encapsulation. <i>Nanoscale</i> , 2019, 11, 7319-7326.	2.8	23
3425	Pivotal Role of Nonmetal Atoms in the Stabilities, Geometries, Electronic Structures, and Isoelectronic Chemistry of $\text{Sc}_3\text{X}@C_{80}$ (X = C, N, and O). <i>Journal of Computational Chemistry</i> , 2019, 40, 2730-2738.	1.5	10
3426	Hydrogen Atom or Proton Coupled Electron Transfer? $\text{C}=\text{H}$ Bond Activation by Transition-Metal Oxides. <i>Journal of the American Chemical Society</i> , 2019, 141, 14603-14611.	6.6	25
3427	Infrared photodissociation spectroscopic and theoretical study of the HC_2nO^+ ($n=3\text{--}6$) cations. <i>Chinese Journal of Chemical Physics</i> , 2019, 32, 77-83.	0.6	4
3428	Theoretical study on the weak interaction and energy performance of nitroformate salts and nitroformate-based propellant formulations. <i>Journal of Molecular Modeling</i> , 2019, 25, 285.	0.8	4
3429	Hopping of $\text{Li}@AR$ (AR = Benzene and Naphthalene) between Electride and Lithium Salt Configurations Brings Considerably Different First Hyperpolarizabilities: Candidate for High-Performance Nonlinear Optical Molecular Switches. <i>Journal of Physical Chemistry C</i> , 2019, 123, 24248-24254.	1.5	5
3430	Double-bond elucidation for arsagermene with a tricoordinate germanium center: a theoretical survey. <i>New Journal of Chemistry</i> , 2019, 43, 15681-15690.	1.4	2

#	ARTICLE	IF	CITATIONS
3431	Performance of doped graphene nanoadsorbents with first-row transition metals (Sc Zn) for the adsorption of water-soluble trivalent arsenicals: A DFT study. <i>Journal of Molecular Liquids</i> , 2019, 294, 111665.	2.3	8
3432	Near-Infrared [Ir(N ^{sup>âˆš</sup>C<sub>2</sub>(N^{sup>âˆš</sup>N)]⁺ Emitters and Their Noncovalent Adducts with Human Serum Albumin: Synthesis and Photophysical and Computational Study. <i>Organometallics</i>, 2019, 38, 3740-3751.}}	1.1	20
3433	Mechanism and origins of ligand-controlled Pd(II)-catalyzed regiodivergent carbonylation of alkynes. <i>Dalton Transactions</i> , 2019, 48, 15059-15067.	1.6	8
3434	Chalcogen bonding of two ligands to hypervalent YF ₄ (Y = S, Se, Te, Po). <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20829-20839.	1.3	27
3435	Sulfamethoxazole degradation by an Fe(II)-activated persulfate process: insight into the reactive sites, product identification and degradation pathways. <i>Environmental Sciences: Processes and Impacts</i> , 2019, 21, 1560-1569.	1.7	55
3436	Theoretical study of nitrogen cation modified aromatics containing thiophene as π -linker for p-type photosensitizers. <i>Journal of Molecular Modeling</i> , 2019, 25, 300.	0.8	2
3437	Substitution induced tunable emission of an airplane-like pyrene-based fluorophore: First-principles study. <i>Chemical Physics Letters</i> , 2019, 734, 136726.	1.2	3
3438	Synthesis of new triazolyl-oxazoline chiral ligands and study of their coordination to Pd(II) metal centers. <i>Inorganica Chimica Acta</i> , 2019, 498, 119129.	1.2	11
3439	Theoretical Study on the Reactions Originating from Solid Char(N): Radical Preference and Possible Surface N ₂ Formation Reactions. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 18021-18026.	1.8	2
3440	A Novel Immunosensing Method Based on the Capture and Enzymatic Release of Sandwich-Type Covalently Conjugated Thionine-Gold Nanoparticles as a New Fluorescence Label Used for Ultrasensitive Detection of Hepatitis B Virus Surface Antigen. <i>ACS Omega</i> , 2019, 4, 15323-15336.	1.6	12
3441	Theoretical insights into tunable optical and electronic properties of graphene quantum dots through phosphorization. <i>Carbon</i> , 2019, 155, 491-498.	5.4	34
3442	Effect of fluorination of the donor unit on the properties of benzodithiophene-triazole based donor-acceptor systems for polymer solar cells: A computational investigation. <i>Computational and Theoretical Chemistry</i> , 2019, 1165, 112564.	1.1	3
3443	Diferrocenyl Thioketone: Reactions with (Bisphosphane)Pt(0) Complexes – Electrochemical and Computational Studies. <i>Materials</i> , 2019, 12, 2832.	1.3	4
3444	DMSO hydration redefined: Unraveling the hydrophobic hydration of solutes with a mixed hydrophilic-hydrophobic characteristic. <i>Journal of Molecular Liquids</i> , 2019, 294, 111661.	2.3	17
3445	Comparison of pnictogen and tetrel bonds in complexes containing CX ₂ carbenes (X = F, Cl, Br, OH,) <i>TJ ETQq0 0 0 rgBT /Overlock 10 Tf 5</i>	1.4	9
3446	Structural evolution and electronic properties of Au ₂ Ge _n ^{+/0} (n=1~8) clusters: Anion photoelectron spectroscopy and theoretical calculations. <i>Chinese Journal of Chemical Physics</i> , 2019, 32, 229-240.	0.6	9
3447	Interaction of H ₂ O with (CuS) _n , (Cu ₂ S) _n , and (ZnS) _n small clusters (n=4, 6): relation to the aggregation characteristics of metal sulfides at aqueous solutions. <i>Journal of Molecular Modeling</i> , 2019, 25, 291.	0.8	11
3448	Insights on [BMIM][BF ₄] and [BMIM][PF ₆] ionic liquids and their binary mixtures with acetone and acetonitrile. <i>Journal of Molecular Liquids</i> , 2019, 294, 111632.	2.3	13

#	ARTICLE	IF	CITATIONS
3449	The facile synthesis of homoleptic phenylpyridazine iridium(III) complexes and their application in high efficiency OLEDs. <i>Organic Electronics</i> , 2019, 75, 105439.	1.4	8
3450	Benchmarking dual-level MS-Tor and DLPNO-CCSD(T) methods for H-abstraction from methyl pentanoate by an OH radical. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20857-20867.	1.3	14
3451	The effect of heteroatoms in carbonaceous surfaces: computational analysis of H chemisorption on to a PANH and Si-doped PAH. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 490, 172-180.	1.6	7
3452	A density functional theory study on complexation processes and intermolecular interactions of triptycene-derived oxacalixarenes. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	34
3453	Role of backbones on the interaction of metal ions with deoxyribonucleic acid and peptide nucleic acid: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 93, 107445.	1.3	11
3454	Theoretical insights into the stability of perovskite clusters by studying water adsorption on (CH ₃ NH ₃) ₄ SnI ₆ . <i>Solar Energy Materials and Solar Cells</i> , 2019, 202, 110126.	3.0	3
3455	Long-Range Charge Transfer Driven by External Electric Field in Alkalides M ⁺ Ca ⁺ M (M = Li or Na, L = Tj ETQq0 0 0 rgBT /Overlock Molecular Optical Switches. <i>Journal of Physical Chemistry C</i> , 2019, 123, 23610-23619.	1.5	21
3456	Application of a Dual-Solvent Method in Separating Paraffin from a Shale Oil: A Combined Experimental and DFT Study. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 17507-17513.	1.8	12
3457	Photo-induced Electron Transfer or Proton-Coupled Electron Transfer in Methylbipyridine/Phenol Complexes: A Time-Dependent Density Functional Theory Investigation. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8122-8129.	1.1	7
3458	Chemical and Physical Viewpoints About the Bonding in Fullerene@Graphene Hybrid Materials: Interaction on Pristine and Fe-Doped Graphene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 24209-24219.	1.5	13
3459	Theoretical study of the ligand effect on NHC-cobalt-catalyzed hydrogenation of ketones. <i>Catalysis Science and Technology</i> , 2019, 9, 5315-5321.	2.1	6
3460	Perylenetetracarboxylic diimide as a high-rate anode for potassium-ion batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 24454-24461.	5.2	55
3461	Systematic study on the structures and properties of (Ag ₂ S) _n (n = 1-8) clusters. <i>Journal of Molecular Modeling</i> , 2019, 25, 310.	0.8	8
3462	Europium-Functionalized Flexible Luminescent Zeolite-like Supramolecular Assembly for Ratiometric Anthrax Biomarker Determination. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 36081-36089.	4.0	34
3463	Regulation of Singlet and Triplet Excitons in a Single Emission Layer: Efficient Fluorescent/Phosphorescent Hybrid White Organic Light-Emitting Diodes. <i>ACS Omega</i> , 2019, 4, 15030-15042.	1.6	16
3464	Pyridine-acetaldehyde, a molecular balance to explore the n-π* interaction. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20566-20570.	1.3	16
3465	Computational characterization of the glutamate receptor antagonist perampanel and its close analogs: density functional exploration of conformational space and molecular docking study. <i>Journal of Molecular Modeling</i> , 2019, 25, 312.	0.8	7
3466	The synergistic effect and microscopic mechanism of co-adsorption of three emerging contaminants and copper ion on gemini surfactant modified montmorillonite. <i>Ecotoxicology and Environmental Safety</i> , 2019, 184, 109610.	2.9	22

#	ARTICLE	IF	CITATIONS
3467	Probing Binding of Ethylated Pillar[5]arene with Pentene and Chlorobutane Positional Isomers. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8391-8396.	1.1	9
3468	2D π - π square and hexagon interactions: a combined crystallographic data analysis and computational study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21568-21576.	1.3	17
3469	Insight into the Relationship between Viscosity and Hydrogen Bond of a Series of Imidazolium Ionic Liquids: A Molecular Dynamics and Density Functional Theory Study. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 18848-18854.	1.8	28
3470	Triplet-State Structures, Energies, and Antiaromaticity of BN Analogues of Benzene and Their Benzo-Fused Derivatives. <i>Journal of Organic Chemistry</i> , 2019, 84, 13582-13594.	1.7	16
3471	Oxidation State-Dependent Electronic Properties of Sulfur-Containing Thermally Activated Delayed Fluorescence Molecules. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8755-8765.	1.1	7
3472	Theoretical study on desulfurization mechanisms of a coal-based model compound 2-methylthiophene during pyrolysis under inert and oxidative atmospheres. <i>Fuel</i> , 2019, 257, 116028.	3.4	15
3473	Doping superalkali on Zn ₁₂ O ₁₂ nanocage constitutes a superior approach to fabricate stable and high-performance nonlinear optical materials. <i>Optics and Laser Technology</i> , 2019, 120, 105753.	2.2	64
3474	Chiral Phosphoric Acid-Catalyzed Enantioselective Direct Arylation of Iminoquinones: A Case Study of the Model Selectivity. <i>Journal of Organic Chemistry</i> , 2019, 84, 13473-13482.	1.7	7
3475	Theoretical Study of the Mechanism of Aggregation-Caused Quenching in Near-Infrared Thermally Activated Delayed Fluorescence Molecules: Hydrogen-Bond Effect. <i>Journal of Physical Chemistry C</i> , 2019, 123, 24705-24713.	1.5	89
3476	Metallalkenyl, Metallacyclopentene, or Metallallylcarbenoid? Ru-Catalyzed Annulation between Benzoic Acid and Alkyne. <i>ACS Catalysis</i> , 2019, 9, 9387-9392.	5.5	19
3477	Theoretical determination of the effects of various linkages between trinitrobenzenes on energetic properties and sensitivity. <i>Journal of Molecular Modeling</i> , 2019, 25, 315.	0.8	7
3478	Photoinduced Charge Separation in Retinoic Acid on TiO ₂ : Comparison of Three Anchoring Modes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 24634-24642.	1.5	8
3479	Evaluation of the molecular inclusion process of β -hexachlorocyclohexane in cyclodextrins. <i>RSC Advances</i> , 2019, 9, 27484-27499.	1.7	12
3480	A Comprehensive Topological Analysis on a New Bromine-Chalcone with Potential Nonlinear Optical Properties. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8632-8643.	1.1	5
3481	Ternary 12-electron CBe ₃ X ₃ ⁺ (X = H, Li, Na, Cu, Ag) clusters: planar tetracoordinate carbons and superalkali cations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22048-22056.	1.3	17
3482	Unusual near infrared (NIR) fluorescent palladium(π) macrocyclic complexes containing M=C bonds with bioimaging capability. <i>Chemical Science</i> , 2019, 10, 10170-10178.	3.7	23
3483	Electrical and Electrochemical Behavior of Carbon Paste Electrodes Modified with Ionic Liquids Based in N-Octylpyridinium Bis(Trifluoromethylsulfonyl)imide. A Theoretical and Experimental Study. <i>Molecules</i> , 2019, 24, 3382.	1.7	8
3484	Multicenter bonding in s-block metals: An insight from theory. <i>Computational and Theoretical Chemistry</i> , 2019, 1167, 112606.	1.1	4

#	ARTICLE	IF	CITATIONS
3485	Superalkali NM4 (M ⁺ =Li, Na, K): Stabilities and electronic structures. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 125952.	0.9	15
3486	[6]Cyclo- <i>para</i> -phenylmethine: An Analog of Benzene Showing Global Aromaticity and Open-Shell Diradical Character. <i>Journal of the American Chemical Society</i> , 2019, 141, 16266-16270.	6.6	41
3487	Predicting the Enthalpies of Sublimation of Cyclic Urea Derivatives Using a Model of the Molecular Electrostatic Potential. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 1896-1901.	0.1	3
3488	Reconstructing the Electron Density of Intermediates of the Hydrolysis of N-Acetylaspartate by Aspartoacylase. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 1873-1879.	0.1	0
3489	Seventeen-coordinate binary metal superatoms: M@Li ₁₇ . <i>Chemical Physics Letters</i> , 2019, 733, 136693.	1.2	1
3490	Cyclometalated Iridium(III) Complexes Incorporating Aromatic Phosphonate Ligands: Syntheses, Structures, and Tunable Optical Properties. <i>ACS Omega</i> , 2019, 4, 16543-16550.	1.6	11
3491	Crystal structure and evaluating C-H⋯N (aryl/chelate) interactions in bis(2-[(2-hydroxyethyl)imino]-methyl)-4,6-diiodophenolato)-palladium(II) Schiff base complex derived from (E)-2-((2-hydroxyethyl)imino)methyl)-4,6-diiodophenol. <i>Inorganica Chimica Acta</i> , 2019, 498, 119118.	1.2	4
3492	Hydrogen bonding interaction of N5H with water: A first principle calculations. <i>Computational and Theoretical Chemistry</i> , 2019, 1165, 112560.	1.1	5
3493	Aluminum-silicon hydride clusters for prospective hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 26459-26468.	3.8	5
3494	Pt doped (8,0) single wall carbon nanotube as hydrogen sensor: A density functional theory study. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 27010-27021.	3.8	41
3495	Reactivity of Polycyclic Aromatic Hydrocarbon Soot Precursors: Implications of Localized $\dot{\text{C}}$ -Radicals on Rim-Based Pentagonal Rings. <i>Journal of Physical Chemistry C</i> , 2019, 123, 26673-26682.	1.5	47
3496	Efficient deep blue OLEDs with extremely low efficiency roll-off at high brightness based on phenanthroimidazole derivatives. <i>Chinese Chemical Letters</i> , 2019, 30, 1989-1993.	4.8	14
3497	How and Why a Protic Ionic Liquid Efficiently Catalyzes Chemical Fixation of CO ₂ to Quinazoline-2,4-(1H,3H)-diones: Electrostatically Controlled Reactivity. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9394-9402.	1.1	10
3498	Ultramild One-Step Encapsulating Method as a Modular Strategy for Protecting Humidity-Susceptible Metal-Organic Frameworks Achieving Tunable Drug Release Profiles. <i>ACS Biomaterials Science and Engineering</i> , 2019, 5, 5180-5188.	2.6	17
3499	Electronic versus steric control in palladium complexes of carboranyl phosphine-iminophosphorane ligands. <i>Dalton Transactions</i> , 2019, 48, 486-503.	1.6	5
3500	A rationally designed vapoluminescent compound with adsorptive channels and responsive luminophores for volatile organic compounds (VOCs). <i>Dalton Transactions</i> , 2019, 48, 1179-1183.	1.6	6
3501	Understanding the axial chirality control of quinidine-derived ammonium cation-directed O-alkylation: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 1916-1923.	1.5	7
3502	Computational insight into the mechanism and origins of high selectivities in the acylation of polyamines with 5-benzoyl-5-phenyl-1,5-dihydro-4H-pyrazol-4-one. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 140-150.	1.5	1

#	ARTICLE	IF	CITATIONS
3503	The effect of different environments on excited-state intramolecular proton transfer in 4-hydroxy-2-methoxy-3-hydroxyflavone. <i>Organic Chemistry Frontiers</i> , 2019, 6, 218-225.	2.3	28
3504	Revealing quantum mechanical effects in enzyme catalysis with large-scale electronic structure simulation. <i>Reaction Chemistry and Engineering</i> , 2019, 4, 298-315.	1.9	33
3505	Global performance evaluation of solar cells using two models: from charge-transfer and recombination mechanisms to photoelectric properties. <i>Journal of Materials Chemistry C</i> , 2019, 7, 1934-1947.	2.7	73
3506	A DFT study of the degradation mechanism of anticancer drug carmustine in an aqueous medium. <i>Structural Chemistry</i> , 2019, 30, 1315-1321.	1.0	9
3507	Amides as models to study the hydration of proteins and peptides – spectroscopic and theoretical approach on hydration in various temperatures. <i>Journal of Molecular Liquids</i> , 2019, 278, 706-715.	2.3	9
3508	Novel aryloxyphenoxypropionate derivatives containing benzofuran moiety: Design, synthesis, herbicidal activity, docking study and theoretical calculation. <i>Pesticide Biochemistry and Physiology</i> , 2019, 154, 78-87.	1.6	18
3509	Hydrogen Bonding Network: Stabilization of the Pentazolate Anion in Two Nonmetallic Energetic Salts. <i>Crystal Growth and Design</i> , 2019, 19, 1853-1859.	1.4	39
3510	Accuracy and reproducibility in crystal structure prediction: the curious case of ROY. <i>CrystEngComm</i> , 2019, 21, 2080-2088.	1.3	55
3511	Valence bonds in planar and quasi-planar boron disks. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 729-735.	1.3	5
3512	π-Hydrogen bonding and aromaticity: a systematic interplay study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 623-630.	1.3	29
3513	Constructing organic superacids from superhalogens is a rational route as verified by DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2804-2815.	1.3	15
3514	Theoretical screening of promising donor and π-linker groups for POM-based Zn porphyrin dyes in dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3822-3831.	1.3	14
3515	Probing enantioselectivity in rhodium-catalyzed Si-C bond cleavage to construct silicon-stereocenters: a theoretical study. <i>Catalysis Science and Technology</i> , 2019, 9, 646-651.	2.1	8
3516	Multi-heteroatom doped graphene-like carbon nanospheres with 3D inverse opal structure: a promising bisphenol-A remediation material. <i>Environmental Science: Nano</i> , 2019, 6, 809-819.	2.2	36
3517	Excellent benzocoumarin-based ratiometric two-photon fluorescent probe for H ₂ O ₂ detection. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 281-291.	1.3	22
3518	Non covalent interactions stabilizing the chiral dimer of CH ₂ ClF: a rotational study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3695-3700.	1.3	5
3519	Highly luminescent copper(II) halide complexes chelated with a tetradentate ligand (PNNP): synthesis, structure, photophysical properties and theoretical studies. <i>Dalton Transactions</i> , 2019, 48, 1418-1426.	1.6	42
3520	Binding affinity of pyridines with Am ^{III} /Cm ^{III} elucidated by density functional theory calculations. <i>Dalton Transactions</i> , 2019, 48, 1613-1623.	1.6	5

#	ARTICLE	IF	CITATIONS
3521	Theoretical study on the influence of electric field direction on the photovoltaic performance of aryl amine organic dyes for dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2019, 43, 651-661.	1.4	7
3522	Theoretical investigation of U(π) arene complexes: is the elusive monovalent oxidation state accessible?. <i>New Journal of Chemistry</i> , 2019, 43, 1469-1477.	1.4	13
3523	Maoericalysins A–D, four novel ent-kaurane diterpenoids from <i>Isodon eriocalyx</i> and their structure determination utilizing quantum chemical calculation in conjunction with quantitative interproton distance analysis. <i>Organic Chemistry Frontiers</i> , 2019, 6, 45-53.	2.3	10
3524	The opposite and amplifying effect of B–N coordination on photophysical properties of regioisomers with an unsymmetrical backbone. <i>Chemical Science</i> , 2019, 10, 1724-1734.	3.7	22
3525	Organic Anions Facilitate in Situ Synthesis of Mesoporous LTA Zeolites. <i>Chemistry of Materials</i> , 2019, 31, 1528-1536.	3.2	15
3526	Competitive hydrogen-bonding and halogen-bonding interactions in the dimerization of hypobromous acid (HOBr) molecules. <i>Structural Chemistry</i> , 2019, 30, 1335-1341.	1.0	0
3527	Electronic excited states of mixed sandwich complexes, (1-7-C7H7)(1-5-C5H5)M (M = V, Cr): Investigation with time-dependent density functional theory. <i>Inorganica Chimica Acta</i> , 2019, 487, 281-286.	1.2	2
3528	Halogen Substituent Effects on Concentration-Controlled Self-Assembly of Fluorenone Derivatives: Halogen Bond versus Hydrogen Bond. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4349-4359.	1.5	25
3529	PtAu ₃ cluster complexes with narrow-band emissions for solution-processed organic light emitting diodes. <i>Journal of Materials Chemistry C</i> , 2019, 7, 2604-2614.	2.7	36
3530	Ellagitannin derivatives and some conjugated metabolites: aqueous-DMSO proton affinities and acidity constants. <i>Structural Chemistry</i> , 2019, 30, 1343-1351.	1.0	1
3531	The unusual improvement of normal alkyl alcohol on solid-state cationic photopolymerization of octadecyl vinyl ether. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 374, 52-57.	2.0	1
3532	Calculation of $V_{S,max}$ and Its Use as a Descriptor for the Theoretical Calculation of pKa Values for Carboxylic Acids. <i>Molecules</i> , 2019, 24, 79.	1.7	13
3533	Effects of Li doping and B3N3 substitution on the static first hyperpolarizabilities of biphenylene nanosheets: A computational and comparative study. <i>Organic Electronics</i> , 2019, 68, 9-14.	1.4	16
3534	Structure evolution of chromium-doped boron clusters: toward the formation of endohedral boron cages. <i>RSC Advances</i> , 2019, 9, 2870-2876.	1.7	18
3535	Use of Single-Metal Fragments for Cluster Building: Synthesis, Structure, and Bonding of Heterometallaboranes. <i>Inorganic Chemistry</i> , 2019, 58, 2744-2754.	1.9	10
3536	Diphosphazane-monoxide and Phosphine-sulfonate Palladium Catalyzed Ethylene Copolymerization with Polar Monomers: A Computational Study. <i>Organometallics</i> , 2019, 38, 638-646.	1.1	25
3537	Structural growth pattern of neutral and negatively charged yttrium-doped silicon clusters YSi _n O [−] ($n = 6-20$): from linked to encapsulated structures. <i>RSC Advances</i> , 2019, 9, 2731-2739.	1.7	15
3538	Electronic structure in the transition metal block and its implications for light harvesting. <i>Science</i> , 2019, 363, 484-488.	6.0	204

#	ARTICLE	IF	CITATIONS
3539	Theoretical studies on the structures, material properties, and IR spectra of polymorphs of 3,4-bis(1H-5-tetrazolyl)furoxan. <i>Journal of Molecular Modeling</i> , 2019, 25, 51.	0.8	3
3540	Structures, metallophilic interactions and electronic excitation energy of linear metal chain complexes $\text{PdmPt}_n[\text{PH}_2(\text{CH}_2\text{PH})_{m+n-2}\text{CH}_2\text{PH}_2]_3$, a theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2019, 1151, 24-30.	1.1	0
3541	Side-On Sulfur Monoxide Complexes of Tantalum, Niobium, and Vanadium Oxyfluorides. <i>Inorganic Chemistry</i> , 2019, 58, 3807-3814.	1.9	14
3542	Spontaneous single-crystal to single-crystal transition with self-healing cracks involving solvent exchange. <i>CrystEngComm</i> , 2019, 21, 1102-1106.	1.3	11
3543	Towards red-light <i>o</i> -carborane derivatives with both aggregation induced emission and thermally activated delayed fluorescence combining quantum chemistry calculation with molecular dynamics simulation. <i>Journal of Materials Chemistry C</i> , 2019, 7, 2699-2709.	2.7	23
3544	A large Stokes shift, sequential, colorimetric fluorescent probe for sensing $\text{Cu}^{2+}/\text{S}^{2-}$ and its applications. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 373, 146-153.	2.0	25
3545	Charge transport properties in organic D-A mixed-stack complexes based on corannulene and sumanene derivatives-a theoretical study. <i>Organic Electronics</i> , 2019, 68, 35-44.	1.4	19
3546	Novel adamantane-based hole transport materials for perovskite solar cells: a computational approach. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3857-3867.	1.3	12
3547	Ultra-Weak Metal-Metal Bonding: Is There a Beryllium-Beryllium Triple Bond?. <i>ChemPhysChem</i> , 2019, 20, 516-518.	1.0	27
3548	Complexation of luteolin with lead (II): Spectroscopy characterization and theoretical researches. <i>Journal of Inorganic Biochemistry</i> , 2019, 193, 25-30.	1.5	19
3549	Colorimetric fluorescence probe detecting Hg^{2+} and OCl^- based on intramolecular charge transfer and excited-state intramolecular proton transfer mechanisms. <i>Journal of Luminescence</i> , 2019, 209, 102-108.	1.5	37
3550	Amino acid ionic liquids based on imidazolium-hydroxyl functionalized cation: New insight from molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , 2019, 279, 51-62.	2.3	5
3551	Investigation of multiple adsorption mechanisms for efficient removal of ofloxacin from water using lignin-based adsorbents. <i>Scientific Reports</i> , 2019, 9, 637.	1.6	38
3552	Fluorescence deactivation mechanism for a new probe detecting phosgene based on ES IPT and TICT. <i>Organic Chemistry Frontiers</i> , 2019, 6, 597-602.	2.3	50
3553	Solvent modulated excited state processes of push-pull molecule with hybridized local excitation and intramolecular charge transfer character. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3894-3902.	1.3	39
3554	Insights into highly selective ring expansion of oxaziridines under Lewis base catalysis: a DFT study. <i>Organic Chemistry Frontiers</i> , 2019, 6, 679-687.	2.3	38
3555	Predicting the halogen- <i>n</i> (<i>n</i> = 3-6) synthons to form the "windmill" pattern bonding based on the halogen-bonded interactions. <i>Journal of Computational Chemistry</i> , 2019, 40, 1219-1226.	1.5	13
3556	Understanding the Role of Fluorination on the Interaction of Electrolytic Carbonates with Li^+ through an Electronic Structure Approach. <i>ChemistrySelect</i> , 2019, 4, 1251-1258.	0.7	9

#	ARTICLE	IF	CITATIONS
3557	Theoretical study for conformational analysis and kinetics on the internal halogen exchange thermally induced of trichloro-(1,1-difluoroethyl)silane in the gas phase. Computational and Theoretical Chemistry, 2019, 1150, 102-109.	1.1	1
3558	Efficient full-colour organic light-emitting diodes based on donor-acceptor electroluminescent materials with a reduced singlet-triplet splitting energy gap. RSC Advances, 2019, 9, 2948-2966.	1.7	11
3559	Computer-Aided Design of Molecularly Imprinted Polymers for Simultaneous Detection of Clenbuterol and Its Metabolites. Polymers, 2019, 11, 17.	2.0	47
3560	Dinuclear Metal-Mediated Guanine-Uracil Base Pairs: Theoretical Studies of GUM22+ (M = Cu, Ag, and Ti). Journal of Physical Chemistry C, 2019, 123, 4007-4021.	1.7	0.7843
3561	The nitron spin trap 5,5-dimethyl-1-pyrroline N-oxide binds to toll-like receptor-2-TIR-BB-loop domain and dampens downstream inflammatory signaling. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2019, 1865, 1152-1159.	1.8	9
3562	Molecular design of organoplatinum(II) complexes through a DFT/TDDFT study: Photophysical properties and intermolecular interactions. Computational and Theoretical Chemistry, 2019, 1150, 91-101.	1.1	2
3563	Introducing Asymmetry Induced by Benzene Substitution in a Rigid Fused π -Spacer of D π A-Type Solar Cells: A Computational Investigation. Journal of Physical Chemistry C, 2019, 123, 4007-4021.	1.5	41
3564	The influence of antenna and anchoring moieties on the improvement of photoelectronic properties in Zn-porphyrin-TiO ₂ as potential dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2019, 21, 4339-4348.	1.3	17
3565	Enhancing effects of π -hole tetrel bonds on the π -hole interactions in complexes involving F2TO (T = Si, Sn, Pb). Journal of Physical Chemistry C, 2019, 123, 4007-4021.	1.0	0.0
3566	The plutonium chemistry of Pu ⁺ O ₂ system: the theoretical investigation of the plutonium-oxygen interaction. Journal of the Iranian Chemical Society, 2019, 16, 1157-1162.	1.2	4
3567	B3Si12: A hexagonal prism with three short B-B single bonds at the center coordinated by a Si ₁₂ cage and reinforced by aromaticity. Journal of Molecular Structure, 2019, 1183, 202-208.	1.8	11
3568	Kinetic understanding of the effect of Na and Mg on pyrolytic behavior of lignin using a distributed activation energy model and density functional theory modeling. Green Chemistry, 2019, 21, 1099-1107.	4.6	33
3569	Revealing the mechanism of contrasting charge transport properties for phenyl and thienyl substituent organic semiconductors. Physical Chemistry Chemical Physics, 2019, 21, 4641-4649.	1.3	5
3570	Mechanism of H ₂ O ₂ /bleach activators and related factors. Cellulose, 2019, 26, 2743-2757.	2.4	14
3571	Trends in the Bond Multiplicity of Cr ₂ , Cr ₃ , and Cr ₂ M (M = Zn, Ni). Journal of Physical Chemistry A, 2019, 123, 1538-1547.	1.1	7
3572	New Crystal Forms for Biologically Active Compounds. Part 1: Noncovalent Interactions in Adducts of Nevirapine with XB Donors. Crystals, 2019, 9, 71.	1.0	16
3573	Is the Fluorine in Molecules Dispersive? Is Molecular Electrostatic Potential a Valid Property to Explore Fluorine-Centered Non-Covalent Interactions?. Molecules, 2019, 24, 379.	1.7	69
3574	Structural effect on the vapor-liquid equilibrium of toluene-ionic liquid systems. Chemical Engineering Science, 2019, 198, 1-15.	1.9	27

#	ARTICLE	IF	CITATIONS
3575	Upgrading of pyrolytic lignin into hexamethylbenzene with high purity: demonstration of the "all-to-one" biochemical production strategy in thermo-chemical conversion. <i>Green Chemistry</i> , 2019, 21, 1000-1005.	4.6	17
3576	Control of the dual emission from a thermally activated delayed fluorescence emitter containing phenothiazine units in organic light-emitting diodes. <i>RSC Advances</i> , 2019, 9, 4336-4343.	1.7	25
3577	Theoretical Studies on the Electronic Structure Parameters and Reactive Activity of Neu5Gc and Neu5Ac under Food Processing Solvent Environment. <i>Molecules</i> , 2019, 24, 313.	1.7	6
3578	Metallaheteroboranes containing group 16 elements: An experimental and theoretical study. <i>Journal of Organometallic Chemistry</i> , 2019, 883, 71-77.	0.8	3
3579	Interaction between the plant alkaloid berberine and fullerene C70: Experimental and quantum-chemical study. <i>Journal of Molecular Liquids</i> , 2019, 278, 452-459.	2.3	12
3580	Performance Regulation of Thieno[3,2-b]benzothiophene π -Spacer-Based D-A Organic Dyes for Dye-Sensitized Solar Cell Applications: Insights From Computational Study. <i>Frontiers in Chemistry</i> , 2018, 6, 676.	1.8	20
3581	Recognition of the π -hole donor ability of iodopentafluorobenzene "a conventional π -hole donor for crystal engineering involving halogen bonding. <i>CrystEngComm</i> , 2019, 21, 616-628.	1.3	56
3582	Possible B-C bonding in the hydroboration of benzonitrile by an external electric field. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18-21.	1.3	11
3583	The effect of two types of dibenzoannulation of pentalene on molecular energies and magnetically induced currents. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3250-3263.	1.3	9
3584	Prediction on the origin of selectivities of NHC-catalyzed asymmetric dearomatization (CADA) reactions. <i>Catalysis Science and Technology</i> , 2019, 9, 465-476.	2.1	50
3585	Experimental and theoretical investigations of cyclometalated ruthenium(ii) complex containing CCC-pincer and anti-inflammatory drugs as ligands: synthesis, characterization, inhibition of cyclooxygenase and in vitro cytotoxicity activities in various cancer cell lines. <i>Dalton Transactions</i> , 2019, 48, 728-740.	1.6	24
3586	Magnetic investigations over reversibly switched chiral (phthalocyaninato)(porphyrinato) dysprosium double-decker compounds. <i>Dalton Transactions</i> , 2019, 48, 1586-1590.	1.6	9
3587	Metal-ligand ring aromaticity in a 2D coordination polymer used as a photosensitive electronic device. <i>New Journal of Chemistry</i> , 2019, 43, 2710-2717.	1.4	27
3588	A dipole-dipole interaction tuning the photoluminescence of silicon quantum dots in a water vapor environment. <i>Nanoscale</i> , 2019, 11, 1790-1797.	2.8	4
3589	Li ₂ B ₂₄ : the simplest combination for a three-ring boron tube. <i>Nanoscale</i> , 2019, 11, 2143-2147.	2.8	52
3590	Molecular assembly-induced charge transfer between a mixed (phthalocyaninato)(porphyrinato) yttrium triple-decker and a fullerene. <i>Inorganic Chemistry Frontiers</i> , 2019, 6, 654-658.	3.0	5
3591	A mechanistic investigation into N-heterocyclic carbene (NHC) catalyzed umpolung of ketones and benzonitriles: is the cyano group better than the classical carbonyl group for the addition of NHC?. <i>Organic Chemistry Frontiers</i> , 2019, 6, 523-531.	2.3	4
3592	Enhancement of intramolecular charge transfer strength in diphenylamine substituted symmetric 1,3,4-oxadiazole derivatives. <i>RSC Advances</i> , 2019, 9, 1-10.	1.7	19

#	ARTICLE	IF	CITATIONS
3593	Formation of Cu _{3,4} (TCA), making the TCA complex a highly selective probe for Cu ²⁺ detection: a TDDFT study. <i>Journal of Materials Chemistry C</i> , 2019, 7, 2443-2456.	2.7	12
3594	Halogen bonding-assisted assembly of bromoantimonate and polybromide-bromoantimonate-based frameworks. <i>CrystEngComm</i> , 2019, 21, 850-856.	1.3	48
3595	Excited-state solvation structure of transition metal complexes from molecular dynamics simulations and assessment of partial atomic charge methods. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4082-4095.	1.3	15
3596	Binuclear heterometallic bonding between a first row transition metal and a second row transition metal: The cyclopentadienyliron molybdenum carbonyls Cp ₂ FeMo(CO) (n = 6, 5, 4, 3, 2). <i>Inorganica Chimica Acta</i> , 2019, 493, 102-111.	1.2	1
3597	Computational and spectroscopic investigations on boronic acid based fluorescent carbohydrate sensor in aqueous solution at physiological pH 7.5. <i>Journal of Molecular Structure</i> , 2019, 1194, 305-319.	1.8	18
3598	On the ability of pnictogen atoms to engage in both π and σ -hole complexes. Heterodimers of ZF ₂ C ₆ H ₅ (Z = P, As, Sb, Bi) and NH ₃ . <i>Journal of Molecular Modeling</i> , 2019, 25, 152.	0.8	29
3599	Ultrafast intramolecular vibrational energy transfer in carbon nitride hydrocolloid examined by femtosecond two-dimensional infrared spectroscopy. <i>Journal of Chemical Physics</i> , 2019, 150, 194703.	1.2	4
3600	Synergistic Effect of i-C ₃ F ₇ CN/CO ₂ and i-C ₃ F ₇ CN/N ₂ Mixtures. <i>IEEE Access</i> , 2019, 7, 50159-50167.	2.6	8
3601	Predicting the Toxicity of Ionic Liquids toward Acetylcholinesterase Enzymes Using Novel QSAR Models. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2186.	1.8	32
3602	Photoinduced charge transfer rate of Cy3/C60 blend material. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 220, 117145.	2.0	5
3603	Modification of a Carbon Nanobelt with Actinides Th ^{IV} Am: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4900-4907.	1.1	3
3604	Controllable and large-scale supramolecular vesicle aggregation: orthogonal light-responsive host-guest and metal-ligand interactions. <i>Journal of Materials Chemistry B</i> , 2019, 7, 4177-4183.	2.9	4
3605	Role of Complexation between Monomethylamine and Triplet Nitromethane Molecules in the Hydrogen Transfer Reaction. <i>High Energy Chemistry</i> , 2019, 53, 103-107.	0.2	3
3606	Hydrogen Bond Induced Green Solvent Processed High Performance Ternary Organic Solar Cells with Good Tolerance on Film Thickness and Blend Ratios. <i>Advanced Functional Materials</i> , 2019, 29, 1902078.	7.8	60
3607	Theoretical insights into the effect of heterocycles of the molecular framework on photochromic magnetic properties of diarylethene compounds. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3973.	0.9	7
3608	Effect of electron-withdrawing groups on photovoltaic performance of thiophene-vinylthiophene derivative and benzochalcogenadiazole based copolymers: A computational study. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25982.	1.0	8
3609	Investigation of interactional behavior and relative photo-physical properties in a group of bioactive compounds. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 381, 111873.	2.0	5
3610	Tetrel Bonding along the Pathways of Transsilylation and Alkylation of <i>N</i> -Trimethylsilyl- <i>N</i> -methylacetamide with Bifunctional (Chloromethyl)fluorosilanes. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5178-5189.	1.1	3

#	ARTICLE	IF	CITATIONS
3611	Stepwise oxidations of a nickel(Ni^{II})–iron(Fe^{III}) heterobimetallic porphyrin dimer: structure, spectroscopic and theoretical investigation. <i>Dalton Transactions</i> , 2019, 48, 10089-10103.	1.6	8
3612	Revisiting ultra-weak metal-metal bonding. <i>Chemical Physics Letters</i> , 2019, 730, 411-415.	1.2	12
3613	An experimental and theoretical investigation of the physicochemical properties on choline chloride LiCl Lactic acid based natural deep eutectic solvent (NADES). <i>Journal of Molecular Liquids</i> , 2019, 290, 110916.	2.3	57
3614	Conformational, spectroscopic (FT-IR, FT-Raman, and UV-Vis), and molecular docking studies of N-(2-hydroxyethyl) succinimide. <i>Journal of Molecular Structure</i> , 2019, 1195, 451-461.	1.8	17
3615	The investigation of fluorine substitution in difluoroanilines with focus on 2,6-difluoroaniline by spectroscopic methods, density functional theory approach, and molecular docking. <i>Journal of Molecular Structure</i> , 2019, 1196, 201-214.	1.8	2
3616	Reunderstanding the photoinduced charge transfer process of ammonium polyoxomolybdate. <i>Dalton Transactions</i> , 2019, 48, 10683-10688.	1.6	18
3617	A new type of halogen bond involving multivalent astatine: an <i>ab initio</i> study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15310-15318.	1.3	39
3618	Dysprosium complexes bearing unsupported Dy^{III} – Ge^{IV} / Sn^{IV} metal–metal bonds as single-ion magnets. <i>Chemical Communications</i> , 2019, 55, 8250-8253.	2.2	20
3619	Synthesis of high-molecular weight isosorbide-based polycarbonates through efficient activation of endo-hydroxyl groups by an ionic liquid. <i>Green Chemistry</i> , 2019, 21, 3891-3901.	4.6	33
3620	Nature and origin of \hat{I}^3 -gauche effect in sulfoxides: A density functional theory and information-theoretic approach study. <i>Chemical Physics Letters</i> , 2019, 730, 451-459.	1.2	12
3621	Recyclable and superior selective CO_2 adsorption of $\text{C}_{40}\text{B}_{32}$ and $\text{Ca}@\text{C}_{40}\text{B}_{32}$: a new category of perfect cubic heteroborospherenes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15541-15550.	1.3	14
3622	Redox-triggered switch based on platinum(Pt^{II}) acetylacetonate complexes bearing an isomeric donor–acceptor conjugation ligand shows a high second-order nonlinear optical response. <i>New Journal of Chemistry</i> , 2019, 43, 11263-11274.	1.4	12
3623	A Comparison of NH_2^+ and CH_5^+ Ions and Deuterated Variants of $\text{NH}_2\text{D}_2^+(5\hat{\alpha}^x)$: Real or Artefactual Rotation?. <i>Journal of Structural Chemistry</i> , 2019, 60, 713-726.	0.3	0
3624	Halogen bonding in differently charged complexes: basic profile, essential interaction terms and intrinsic f -hole. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15106-15119.	1.3	37
3625	$[\text{E}(\hat{1}/4\text{-NBbp})]_2$ (E = P, As) d^0 group 15 biradicals synthesized from acyclic precursors. <i>Dalton Transactions</i> , 2019, 48, 11103-11111.	1.6	12
3626	Chirality-activated mechanoluminescence from aggregation-induced emission enantiomers with high contrast mechanochromism and force-induced delayed fluorescence. <i>Materials Chemistry Frontiers</i> , 2019, 3, 1800-1806.	3.2	81
3627	Quad-rotor-shaped non-fullerene electron acceptor materials with potential to enhance the photoelectric performance of organic solar cells. <i>Journal of Materials Chemistry A</i> , 2019, 7, 18150-18157.	5.2	23
3628	How does the pH influences the Ru^{II} –NO coordination compounds?. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25999.	1.0	2

#	ARTICLE	IF	CITATIONS
3629	Theoretical study and experimental validation on the optical emission processes in "free" and "locked" pyrazine derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 223, 117296.	2.0	3
3630	Gain-of-Function SHP2 E76Q Mutant Rescuing Autoinhibition Mechanism Associated with Juvenile Myelomonocytic Leukemia. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3229-3239.	2.5	37
3631	Face-Sharing Homo- and Hetero-Bitetrahedral Superatomic Molecules $M_1M_2@Li_{20}$ ($M_1/M_2 = Ti$ and W). <i>Journal of Physical Chemistry A</i> , 2019, 123, 5517-5524.	1.1	6
3632	A fast and specific fluorescent probe for thioredoxin reductase that works via disulphide bond cleavage. <i>Nature Communications</i> , 2019, 10, 2745.	5.8	70
3633	Revelation solvent effects: excited state hydrogen bond and proton transfer of 2-(benzo[<i>d</i>]thiazol-2-yl)-3-methoxynaphthalen-1-ol. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2780-2787.	2.3	19
3634	Study on Structural Evolution, Thermochemistry and Electron Affinity of Neutral, Mono- and Di-Anionic Zirconium-Doped Silicon Clusters $ZrSi_nO_{-2}$ ($n = 6-16$). <i>International Journal of Molecular Sciences</i> , 2019, 20, 2933.	1.8	9
3635	Physical adsorption of hydrogen molecules on single-walled carbon nanotubes and carbon-boron-nitrogen heteronanotubes: A comparative DFT study. <i>Vacuum</i> , 2019, 167, 280-286.	1.6	40
3636	Tri-spiral Donor for High Efficiency and Versatile Blue Thermally Activated Delayed Fluorescence Materials. <i>Angewandte Chemie</i> , 2019, 131, 11423-11427.	1.6	28
3637	New insight into the mechanism of $LiPO_2F_2$ on the interface of high-voltage cathode $LiNi_{0.5}Mn_{1.5}O_4$ with truncated octahedral structure. <i>Applied Surface Science</i> , 2019, 491, 595-606.	3.1	36
3638	Two-photon-excited ultralong organic room temperature phosphorescence by dual-channel triplet harvesting. <i>Chemical Science</i> , 2019, 10, 7352-7357.	3.7	98
3639	Four-center Nodes: Supramolecular Synthons Based on Cyclic Halogen Bonding. <i>Chemistry - A European Journal</i> , 2019, 25, 13671-13675.	1.7	28
3640	A joint experimental and theoretical Raman study on the interactions of pyridine adsorbed on chemically pure Ag_{18} clusters. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 1477-1484.	1.2	3
3641	Degradation kinetics, byproducts formation and estimated toxicity of metronidazole (MNZ) during chlor(am)ination. <i>Chemosphere</i> , 2019, 235, 21-31.	4.2	18
3642	Synthesis and Characterization of Heterobimetallic Carbonyl Clusters with Direct Au-Fe and Au-Au Interactions Supported by <i>N</i> -heterocyclic Carbene and Phosphine Ligands. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 3084-3093.	1.0	16
3643	Metal cation saturation on montmorillonites facilitates the adsorption of DNA via cation bridging. <i>Chemosphere</i> , 2019, 235, 670-678.	4.2	43
3644	Theoretical investigation on the interaction of benzazaborole derivatives with iodide ion: Structural, binding and fluorescence properties analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 92, 32-43.	1.3	3
3645	A coumarin-based near-infrared fluorescent probe with a large stokes shift for the sequential recognition of Ni^{2+} and CN^- : Performance research and quantum calculation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 382, 111943.	2.0	29
3646	Spectroscopic (FT-IR, FT-Raman, NMR and UV-Vis), ELF, LOL, NBO, and Fukui function investigations on (5-bromo-benzofuran-3-yl)-acetic acid hydrazide (5BBAH): Experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2019, 1196, 280-290.	1.8	51

#	ARTICLE	IF	CITATIONS
3647	The structure and hydrogen-bond behaviours of binary systems containing ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate and methanol/ethanol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 223, 117312.	2.0	16
3648	Phthalocyanine and Metal Phthalocyanines Adsorbed on Graphene: A Density Functional Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16614-16620.	1.5	33
3649	A 3,2-Hydroxypyridinone-based Decorporation Agent that Removes Uranium from Bones In Vivo. <i>Nature Communications</i> , 2019, 10, 2570.	5.8	107
3650	Coordination mode engineering in stacked-nanosheet metal-organic frameworks to enhance catalytic reactivity and structural robustness. <i>Nature Communications</i> , 2019, 10, 2779.	5.8	89
3651	Probing effects of molecular conformation on the electronic and charge transport properties in two- and three-dimensional small molecule hole-transporting materials: a theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15206-15214.	1.3	24
3652	Three new carbazole derivatives with high thermal stability as host for efficient green phosphorescent organic-light emitting diodes. <i>Dyes and Pigments</i> , 2019, 171, 107670.	2.0	9
3653	The mechanism of the excited-state proton transfer of Salicylaldehyde azine and 2,2'-[1,4-Phenylenebis{(E)-nitrilomethylidyne}] bisphenol: Via single or double proton transfer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 223, 117321.	2.0	8
3654	Separation of GaCl_3 from AlCl_3 by Solid-Liquid Extraction and Stripping Using Anhydrous <i>n</i> -Dodecane and NaCl. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 12459-12464.	1.8	3
3655	Quantum Mechanical Description of Electrostatics Provides a Unified Picture of Catalytic Action Across Methyltransferases. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3779-3787.	2.1	21
3656	A DFT Analysis on Antioxidant and Antiradical Activities from Anthraquinones Isolated from the Cameroonian Flora. <i>Journal of Chemistry</i> , 2019, 2019, 1-13.	0.9	5
3657	Experimental and theoretical study of corrosion inhibition performance of N-phenylthiourea for mild steel in hydrochloric acid and sodium chloride solution. <i>Journal of Molecular Modeling</i> , 2019, 25, 204.	0.8	10
3658	Theoretical Insight into the Mechanism and Origin of Divergent Reactivity in the Synthesis of Benzo-Heterocycles from <i>o</i> -Alkynylbenzamides Catalyzed by Gold and Platinum Complexes. <i>Journal of Organic Chemistry</i> , 2019, 84, 9705-9713.	1.7	17
3659	Strategy for tuning the up-conversion intersystem crossing rates in a series of organic light-emitting diodes emitters relevant for thermally activated delayed fluorescence. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 221, 117214.	2.0	4
3660	A microwave spectroscopic and <i>ab initio</i> study of keto-enol tautomerism and isomerism in the cyclohexanone-water complex. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12872-12880.	1.3	10
3661	Syntheses, Structures, and Bonding of $\text{NgF}_2 \cdot \text{CrOF}_4$, $\text{NgF}_2 \cdot 2\text{CrOF}_4$ (Ng=Kr, Xe), and $(\text{CrOF}_4)_z$. <i>Chemistry - A European Journal</i> , 2019, 25, 12105-12119.	1.7	18
3662	Is the pericyclic transition structure of aza-Diels-Alder reaction aromatic?. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 91, 119-129.	1.3	4
3663	Spectroscopic, chemical reactivity, molecular docking investigation and QSAR analyses of (2E)-1-(3-bromo-2-thienyl)-3-(2,5-dimethoxyphenyl)prop-2-en-1-one. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 222, 117190.	2.0	18
3664	Theoretical Spectroscopic Study on the Au, Ag, Au/Ag, and Ag/Au Nanosurfaces and Their Cytosine/Nanosurface Complexes: UV, IR, and Charge-Transfer SERS Spectra. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16345-16358.	1.5	5

#	ARTICLE	IF	CITATIONS
3665	Over 16% efficiency organic photovoltaic cells enabled by a chlorinated acceptor with increased open-circuit voltages. <i>Nature Communications</i> , 2019, 10, 2515.	5.8	1,431
3666	On the nature of organic electron density transfer complexes within molecular electron density theory. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 6478-6488.	1.5	12
3667	Dimeric conformation sensitive electronic excited states of tetracene congeners and their unconventional non-fluorescent behaviour. <i>Journal of Chemical Sciences</i> , 2019, 131, 1.	0.7	3
3668	RNA aptasensor based on gold nanoparticles for selective detection of neomycin B, molecular approach. <i>Journal of the Iranian Chemical Society</i> , 2019, 16, 2389-2400.	1.2	11
3669	Shorter interval and multiple flooding-drying cycling enhanced the mineralization of 14C-DDT in a paddy soil. <i>Science of the Total Environment</i> , 2019, 676, 420-428.	3.9	6
3670	Synthesis, characterization, photoluminescence, anti-tumor activity, DFT calculations and molecular docking with proteins of zinc(ⁱⁱ) halogen substituted terpyridine compounds. <i>Dalton Transactions</i> , 2019, 48, 10488-10504.	1.6	40
3671	The first water-soluble polynuclear metallamacrocyclic Sr(ⁱⁱ)-Cu(ⁱⁱ) complex based on simple glycinehydroximate ligands. <i>Dalton Transactions</i> , 2019, 48, 10479-10487.	1.6	8
3672	Bis-pyrazolyl-s-triazine Ni(II) pincer complexes as selective gram positive antibacterial agents; synthesis, structural and antimicrobial studies. <i>Journal of Molecular Structure</i> , 2019, 1195, 315-322.	1.8	22
3673	A Search for X-ray Crystallographic Evidence of π - π^* Interactions in a Series of Substituted 2-(Dimethylamino)biphenyl-2-carboxaldehydes. <i>Crystal Growth and Design</i> , 2019, 19, 3895-3904.	1.4	9
3674	Unveiling the electronic structures and ligation effect of the superatom-like polymeric zirconium oxide clusters: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14865-14872.	1.3	17
3675	Theoretical study on the mechanism and chemoselectivity in gold(ⁱ)-catalyzed cycloisomerization of β,β -disubstituted <i>ortho</i> -(alkynyl)styrenes. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2701-2712.	2.3	13
3676	Mechanistic investigation-inspired activation mode of DBU and the function of the β -diazo group in the reaction of the β -amino ketone compound and EDA: [DBU-H] ⁺ -DMF-H ₂ O and β -diazo as strong N-terminal nucleophiles. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2678-2686.	2.3	2
3677	Crystallographic and first-principles density functional theory study on the structure, noncovalent interactions, and chemical reactivity of 1,5-benzodiazepin-2-ones derivatives. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e26000.	1.0	30
3678	Molecular design of D- π -D-typed hole-transporting materials for perovskite solar cells based on the π -conjugated cores. <i>Synthetic Metals</i> , 2019, 254, 34-41.	2.1	18
3679	Fused Aromatics To Restore Molecular Packing of Aged Bituminous Materials. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 11939-11953.	1.8	31
3680	Chiral Spiro Phosphoric Acid-Catalyzed Friedel-Crafts Conjugate Addition/Enantioselective Protonation Reactions. <i>ACS Catalysis</i> , 2019, 9, 6522-6529.	5.5	58
3681	Design of Energetic Materials Based on Asymmetric Oxadiazole. <i>ChemistryOpen</i> , 2019, 8, 692-700.	0.9	6
3682	Anion-binding properties of π -electron deficient cavity in tetraoxacalix[2]arene[2]triazine by a computational study. <i>Journal of Molecular Liquids</i> , 2019, 288, 111007.	2.3	2

#	ARTICLE	IF	CITATIONS
3683	From BTO ²⁺ to HBTO ⁺ insensitive energetic salt: a route to boost energy. <i>CrystEngComm</i> , 2019, 21, 3873-3880.	1.3	3
3684	A nonlinear optical switch induced by an external electric field: inorganic alkaline-earth alkalide. <i>RSC Advances</i> , 2019, 9, 16718-16728.	1.7	27
3685	Nano Molecular Motor of Azo Antibiotics on Edge-Carboxylated Graphene: A UV and Visible-Switchable Sensors. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 324-332.	0.1	1
3686	Donor-acceptor coordination interactions in 1,3-bis(NHC)triazenyl Cations: An electronic structure analysis. <i>Journal of Computational Chemistry</i> , 2019, 40, 2207-2215.	1.5	5
3687	The dependence of oxygen sensitivity on the molecular structures of Ir(III) complexes and their application for photostable and reversible luminescent oxygen sensing. <i>RSC Advances</i> , 2019, 9, 15370-15380.	1.7	10
3688	PIDAZTA: Structurally Constrained Chelators for the Efficient Formation of Stable Gallium-68 Complexes at Physiological pH. <i>Chemistry - A European Journal</i> , 2019, 25, 10698-10709.	1.7	11
3689	A theoretical research on intersystem crossing, radiative and nonradiative rates of cyclometalated platinum(II) complexes. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	4
3690	Heteroatom substitution effect on electronic structures, photophysical properties, and excited-state intramolecular proton transfer processes of 3-hydroxyflavone and its analogues: A TD-DFT study. <i>Journal of Molecular Structure</i> , 2019, 1195, 280-292.	1.8	19
3691	The physical mechanism of electron excitation spectrum for photo redox device controlled by gate voltage, a first-principles study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 223, 117225.	2.0	0
3692	Substitution of Nitrogen-Rich Linkers with Insensitive Linkers in Azide-Based Energetic Coordination Polymers toward Safe Energetic Materials. <i>Crystal Growth and Design</i> , 2019, 19, 3934-3944.	1.4	48
3693	Bond orders of the diatomic molecules. <i>RSC Advances</i> , 2019, 9, 17072-17092.	1.7	18
3694	Epitaxial Graphene Sensors Combined with 3D-Printed Microfluidic Chip for Heavy Metals Detection. <i>Sensors</i> , 2019, 19, 2393.	2.1	24
3695	Spectroscopic, quantum computational and molecular docking studies on 1-phenylcyclopentane carboxylic acid. <i>Computational Biology and Chemistry</i> , 2019, 82, 44-56.	1.1	36
3696	Exploring the electronic structure and stability of HgF ₆ : Exact 2-Component (X2C) relativistic DFT and NEVPT2 studies. <i>Computational and Theoretical Chemistry</i> , 2019, 1160, 14-18.	1.1	8
3697	Implementation of the Molecular Electrostatic Potential over Graphics Processing Units. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3120-3127.	2.5	16
3698	Spectroscopic speciation of aqueous Am(III)-oxalate complexes. <i>Dalton Transactions</i> , 2019, 48, 10023-10032.	1.6	13
3699	Ab initio investigation of cationic water cluster (H ₂ O) ₊₁₃ via particle swarm optimization algorithm. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	4
3700	Theoretical study on alkaloid encapsulating via monohydroxy-cucurbit[n]uril (n=8,10)/graphene oxide composite. <i>Journal of Molecular Liquids</i> , 2019, 288, 111085.	2.3	5

#	ARTICLE	IF	CITATIONS
3701	A computational study of the effects of axial halogen substitutions of boron subphthalocyanines on their electronic spectra in solution and in the solid state. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 222, 117180.	2.0	9
3702	Computational evaluation of the reactivity and pharmaceutical potential of an organic amine: A DFT, molecular dynamics simulations and molecular docking approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 222, 117188.	2.0	80
3703	Carboxylation as an effective approach to improve the adsorption performance of graphene materials for Cu ²⁺ removal. <i>Science of the Total Environment</i> , 2019, 682, 591-600.	3.9	28
3704	•••Radical Formation by Pyrrolic H Abstraction of Phthalocyanine Molecules on Molybdenum Disulfide. <i>ACS Nano</i> , 2019, 13, 7031-7035.	7.3	9
3705	Using Pauli energy to appraise the quality of approximate semilocal non-interacting kinetic energy density functionals. <i>Journal of Chemical Physics</i> , 2019, 150, 204106.	1.2	26
3706	Structural Mechanism of Barriers to Interspecies Seeding Transmissibility of Full-length Prion Protein Amyloid. <i>ChemBioChem</i> , 2019, 20, 2757-2766.	1.3	3
3707	Molecular Encapsulation of Trimeric Chromium Carboxylate Clusters in Metal-Organic Frameworks and Propylene Sorption. <i>Chemistry - A European Journal</i> , 2019, 25, 12889-12894.	1.7	8
3708	Theoretical insights on the comparison of champion dyes SM315 and C275 used for DSSCs reaching over 12% efficiency and the further optimization of C275. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 222, 117217.	2.0	5
3709	Complete Reaction Mechanisms of Mercury Binding on Petroleum Coke and Brominated Petroleum Coke. <i>Energy & Fuels</i> , 2019, 33, 5488-5497.	2.5	5
3710	B10M2 (M = Rh, Ir): finally a stable boron-based icosahedral cluster. <i>Chemical Communications</i> , 2019, 55, 7490-7493.	2.2	22
3711	Mechanistic study of the role of hydrogen bond donors in the two-component organocatalysis of the ring-opening reaction of epoxides. <i>Molecular Catalysis</i> , 2019, 474, 110425.	1.0	8
3712	Origin of High Selectivity of Dimethyl Ether Carbonylation in the 8-Membered Ring Channel of Mordenite Zeolite. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15503-15512.	1.5	28
3713	Poly(ionic liquid)s as a distinct receptor material to create a highly-integrated sensing platform for efficiently identifying numerous saccharides. <i>Chemical Science</i> , 2019, 10, 6617-6623.	3.7	29
3714	Theoretical predictions of the nitrogen heterocyclic compounds with metal and noble gas (metal-Cu, N ₂) Tj FJQq1 1 0.784314	1.0	2
3715	Effect of heterocyclic spacer on property of hole-transporting materials with silafluorene core for perovskite solar cells. <i>Computational and Theoretical Chemistry</i> , 2019, 1161, 10-17.	1.1	18
3716	Computational screening of carbon monoxide (CO) adsorption over neutral and charged Al ₇ clusters. <i>Heliyon</i> , 2019, 5, e01762.	1.4	3
3717	Interaction of trivalent arsenic on different topologies of Fe-doped graphene nanosheets at water environments: A computational study. <i>Journal of Molecular Liquids</i> , 2019, 289, 111137.	2.3	16
3718	Polynuclear Glycinehydroximate Cu(II)-Gd(III) Metallamacrocyclic Complexes: Halochromic Properties. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2019, 45, 356-360.	0.3	5

#	ARTICLE	IF	CITATIONS
3719	Modification of NFA-Conjugated Bridges with Symmetric Structures for High-Efficiency Non-Fullerene PSCs. <i>Polymers</i> , 2019, 11, 958.	2.0	16
3720	Fluorenone-based thermally activated delayed fluorescence materials for orange-red emission. <i>Organic Electronics</i> , 2019, 73, 240-246.	1.4	13
3721	Calcium-Ion Batteries: Identifying Ideal Electrolytes for Next-Generation Energy Storage Using Computational Analysis. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15885-15896.	1.5	29
3722	Tri-spiral Donor for High Efficiency and Versatile Blue Thermally Activated Delayed Fluorescence Materials. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 11301-11305.	7.2	198
3723	Theory and practice of modeling van der Waals interactions in electronic-structure calculations. <i>Chemical Society Reviews</i> , 2019, 48, 4118-4154.	18.7	114
3724	Stability, Electronic, and Structural Features of the Conformers of 2-Methyl-1,3,2-Diheterophosphinane 2-Oxide (Heteroatom = O, S, Se): DFT and NBO Investigations. <i>Journal of Structural Chemistry</i> , 2019, 60, 746-754.	0.3	5
3725	The interface effect between ZIF crystal surface and C60: Strong charge-transfer (CT) vs weak CT state. <i>Chemical Physics Letters</i> , 2019, 730, 266-270.	1.2	1
3726	Single crystal structure, hydrogen bonding interaction, charge transfer and thermal properties of a new guanidine derivative crystal: Phosphate bis-guanidinoacetate. <i>Journal of Molecular Structure</i> , 2019, 1195, 883-890.	1.8	1
3727	Bicolor switching mechanism of multifunctional light-emitting molecular material in solid phase. <i>Organic Electronics</i> , 2019, 71, 212-219.	1.4	23
3728	Natural Bond Orbital (NBO) and Quantum Theory of Atoms in Molecules (QTAIM) Analyses of Iron-Substituted Borirene and Boryl Isomers. <i>Russian Journal of Inorganic Chemistry</i> , 2019, 64, 472-477.	0.3	2
3729	Thermal and Sensitiveness Determination of Cubanes: Towards Cubane-Based Fuels for Infrared Countermeasures. <i>Chemistry - A European Journal</i> , 2019, 25, 8344-8352.	1.7	9
3730	Blue wine, a color obtained with synthetic blue dye addition: two case studies. <i>European Food Research and Technology</i> , 2019, 245, 1777-1782.	1.6	4
3731	Target prediction and antioxidant analysis on isoflavones of demethyltaxasin: a DFT study. <i>Journal of Molecular Modeling</i> , 2019, 25, 169.	0.8	6
3732	DFT studies of the electron density distribution and donor-acceptor interactions in water-soluble aminohydroximate metallamacrocyclic Cu(I) and Y(III) complexes. <i>Russian Chemical Bulletin</i> , 2019, 68, 743-750.	0.4	10
3733	Photoelectron imaging spectroscopic study and chemical-bonding analysis of AgOH and AgSH anions. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2019, 233, 52-56.	1.1	1
3734	Effects of intramolecular and intermolecular interactions on excited state properties of two isomeric Cu complexes with AIE and TADF mechanisms in solid phase: A QM/MM study. <i>Organic Electronics</i> , 2019, 71, 113-122.	1.4	40
3735	Adsorption behavior of mercuric oxide clusters on activated carbon and the effect of SO ₂ on this adsorption: a theoretical investigation. <i>Journal of Molecular Modeling</i> , 2019, 25, 142.	0.8	18
3736	Interactions of (MY) ₆ (M = Zn, Cd; Y = O, S, Se) quantum dots with N-bases. <i>Structural Chemistry</i> , 2019, 30, 1003-1014.	1.0	2

#	ARTICLE	IF	CITATIONS
3737	Mechanism of the charge separation improvement in carbon-nanodot sensitized g-C ₃ N ₄ . <i>Applied Surface Science</i> , 2019, 487, 151-158.	3.1	27
3738	Computational quest of adsorbents based on doped graphene nanosheets for phosgene uptake, and analysis of the co-adsorption phenomena. <i>Synthetic Metals</i> , 2019, 252, 142-150.	2.1	24
3739	Nature of the Lowest Singlet and Triplet Excited States of Organic Thermally Activated Delayed Fluorescence Emitters: A Self-Consistent Quantum Mechanics/Embedded Charge Study. <i>Chemistry of Materials</i> , 2019, 31, 6665-6671.	3.2	46
3740	â€œCâ€“Hâ€“ Interactionâ€•regulates the stereoselectivity in olefin polymerization. <i>Chemical Communications</i> , 2019, 55, 6689-6692.	2.2	15
3741	Theoretical study on lithiation mechanism of benzoquinone-based macrocyclic compounds as cathode for lithium-ion batteries. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11004-11010.	1.3	7
3742	Synthesis, structures and luminescence of multinuclear silver(<i>scp</i>) pyrazolate adducts with 1,10-phenanthroline derivatives. <i>Dalton Transactions</i> , 2019, 48, 8410-8417.	1.6	29
3743	Synthesis, Molecular and Supramolecular Structures of New Cd(II) Pincer-Type Complexes with s-TriazineCore Ligand. <i>Crystals</i> , 2019, 9, 226.	1.0	19
3744	Searching for Diradicaloid Chromophores with Efficient Singlet Fission: Cyanoâ€•Group Substitution of Difurophyrene Systems. <i>ChemPhotoChem</i> , 2019, 3, 652-659.	1.5	4
3745	Furthering the reaction mechanism of cationic vanadium clusters towards oxygen. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11234-11241.	1.3	18
3746	Emissions and the application of a series of twisted fluorophores with intramolecular weak hydrogen bonds. <i>RSC Advances</i> , 2019, 9, 13214-13219.	1.7	1
3747	Modulation of the conductance in platinum(<i>scp</i>) bis(acetylide) molecules through â€œgatingâ€• metal ions. <i>Journal of Materials Chemistry C</i> , 2019, 7, 7259-7266.	2.7	12
3748	Interaction in Li@Fullerenes and Li+@Fullerenes: First Principle Insights to Li-Based Endohedral Fullerenes. <i>Nanomaterials</i> , 2019, 9, 630.	1.9	23
3749	Probing non-covalent interactions of phosphine and arsine derivatives: an energy decomposition analysis using localized molecular orbitals. <i>Structural Chemistry</i> , 2019, 30, 2191-2204.	1.0	0
3750	Th doped carbon clusters ThC _n (nâ€“=â€“1â€“7): Stability and bonding natures. <i>Computational and Theoretical Chemistry</i> , 2019, 1159, 7-11.	1.1	4
3751	Dimethylamine substituted bisbenzocoumarin amides with solvatochromic and mechanochromic properties. <i>Tetrahedron</i> , 2019, 75, 3504-3509.	1.0	8
3752	Visualization of Photoinduced Charge Transfer and Electronâ€“Hole Coherence in Two-Photon Absorption. <i>Journal of Physical Chemistry C</i> , 2019, 123, 14132-14143.	1.5	81
3753	Dynamical fluxionality, multiplicity of structural forms, and electronic properties of the B ₃ Si ₁₁ cluster: anion photoelectron spectroscopy and theoretical calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12241-12249.	1.3	6
3754	Experimental, DFT dimeric modeling and AIM study of H-bond-mediated composite vibrational structure of Chelidonic acid. <i>Heliyon</i> , 2019, 5, e01586.	1.4	15

#	ARTICLE	IF	CITATIONS
3755	A DFT Study of the Modulation of the Antiaromatic and Open-Shell Character of Dibenzopentalene by Employing Three Strategies: Additional Benzoannulation, BN/CC Isosterism, and Substitution. <i>Chemistry - A European Journal</i> , 2019, 25, 9747-9757.	1.7	19
3756	Design, synthesis and fungicidal activity evaluation of novel pyrimidinamine derivatives containing phenyl-thiazole/oxazole moiety. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 3218-3228.	1.4	36
3757	Aryl modification of diketopyrrolopyrrole-based quaternary ammonium salts and their applications in copper electrodeposition. <i>Dyes and Pigments</i> , 2019, 170, 107559.	2.0	21
3758	On the spectral profile change in the Q band absorption spectra of metalloporphyrins (Mg, Zn, and) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.2	8
3759	Revisiting the structural and electronic properties of neutral, mono- and dianionic titanium-doped silicon clusters $TiSi_n O_n / 2n^+ (n = 6-16)$. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25978.	1.0	5
3760	Microsolvation of lithium-phosphorus double helix: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	2
3761	A DFT approach for theoretical and experimental study of structure, electronic, Hirshfeld surface and spectroscopic properties of 12-(4-bromophenyl)-2-(prop-2-ynoxy)-9,10-dihydro-8H-benzo[a]xanthen-11(12H)-on single crystal. <i>Chemical Physics</i> , 2019, 524, 1-13.	0.9	23
3762	Quick-Silver from a Systematic Study of Highly Luminescent, Two-Coordinate, d^{10} Coinage Metal Complexes. <i>Journal of the American Chemical Society</i> , 2019, 141, 8616-8626.	6.6	187
3763	Using molecular dynamics simulation to explore the binding of the three potent anticancer drugs sorafenib, streptozotocin, and sunitinib to functionalized carbon nanotubes. <i>Journal of Molecular Modeling</i> , 2019, 25, 159.	0.8	24
3764	Clean and Efficient Transformation of CO_2 to Isocyanic Acid: The Important Role of Triatomic Cation $ScNH^+$. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5762-5767.	1.1	7
3765	Anion Complexes of Halides with <i>p</i> -Benzoquinones: Structures, Thermodynamics, and Criteria of Charge Transfer to Electron Transfer Transition. <i>Journal of the American Chemical Society</i> , 2019, 141, 9338-9348.	6.6	52
3766	Adiabatic deprotonation as an important competing pathway to ESIPT in photoacidic 2-phenylphenols. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12231-12240.	1.3	7
3767	Theoretical investigations of the reactivity of neutral molecules that feature an M^m ($M = B, Al, Ga, In$) Tj ETQq0 0,0,rgBT /Overlock 10	1.4	10
3768	Oxygen-Bridged $Ga_2(Et)_3(OTeF_5)_3$ and the Weakly Coordinating Anions $[Ga(Et)(OTeF_5)_3]^-$ and $[Ga(OTeF_5)_4]^-$. <i>Chemistry - A European Journal</i> , 2019, 25, 10441-10449.	1.7	8
3769	π - π^* Interaction Promoted Charge Carrier Transfer between Helical SWNTs and a 4-(1-Pyrenyl)phenyl Group. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13976-13982.	1.5	3
3770	Metal-coordination driven intramolecular twisting: a turn-on fluorescent-redox probe for Hg^{2+} ions through the interaction of ferrocene nonbonding orbitals and dibenzylidenehydrazine. <i>Dalton Transactions</i> , 2019, 48, 8209-8220.	1.6	10
3771	Selective Adsorption-Based Separation of Flue Gas and Natural Gas in Zirconium Metal-Organic Frameworks Nanocrystals. <i>Molecules</i> , 2019, 24, 1822.	1.7	20
3772	A Reliable Database for Ionic Volume and Surface: Its Application To Predict Molar Volume and Density of Ionic Liquid. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 10073-10083.	1.8	8

#	ARTICLE	IF	CITATIONS
3773	Local Excitation/Charge-Transfer Hybridization Simultaneously Promotes Charge Generation and Reduces Nonradiative Voltage Loss in Nonfullerene Organic Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2911-2918.	2.1	73
3774	A non-conjugated polyethylenimine copolymer-based unorthodox nanoprobe for bioimaging and related mechanism exploration. <i>Biomaterials Science</i> , 2019, 7, 3016-3024.	2.6	20
3775	A thorough understanding of the nonlinear optical properties of BODIPY/carborane/diketopyrrolopyrrole hybrid chromophores: module contribution, linear combination, one-/two-dimensional difference and carborane's arrangement. <i>Journal of Materials Chemistry C</i> , 2019, 7, 7531-7547.	2.7	36
3776	Experimental and quantum-chemical study of differential absorbance spectra of environmentally relevant species: A study of quercetin deprotonation and its interactions with copper (II) ions. <i>Science of the Total Environment</i> , 2019, 679, 229-236.	3.9	12
3777	Following Bimolecular Excited-State Proton Transfer between Hydroxycoumarin and Imidazole Derivatives. <i>Journal of Physical Chemistry B</i> , 2019, 123, 4745-4756.	1.2	11
3778	Tunable optoelectronic properties of D-A- π -A type dyes by altering auxiliary acceptor position and atomic electronegativity. <i>Journal of Molecular Liquids</i> , 2019, 287, 110883.	2.3	17
3779	Preparation and crystal structure of the boranehydrazine complex [RuCl(η^1 -NH ₂ NH ₂ BPh ₃){P(OEt) ₃] ₄ BPh ₄ . <i>Polyhedron</i> , 2019, 169, 78-83.	1.0	0
3780	Through-space Spin Coupling in a Silver(II) Porphyrin Dimer upon Stepwise Oxidations: Ag II \rightarrow Ag II ₇ , Ag II ₇ \rightarrow Ag III, and Ag III \rightarrow Ag III Metallophilic Interactions. <i>Chemistry - A European Journal</i> , 2019, 25, 10098-10110.	1.7	10
3781	A Computational Investigation of Unconventional Lone Pair Hole Interactions of Group V \leftarrow VIII Elements. <i>ChemistrySelect</i> , 2019, 4, 5489-5495.	0.7	17
3782	The fate of rhenium in polyaminocarboxy solution: Hourglass crystal and its speciation study. <i>Journal of Hazardous Materials</i> , 2019, 375, 78-85.	6.5	6
3783	Narrowing Segments of Helical Carbon Nanotubes with Curved Aromatic Panels. <i>Angewandte Chemie</i> , 2019, 131, 7463-7467.	1.6	16
3784	Theoretical insight into the photodeactivation pathway of the tetradentate Pt (II) complex with different inductive substituents. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4879.	1.7	7
3785	Pentapnictogen heterocyclic monoanions: Structure, stability, and aromaticity. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25961.	1.0	3
3786	Amorphous agomelatine stabilization in the presence of pyrogenic silica: Molecular mobility and intermolecular interaction studies. <i>European Journal of Pharmaceutics and Biopharmaceutics</i> , 2019, 139, 291-300.	2.0	7
3787	Atomic-scale insights into zeolite-based catalysis in N ₂ O decomposition. <i>Science of the Total Environment</i> , 2019, 673, 266-271.	3.9	15
3788	Insights into N-Heterocyclic Carbene-Catalyzed Oxidative α -C(sp ³)-H Activation of Aliphatic Aldehydes and Cascade [2 + 2] Cycloaddition with Ketimines. <i>Journal of Organic Chemistry</i> , 2019, 84, 6117-6125.	1.7	42
3789	Confining an Ag ₁₀ Core in an Ag ₁₂ Shell: A Four-Electron Superatom with Enhanced Photoluminescence upon Crystallization. <i>ACS Nano</i> , 2019, 13, 5753-5759.	7.3	70
3790	A novel structure of grid spirofluorene: a new organic semiconductor with low reorganization energy. <i>New Journal of Chemistry</i> , 2019, 43, 7790-7796.	1.4	14

#	ARTICLE	IF	CITATIONS
3791	1-Titanacyclobuta-2,3-diene – an elusive four-membered cyclic allene. <i>Chemical Science</i> , 2019, 10, 5319-5325.	3.7	26
3792	Nonbonding interaction analyses on PVDF/[BMIM][BF ₄] complex system in gas and solution phase. <i>Journal of Molecular Modeling</i> , 2019, 25, 131.	0.8	21
3793	Amoxicillin on polyglutamic acid composite three-dimensional graphene modified electrode: Reaction mechanism of amoxicillin insights by computational simulations. <i>Analytica Chimica Acta</i> , 2019, 1073, 22-29.	2.6	30
3794	The Protein's Role in Substrate Positioning and Reactivity for Biosynthetic Enzyme Complexes: The Case of SyrB2/SyrB1. <i>ACS Catalysis</i> , 2019, 9, 4930-4943.	5.5	28
3795	Understanding the sequence of the electronic flow along the HCN/CNH isomerization within a bonding evolution theory quantum topological framework. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	4
3796	Mechanistic investigation of molecular geometry, intermolecular interactions and spectroscopic properties of pyridinium nitrate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 219, 53-67.	2.0	13
3797	Theoretical arrangement of thermally activated delayed fluorescence as host for fluorescent emitter with blue to red emission. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 219, 44-52.	2.0	2
3798	Insight into Coordination of Uranyl Ions with N,N'-bis(2- ϵ -membered) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 462 Td	1.7	10
3799	Impact of the dielectric constant on the first hyperpolarizabilities and the Singlet-Triplet gap in T- and V-Shaped donor-acceptor-donor molecules. <i>Organic Electronics</i> , 2019, 70, 193-204.	1.4	12
3800	Novel Deep Eutectic Solvents for Highly Efficient and Reversible Absorption of SO ₂ by Preorganization Strategy. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 8347-8357.	3.2	63
3801	Does aromaticity account for an enhanced thermodynamic stability? The case of monosubstituted azaborines and the stereoelectronic chameleonism of the NH ₂ group. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9465-9476.	1.3	5
3802	Comparison of third-order nonlinear optical properties of benzothiazolium salt and neutral benzothiazole derivative: Broadband absorption response and transient dynamic analysis. <i>Dyes and Pigments</i> , 2019, 168, 28-35.	2.0	12
3803	Explaining the interactions between metaldehyde and acidic surface groups of activated carbon under different pH conditions. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 90, 94-103.	1.3	8
3804	An Updated Strategy for Designing Non-Fullerene Acceptors by the Lowest Singlet and Triplet States Excitation: Influence of Periodical Substitution from O, S, and Se to Te for BAE Derivatives. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11397-11405.	1.5	14
3805	Mechanistic Insights into the Ruthenium-Catalyzed [4 + 1] Annulation of Benzamides and Propargyl Alcohols by DFT Studies. <i>Organometallics</i> , 2019, 38, 1877-1886.	1.1	23
3806	Quaternary Ammonium Salt Based NIR Probes for In Vivo Imaging. <i>Advanced Optical Materials</i> , 2019, 7, 1900229.	3.6	66
3807	Insight into the origins of the reactivity and selectivity for the aminocatalytic [2+2] cycloaddition reaction. <i>Tetrahedron</i> , 2019, 75, 3421-3431.	1.0	3
3808	Highly Efficient Orange-Red/Red Excimer Fluorescence from Dimeric π - π Stacking of Perylene and Its Nanoparticle Applications. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13047-13056.	1.5	53

#	ARTICLE	IF	CITATIONS
3809	Design of arginine-based therapeutic deep eutectic solvents as drug solubilization vehicles for active pharmaceutical ingredients. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10621-10634.	1.3	54
3810	Facile color tuning of thermally activated delayed fluorescence by substituted ortho-carbazole-appended triarylboron emitters. <i>Dyes and Pigments</i> , 2019, 168, 273-280.	2.0	8
3811	Synthesis, crystal structure and DFT calculations of a new coumarin-amide binuclear Cu (II) complex. <i>Journal of Molecular Structure</i> , 2019, 1192, 115-121.	1.8	5
3812	Through-Space Conjugation: An Effective Strategy for Stabilizing Intramolecular Charge-Transfer States. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2648-2656.	2.1	26
3813	Influence of monomer deformation on the competition between two types of σ -holes in tetrel bonds. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10336-10346.	1.3	20
3814	Theoretical Study of the Interaction between Graphyne and cis-PtCl ₂ (NH ₃) ₂ Complex. <i>Russian Journal of Inorganic Chemistry</i> , 2019, 64, 369-376.	0.3	1
3815	A de novo strategy for predictive crystal engineering to tune excitonic coupling. <i>Nature Communications</i> , 2019, 10, 2048.	5.8	44
3816	Combined Experimental and Theoretical Study on High Pressure Methane Solubility in Natural Deep Eutectic Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 8097-8111.	1.8	34
3817	Direct Access to IMes ^F and IMes ^{F₂} by Electrophilic Fluorination of Abnormal N-Heterocyclic Carbenes. <i>Organometallics</i> , 2019, 38, 2330-2337.	1.1	19
3818	Dithiothreitol-assisted polysulfide reduction in the interlayer of lithium-sulfur batteries: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16435-16443.	1.3	7
3819	Hydrogen bond-mediated strong adsorbent ³⁺ interactions enable high-efficiency radioiodine capture. <i>Materials Horizons</i> , 2019, 6, 1517-1525.	6.4	43
3820	Removing phenol contaminants from wastewater using graphene nanobuds: DFT and reactive MD simulation investigations. <i>Journal of Molecular Liquids</i> , 2019, 286, 110872.	2.3	11
3821	Account of chemical bonding and enhanced reactivity of vanadium-doped rhodium clusters toward C-H activation: a DFT investigation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9935-9948.	1.3	8
3822	Rigidified and expanded N-annulated perylenes as efficient donors in organic sensitizers for application in solar cells. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10488-10496.	1.3	11
3823	Decorating BODIPY with electron-rich unit THDTAP: An ICT-based fluorometric sensor toward peroxide, acid, and electrochemical stimuli. <i>Dyes and Pigments</i> , 2019, 168, 235-247.	2.0	10
3824	A Theoretical Study on Divalent Heavier Group 14 Complexes as Promising Donor Ligands for Building Uranium-Metal Bonds. <i>Organometallics</i> , 2019, 38, 1963-1972.	1.1	10
3825	Incorporating a tercarbazole donor in a spiro-type host material for efficient RGB phosphorescent organic light-emitting diodes. <i>Journal of Materials Chemistry C</i> , 2019, 7, 6714-6720.	2.7	36
3826	Chlorocuprate(ionic liquid) as an efficient and stable Cu-based catalyst for hydrochlorination of acetylene. <i>Catalysis Science and Technology</i> , 2019, 9, 2868-2878.	2.1	30

#	ARTICLE	IF	CITATIONS
3827	Energetic furazan-triazole hybrid with dinitromethyl and nitramino groups: decreasing sensitivity via the formation of a planar anion. Dalton Transactions, 2019, 48, 7677-7684.	1.6	39
3828	Investigation on two triphenylene based electron transport materials. Science China Chemistry, 2019, 62, 775-783.	4.2	5
3829	Spectroscopic, electrochemical and electrocolorimetric properties of novel 2-(2-pyridyl)-1H-benzimidazole appended bay-substituted perylene diimide triads. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 379, 54-62.	2.0	6
3830	Donor Halogenation Effects on Electronic Structures and Electron Process Rates of Donor/C ₆₀ Heterojunction Interface: A Theoretical Study on F _n ZnPc (n = 0, 4, 8, 16) and Cl _n SubPc (n = 0, 6). Journal of Physical Chemistry A, 2019, 123, 4034-4047.	1.1	26
3831	Coinage metal complexes of N-heterocyclic carbene bearing nitrile functionalization: Synthesis and photophysical properties. Applied Organometallic Chemistry, 2019, 33, e4927.	1.7	8
3832	Superhalogens as Building Blocks of Super Lewis Acids. ChemPhysChem, 2019, 20, 1607-1612.	1.0	11
3833	Density Functional Theory Descriptors for Ionic Liquids and the Introduction of a Coulomb Correction. Journal of Physical Chemistry A, 2019, 123, 4188-4200.	1.1	16
3834	The QM/MM-QTAIM approach reveals the nature of the different reactivity of cephalosporins in the active site of L1 metallo-β-lactamase. New Journal of Chemistry, 2019, 43, 7329-7338.	1.4	25
3835	Comparative studies on the effect of CB[8] on the charge transfer interaction. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	2
3836	Four 14(13-abeolanostane) Triterpenoids with 6/6/5/6-Fused Ring System from the Roots of Kadsura coccinea. Natural Products and Bioprospecting, 2019, 9, 165-173.	2.0	11
3837	High pressure behavior of crystal [2,2-bi(1,3,4-oxadiazole)]-5,5-dinitramide: A DFT investigation. Journal of Molecular Graphics and Modelling, 2019, 90, 87-93.	1.3	3
3838	Synthesis and structural characterisation of 1 TM -(diphenylphosphino)ferrocene-1-phosphonic acid, its ammonium salts and Pd(II) complexes. Journal of Organometallic Chemistry, 2019, 891, 44-53.	0.8	13
3839	On the capability of metal-halogen groups to participate in halogen bonds. CrystEngComm, 2019, 21, 2875-2883.	1.3	18
3840	A computational investigation of the interaction between As ³⁺ and deoxynucleotides. Molecular Simulation, 2019, 45, 769-776.	0.9	2
3841	Effect of CO ₂ in Flue Gas on Arsenic Adsorption over a Carbonaceous Surface. Energy & Fuels, 2019, 33, 4412-4419.	2.5	16
3842	A Large Family of Synthetic Two-Dimensional Metal Hydrides. Journal of the American Chemical Society, 2019, 141, 7899-7905.	6.6	25
3843	A theoretical exploration on why the replacement of hexyl group by alkoxycarbonyl in P3HT could greatly improve the performance of non-fullerene organic solar cell. Journal of the Taiwan Institute of Chemical Engineers, 2019, 100, 160-167.	2.7	4
3844	Amino-tetrazole functionalized fused triazolo-triazine and tetrazolo-triazine energetic materials. Chemical Communications, 2019, 55, 6062-6065.	2.2	77

#	ARTICLE	IF	CITATIONS
3845	Theoretical design of a fluorescence sensor with configuration-transformed metal ion recognition of aza-18-crown-6. <i>Supramolecular Chemistry</i> , 2019, 31, 402-411.	1.5	0
3846	Dibromomanganese(II) complexes with hexamethylphosphoramide and phenylphosphonic bis(diamide) ligands. <i>Journal of Coordination Chemistry</i> , 2019, 72, 309-327.	0.8	18
3847	Formation of Hetero-binuclear Pt(II)-M(II) Complexes Based on (2-(1 <i>H</i> -Tetrazol-5-yl)phenyl)diphenylphosphine Oxide for Superior Phosphorescence of Monomers. <i>Inorganic Chemistry</i> , 2019, 58, 4253-4261.	1.9	11
3848	Pressure-Dependent Luminescence and Absorption in 3,3'-Diamino-4,4'-azoxyfuran: Secondary Bonding Interaction in Molecular Crystals. <i>Journal of Physical Chemistry C</i> , 2019, 123, 8731-8739.	1.5	7
3849	Lone pair- π interaction versus σ -hole appearance in metal-bonded halogens. <i>CrystEngComm</i> , 2019, 21, 2929-2939.	1.3	3
3850	A quantitative description of photoluminescence efficiency of a carbazole-based thermally activated delayed fluorescence emitter. <i>New Journal of Chemistry</i> , 2019, 43, 6032-6039.	1.4	4
3851	Carbonyl-based polyimide and polyquinoneimide for potassium-ion batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 9997-10003.	5.2	102
3852	Silver cluster-amino acid interactions: a quantum-chemical study. <i>Amino Acids</i> , 2019, 51, 855-864.	1.2	25
3853	New insights into the dihydrogen bonds ($MH^{\delta+} \cdots \hat{A} \cdots \hat{A} \cdots H^{\delta+} + X$) in $CpM(PMe_3)(L)2H\hat{A} \cdots \hat{A} \cdots HX$ ($M=Cr, Mo, W$; $L=PMe_3, CO$); $Tj ETQqO O O rg$	1.0	1
3854	Mechanism and Origins of Regioselectivity of Copper-Catalyzed Borocyanation of 2-Aryl-Substituted 1,3-Dienes: A Computational Study. <i>Journal of Organic Chemistry</i> , 2019, 84, 5514-5523.	1.7	42
3855	Structures, Stabilities, and Spectral Properties of Endohedral Borospherenes $M@B_{40}^{sup>O} / \hat{A}^{sup}$ ($M = H_2, HF$, and H_2O). <i>ACS Omega</i> , 2019, 4, 5705-5713.	1.6	12
3856	Sulfuryl Fluoride Absorption from Fumigation Exhaust Gas by Biobased Solvents: Thermodynamic and Quantum Chemical Analysis. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 5018-5029.	1.8	4
3857	Theoretical Investigations into the Electron and Ambipolar Transport Properties of Anthracene-Based Derivatives. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3300-3314.	1.1	10
3858	Bowl-Shaped Carbon Nanobelts Showing Size-Dependent Properties and Selective Encapsulation of C_{70} . <i>Journal of the American Chemical Society</i> , 2019, 141, 5934-5941.	6.6	58
3859	Bond stretch isomerism in Be_3^{2+} driven by the Renner-Teller effect. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7996-8003.	1.3	10
3860	Single-Molecule Imaging and Computational Microscopy Approaches Clarify the Mechanism of the Dimerization and Membrane Interactions of Green Fluorescent Protein. <i>International Journal of Molecular Sciences</i> , 2019, 20, 1410.	1.8	7
3861	A Computational Study of Model Parent Systems and Reported Aza(Iso)Nazarov/Aza(Iso)Piancatelli Electrocyclic Reactions. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 2539-2551.	1.2	8
3862	Theoretical insights into the sensing mechanism of a series of terpyridine-based chemosensors for TNP. <i>Chemical Physics Letters</i> , 2019, 725, 45-51.	1.2	15

#	ARTICLE	IF	CITATIONS
3863	Binaphthanol-based organic fluorophores with color tunability and their optical properties. <i>CrystEngComm</i> , 2019, 21, 2809-2817.	1.3	14
3864	Platinum(II)-mediated aminonitrone- π -isocyanide interplay: A new route to acyclic diaminocarbene complexes. <i>Inorganica Chimica Acta</i> , 2019, 490, 267-271.	1.2	13
3865	New insights on the understanding of the high adsorption of bisphenol compounds on reduced graphene oxide at high pH values via charge assisted hydrogen bond. <i>Journal of Hazardous Materials</i> , 2019, 371, 513-520.	6.5	30
3866	Role of Water in the Reaction Mechanism and endo / exo Selectivity of 1,3-Dipolar Cycloadditions Elucidated by Quantum Chemistry and Machine Learning. <i>Chemistry - A European Journal</i> , 2019, 25, 8289-8303.	1.7	3
3867	The effect of substituent number on mechanochromic luminescence of β^2 -diketones and the corresponding boron complexes. <i>Dyes and Pigments</i> , 2019, 166, 159-167.	2.0	12
3868	Rational design of (D-A) copolymers towards high efficiency organic solar cells: DFT and TD-DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 89, 139-146.	1.3	6
3869	Atmospheric Chemistry of Enols: Vinyl Alcohol + OH + O ₂ Reaction Revisited. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3205-3213.	1.1	18
3870	Dual Aromaticity in Both the T ₀ and S ₁ States: Osmapyridinium with Phosphonium Substituents. <i>Journal of the American Chemical Society</i> , 2019, 141, 5720-5727.	6.6	62
3871	Theoretical Study of the Addition of Cu ⁺ Carbenes to Acetylenes to Form Chiral Allenes. <i>Journal of the American Chemical Society</i> , 2019, 141, 5772-5780.	6.6	35
3872	Size-selected anion photoelectron spectroscopy and density functional theory study of MnCn ^{+/0} (n = 1-10). <i>Journal of Physical Chemistry A</i> , 2019, 123, 10743-10744.	1.2	5
3873	Interactions between the Aryldiazonium Cations and Graphene Oxide: A DFT Study. <i>Journal of Chemistry</i> , 2019, 2019, 1-5.	0.9	63
3874	Identification of the Tetrel Bonds between Halide Anions and Carbon Atom of Methyl Groups Using Electronic Criterion. <i>Molecules</i> , 2019, 24, 1083.	1.7	30
3875	Mechanistic Insights into Formaldehyde-Blocked Lignin Condensation: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 8640-8648.	1.5	14
3876	Nickel-catalyzed C-N bond activation: activated primary amines as alkylating reagents in reductive cross-coupling. <i>Chemical Science</i> , 2019, 10, 4430-4435.	3.7	131
3877	Capturing volatile ester compounds from gas mixture with ionic liquids. <i>Journal of Molecular Liquids</i> , 2019, 281, 517-527.	2.3	16
3878	Suzuki coupling catalyzed by chloro(2-[mesityl(quinolin-8-yl- π -N)boryl]-3,5-dimethylphenyl)methyl- π -Cpalladium(II). <i>Tetrahedron</i> , 2019, 75, 2365-2370.	1.0	7
3879	Unraveling Excitonic Effects for the First Hyperpolarizabilities of Chromophore Aggregates. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13818-13836.	1.5	8
3880	Exploring the necessity of an acidic additive for Pd-catalyzed exclusive C4-fluoroalkylation of 3-acetylindole: a detailed DFT study on the mechanism and regioselectivity. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2607-2618.	2.3	14

#	ARTICLE	IF	CITATIONS
3881	DFT study of small gas molecules adsorbed on undoped and N-, Si-, B-, and Al-doped graphene quantum dots. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	38
3882	Understanding the spontaneous formation of pyridofuroxan from 2-azido-3-nitropyridine: A theoretical evaluation. <i>Computational and Theoretical Chemistry</i> , 2019, 1154, 31-36.	1.1	1
3883	Experimental and theoretical investigations of Cs ⁺ adsorption on crown ethers modified magnetic adsorbent. <i>Journal of Hazardous Materials</i> , 2019, 371, 712-720.	6.5	66
3884	Isoforrethins Aâ€”D, four ent- <i>abietane</i> diterpenoids from <i>Isodon forrestii</i> var. <i>forrestii</i> . <i>FÃ—totera pÃ—Ã—</i> , 2019, 134, 158-164.	1.1	3
3885	Hexagonal boron nitride nanosheet as novel drug delivery system for anticancer drugs: Insights from DFT calculations and molecular dynamics simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 89, 50-59.	1.3	123
3886	Hydrogen bonding capabilities of group 14 homologues of HCN and HNC. <i>RSC Advances</i> , 2019, 9, 5937-5941.	1.7	2
3887	Aggregation behavior and nonâ€”covalent functionalization of borofullerenes B 28 , B 38 , and B 40 : A density functional theory investigation. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25921.	1.0	4
3888	Stabilization and Extraction of Fluoride Anion Using a Tetralactam Receptor. <i>Journal of Organic Chemistry</i> , 2019, 84, 4050-4057.	1.7	21
3889	Derivatives of Cyanonaphthyl-Substituted Phenanthroimidazole as Blue Emitters for Nondoped Organic Light-Emitting Diodes. <i>ACS Omega</i> , 2019, 4, 4553-4570.	1.6	16
3890	An ideal platform of light-emitting materials from phenothiazine: facile preparation, tunable red/NIR fluorescence, bent geometry-promoted AIE behaviour and selective lipid-droplet (LD) tracking ability. <i>Journal of Materials Chemistry C</i> , 2019, 7, 4185-4190.	2.7	32
3891	Inâ€”depth probe of researching interfacial charge transfer process for organic solar cells: A promising bisadduct fullerene derivatives acceptor. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25938.	1.0	9
3892	DFT and QTAIM based investigation on the structure and antioxidant behavior of lichen substances Atranorin, Evernic acid and Diffractaic acid. <i>Computational Biology and Chemistry</i> , 2019, 80, 66-78.	1.1	31
3893	Noncovalent interactions within 3D molecular structure of diastereoisomers: A background for stereodependent redox activity. <i>Electrochimica Acta</i> , 2019, 306, 568-574.	2.6	9
3894	A theoretical study on cage-like clusters (C12Ti6 and C12Ti62+) for dihydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 10763-10769.	3.8	6
3895	Experimental and theoretical study on cetylpyridinium dipicrylamide â€” A promising ion-exchanger for cetylpyridinium selective electrodes. <i>Journal of Molecular Structure</i> , 2019, 1187, 77-85.	1.8	28
3896	Bidentate Sulfur Dioxide Complexes of Scandium, Yttrium, and Lanthanum Difluorides. <i>Inorganic Chemistry</i> , 2019, 58, 5281-5288.	1.9	8
3897	Solvent-Polarity-Dependent Excited-State Behavior and Thermally Active Delayed Fluorescence for Triquinolonobenzene. <i>ACS Applied Bio Materials</i> , 2019, 2, 2060-2068.	2.3	50
3898	Novel Colorimetric Method for Simultaneous Detection and Identification of Multimetal Ions in Water: Sensitivity, Selectivity, and Recognition Mechanism. <i>ACS Omega</i> , 2019, 4, 5915-5922.	1.6	34

#	ARTICLE	IF	CITATIONS
3899	A novel turn-on fluorescent probe for selective sensing and imaging of glutathione in live cells and organisms. <i>Analyst</i> , The, 2019, 144, 3260-3266.	1.7	19
3900	What accounts for the color purity of tetradentate Pt complexes? A computational analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8073-8080.	1.3	15
3901	A comparative study of Cu _n X (X = Sc, Y; n = 1–10) clusters based on the structures, and electronic and aromatic properties. <i>New Journal of Chemistry</i> , 2019, 43, 6597-6606.	1.4	17
3902	Structural and electronic properties of MB ₂₂ ⁺ (M = Na, K) clusters: tubular boron versus quasi-planar boron forms. <i>New Journal of Chemistry</i> , 2019, 43, 6507-6512.	1.4	17
3903	Chalcogen-substitution modulated supramolecular chirality and gas sensing properties in perylenediimides. <i>Chemical Communications</i> , 2019, 55, 4379-4382.	2.2	20
3904	Investigation of ECD conformational transition mechanism of GLP-1R by molecular dynamics simulations and Markov state model. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8470-8481.	1.3	19
3905	Applicability of NBO and AIM Topology Analyses to Chemical Bonding in Some Diacetylplatinum(II) Complexes. <i>Asian Journal of Chemistry</i> , 2019, 31, 925-937.	0.1	1
3906	An experimental and theoretical study on 2-hydroxyethylammonium acetate ionic liquid. <i>Journal of Molecular Liquids</i> , 2019, 284, 271-281.	2.3	13
3907	A dual-site modulated FRET-based two-photon ratiometric fluorescent probe for tracking lysosomal pH changes in living cells, tissues and zebrafish. <i>Sensors and Actuators B: Chemical</i> , 2019, 290, 79-86.	4.0	47
3908	Reductive Debromination of Polybrominated Diphenyl Ethers: Dependence on Br Number of the Br-Rich Phenyl Ring. <i>Environmental Science & Technology</i> , 2019, 53, 4433-4439.	4.6	28
3909	Describing Molecular Polarizability by a Bond Capacity Model. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3093-3107.	2.3	22
3910	Visible Light Rewritable and Long-Lived Colors in Cholesteric Liquid Crystals: A Facile Co-Doping Strategy. <i>Macromolecular Rapid Communications</i> , 2019, 40, e1900037.	2.0	17
3911	Theoretical study of aerobic oxidation of alcohols over Au ₃₈ nanocluster by a two-step-modeling approach. <i>Chemical Physics Letters</i> , 2019, 724, 115-121.	1.2	7
3912	¹³ C NMR Shifts as an Indicator of U–C Bond Covalency in Uranium(VI) Acetylide Complexes: An Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2019, 58, 4152-4163.	1.9	34
3913	Fabrication of Hydrazone-Linked Covalent Organic Frameworks Using Alkyl Amine as Building Block for High Adsorption Capacity of Metal Ions. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 11706-11714.	4.0	139
3914	Analysis of pseudo jahn–teller distortion based on natural bond orbital theory: Case study for silicene. <i>Journal of Computational Chemistry</i> , 2019, 40, 1488-1495.	1.5	14
3915	Theoretical study on the light-emitting mechanism of circularly polarized luminescence molecules with both thermally activated delayed fluorescence and aggregation-induced emission. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7288-7297.	1.3	20
3916	Impact sensitivity of aryl diazonium chlorides: Limitations of molecular and solid-state approach. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 89, 114-121.	1.3	14

#	ARTICLE	IF	CITATIONS
3917	A Quantum Mechanism Study of the C-C Bond Cleavage to Predict the Bio-Catalytic Polyethylene Degradation. <i>Frontiers in Microbiology</i> , 2019, 10, 489.	1.5	26
3918	Interpreting Aromaticity and Antiaromaticity through Bifurcation Analysis of the Induced Magnetic Field. <i>ChemistryOpen</i> , 2019, 8, 321-326.	0.9	9
3919	A multifunctional bipolar host material based on phenanthroimidazole for efficient green and red PhOLEDs with low turn-on voltage. <i>Organic Electronics</i> , 2019, 69, 85-91.	1.4	20
3920	Theoretical study on a boron phosphide nanocage doped with superalkalis: novel electrides having significant nonlinear optical response. <i>New Journal of Chemistry</i> , 2019, 43, 5727-5736.	1.4	73
3921	<i>exo/endo</i> Selectivity Control in Diels-Alder Reactions of Geminal Bis(silyl) Dienes: Theoretical and Experimental Studies. <i>Journal of Organic Chemistry</i> , 2019, 84, 3940-3952.	1.7	12
3922	Phantom Reactivity in Organic and Catalytic Reactions as a Consequence of Microscale Destruction and Contamination-Trapping Effects of Magnetic Stir Bars. <i>ACS Catalysis</i> , 2019, 9, 3070-3081.	5.5	106
3923	Organochlorinated pesticides expedite the enzymatic degradation of DNA. <i>Communications Biology</i> , 2019, 2, 81.	2.0	11
3924	Rydberg state mediated multiphoton ionization of $(\text{I}^{\text{I}^{\text{I}}}\text{-C}^{\text{I}^{\text{I}}}\text{H}^{\text{I}^{\text{I}}})^{\text{I}^{\text{I}}}\text{-C}^{\text{I}^{\text{I}}}\text{H}^{\text{I}^{\text{I}}}$: DFT-supported experimental insights into the molecular and electronic structures of excited sandwich complexes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9665-9671.	1.3	2
3925	Initial Mechanisms for the Unimolecular Thermal Decomposition of 2,6-Diamino-3,5-dinitropyrazine-1-oxide. <i>Molecules</i> , 2019, 24, 125.	1.7	18
3926	DFT Studies on Second-order Nonlinear Optical Response of $\text{Ir}(\text{C}^{\text{N}})_2(\text{pic})$ Complexes. <i>Chemical Research in Chinese Universities</i> , 2019, 35, 333-339.	1.3	4
3927	Selective Separation and Complexation of Trivalent Actinide and Lanthanide by a Tetradentate Soft-Hard Donor Ligand: Solvent Extraction, Spectroscopy, and DFT Calculations. <i>Inorganic Chemistry</i> , 2019, 58, 4420-4430.	1.9	84
3928	Halo-1,2,3-triazolium Salts as Halogen Bond Donors for the Activation of Imines in Dihydropyridinone Synthesis. <i>Journal of Organic Chemistry</i> , 2019, 84, 4294-4303.	1.7	52
3929	Mechanism and stereoselectivity in NHC-catalyzed I^2 -functionalization of saturated carboxylic ester. <i>RSC Advances</i> , 2019, 9, 7635-7644.	1.7	9
3930	Efficient electroluminescent hybridized local and charge-transfer host materials with small singlet-triplet splitting to enhance exciton utilization efficiency: excited state transition configuration. <i>RSC Advances</i> , 2019, 9, 6658-6680.	1.7	12
3931	Halogen Bonding: A Halogen-Centered Noncovalent Interaction Yet to Be Understood. <i>Inorganics</i> , 2019, 7, 40.	1.2	115
3932	A Spectroscopic Study of Tautomeric Equilibrium of Salicylideneaniline in ZSM-5 Zeolites. <i>Molecules</i> , 2019, 24, 795.	1.7	1
3933	A facile approach for the synthesis of novel xanthene derivatives with Vilsmeier-Haack reagent. <i>Chemistry of Heterocyclic Compounds</i> , 2019, 55, 38-46.	0.6	14
3934	Second-order NLO properties of bis-cyclometalated iridium($\lambda\text{-}\text{C}$) complexes: Substituent effect and redox switch. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 89, 131-138.	1.3	18

#	ARTICLE	IF	CITATIONS
3935	A theoretical insight into the role of counter anions and their interactions in nitropentaamminecobalt(III) toward linkage isomerism-induced photochemical motion. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25929.	1.0	6
3936	Molecular design of ionic liquids as novel non-metal catalysts for the acetylene hydrochlorination reaction. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7635-7644.	1.3	7
3937	Study on the spectral complementary composite dye molecules designed for high performance dye-sensitized solar cells: A theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2019, 1154, 44-49.	1.1	9
3938	Theoretical study on the sensing mechanism of a fluorescence chemosensor for the cyanide anion. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 216, 258-264.	2.0	7
3939	Solvent effect on the formation of NTO/TZTN cocrystal explosives. <i>Computational Materials Science</i> , 2019, 163, 308-314.	1.4	9
3940	Density functional theory analysis for the limitations of fluoranthene-fused imide based small molecule acceptor materials in photovoltaic performance. <i>Computational and Theoretical Chemistry</i> , 2019, 1156, 37-42.	1.1	3
3941	The scandium doped boron cluster $B_{27}Sc_2^{+}$: a fruit can-like structure. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8933-8939.	1.3	14
3942	A computational investigation on core-expanded subphthalocyanines. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25942.	1.0	8
3943	TCA self-assembled fluorescence probe for Cu (II) ion based on the unique configuration of extra nuclear electrons of metal ions: A TDDFT study. <i>Computational and Theoretical Chemistry</i> , 2019, 1157, 1-10.	1.1	0
3944	Combined Theoretical and Experimental Study on Intramolecular Charge Transfer Processes in Star-Shaped Conjugated Molecules. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11179-11188.	1.5	7
3945	Deeper Insights into Conformational Analysis of <i>cis</i> -Butene and 1-Alkenes as Monomers and Dimers: QAIM, NCI, and DFT Approach. <i>Journal of Chemistry</i> , 2019, 2019, 1-13.	0.9	1
3946	(Isocyano Group Hole) ... [d ^{II}] Interactions of (Isocyanide)[M ^{II}] Complexes, in which Positively Charged Metal Centers (d ⁸) Act as Nucleophiles. <i>Chemistry - A European Journal</i> , 2019, 25, 8590-8598.	1.7	53
3947	Crystal Structure Characterization, Independent Gradient Model Analysis, and Gas-Phase Mediated Transformation of Nicosulfuron DMF Solvate and Hydrate. <i>Crystal Research and Technology</i> , 2019, 54, 1800244.	0.6	4
3948	The complexation reaction of oxotitanium(IV) tetraphenylporphyrin with benzoyl peroxide: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	2
3949	Complexes of damirone A/C, batzelline A/D, makaluvamine O and makaluvone with guanidinium and magnesium cations: a theoretical study. <i>Structural Chemistry</i> , 2019, 30, 1635-1646.	1.0	0
3950	The effect of molecular structure on intramolecular charge-transfer in 1,3,4-oxadiazole derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 377, 309-317.	2.0	17
3951	Insights into NHC-catalyzed oxidative $\hat{C}(sp^3)\text{-H}$ activation of aliphatic aldehydes and cascade [2 + 3] cycloaddition with azomethine imines. <i>Catalysis Science and Technology</i> , 2019, 9, 2514-2522.	2.1	48
3952	Computational design of species with ultrashort Be-Be distances using planar hexacoordinate carbon structures as the templates. <i>Dalton Transactions</i> , 2019, 48, 6581-6587.	1.6	7

#	ARTICLE	IF	CITATIONS
3953	Exploring the effect of aggregation-induced emission on the excited state intramolecular proton transfer for a bis-imine derivative by quantum mechanics and our own <i>n</i> -layered integrated molecular orbital and molecular mechanics calculations. <i>Chinese Physics B</i> , 2019, 28, 018201.	0.7	7
3954	Theoretical design on molecular tweezers of sodium cyanide by zinc porphyrin-crown ether triads receptor. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3963.	0.9	5
3955	B ₁₂ @Mg ₂₀ B ₁₂ : A Stable Molecular Pentakis Dodecahedron. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17639-17643.	1.5	7
3956	Toward an Accurate Description of Thermally Activated Delayed Fluorescence: Equal Importance of Electronic and Geometric Factors. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13869-13876.	1.5	11
3957	Mechanistic insight into the self-coupling of 5-hydroxymethyl furfural to C12 fuel intermediate catalyzed by ionic liquids. <i>RSC Advances</i> , 2019, 9, 10825-10831.	1.7	2
3958	Local-structure effects on 31P NMR chemical shift tensors in solid state. <i>Journal of Chemical Physics</i> , 2019, 150, 144706.	1.2	18
3959	Experimental and theoretical investigation on photodegradation mechanisms of naproxen and its photoproducts. <i>Chemosphere</i> , 2019, 227, 142-150.	4.2	31
3960	Methyl Thioether Functionalization of a Polymeric Donor for Efficient Solar Cells Processed from Non-Halogenated Solvents. <i>Chemistry of Materials</i> , 2019, 31, 3025-3033.	3.2	23
3961	Asymmetric Construction of 4-H-Pyrano[3,2- <i>b</i>]indoles via Cinchonine-Catalyzed 1,4-Addition of 2-Ylideneoxindole with Malononitrile. <i>Journal of Organic Chemistry</i> , 2019, 84, 5450-5459.	1.7	16
3962	A rational design of manganese electrocatalysts for Lewis acid-assisted carbon dioxide reduction. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8849-8855.	1.3	12
3963	On the nature of ion-stabilized cytosine pairs in DNA motifs: The importance of charge transfer processes. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25933.	1.0	10
3964	Stability and bonding in rare gas inserted interhalogens FR _n X _n (X = Br and I, n = 0 and 2). <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25940.	1.0	1
3965	A pyrocarbonate intermediate for CO ₂ activation and selective conversion in bifunctional metal-organic frameworks. <i>Journal of Catalysis</i> , 2019, 373, 37-47.	3.1	12
3966	Dynamic Excited-State Intramolecular Proton Transfer Mechanisms of Two Novel 3-Hydroxyflavone-Based Chromophores in Two Different Surroundings. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3937-3948.	1.1	11
3967	Synergistic use of NMR computation and quantitative interproton distance analysis in the structural determination of neokadococitane A, a rearranged triterpenoid featuring an aromatic ring D from <i>Kadsura coccinea</i> . <i>Organic Chemistry Frontiers</i> , 2019, 6, 1619-1626.	2.3	18
3968	A series of energetic cyclo-pentazolate salts: rapid synthesis, characterization, and promising performance. <i>Journal of Materials Chemistry A</i> , 2019, 7, 12468-12479.	5.2	105
3969	Possible low-energy isomers of OH (H ₂ O) ₄ (n ⁻ = ⁻ 0, $\hat{A}\pm 1$) clusters via the particle swarm optimization algorithm: An ab initio study. <i>Computational and Theoretical Chemistry</i> , 2019, 1155, 20-30.	1.1	1
3970	Conformational landscape and inertial defect of methoxyphenol isomers studied by mm-wave spectroscopy and quantum chemistry calculations. <i>Journal of Chemical Physics</i> , 2019, 150, 104303.	1.2	6

#	ARTICLE	IF	CITATIONS
3971	CH ₃ NH ₃ Formed by Electron Injection at Heterojunction Inducing Peculiar Properties of CH ₃ NH ₃ PbI ₃ Material. Chinese Physics Letters, 2019, 36, 026701.	1.3	0
3972	Theoretical Study on the Growth Behavior and Photoelectron Spectroscopy of Lanthanum-Doped Silicon Clusters LaSi _n O _n (n=20). Journal of Cluster Science, 2019, 30, 789-796.	1.7	13
3973	Interfacial charge-transfer in Cu-TiO ₂ -HBDPPIN-Ag film and AIEE-active chemosensor. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 377, 318-338.	2.0	1
3974	The First Naked Bismuth-Chalcogen Metal Carbonyl Clusters: Extraordinary Nucleophilicity of the Bi Atom and Semiconducting Characteristics. Inorganic Chemistry, 2019, 58, 6706-6721.	1.9	7
3975	Solid state properties of hydroxyurea: Optical absorption measurement and DFT calculations. Journal of Applied Physics, 2019, 125, 134901.	1.1	4
3976	Narrowing Segments of Helical Carbon Nanotubes with Curved Aromatic Panels. Angewandte Chemie - International Edition, 2019, 58, 7385-7389.	7.2	42
3977	Exploring the structural and electronic properties of double-Fe atom-doped Si ₂₀ cluster by quantum chemical calculations. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	15
3978	A comparative study of S-As chalcogen bonds between SF ₂ or SFH and C-C multiple bonds. Journal of Molecular Structure, 2019, 1188, 62-68.	1.8	3
3979	Carbon rings decorated with group 14 elements: new aromatic clusters containing planar tetracoordinate carbon. New Journal of Chemistry, 2019, 43, 6781-6785.	1.4	31
3980	The solvent effect on the excited-state intramolecular proton transfer of cyanine derivative molecules. Organic Chemistry Frontiers, 2019, 6, 1674-1680.	2.3	27
3981	Aromaticity-promoted C-F Bond Activation in Rhodium Complex: A Facile Tautomerization. Chemistry - an Asian Journal, 2019, 14, 1937-1940.	1.7	20
3982	A greener catalyst for hydroboration of imines-external electric field modify the reaction mechanism. Journal of Computational Chemistry, 2019, 40, 1772-1779.	1.5	11
3983	Room-Temperature Cavity Ring-Down Spectroscopy of Methylallyl Peroxy Radicals. Journal of Physical Chemistry A, 2019, 123, 3510-3517.	1.1	4
3984	Insight into the structure and interaction properties of 1-propylnitrile-3-methylimidazolium bis(trifluoromethylsulfonyl)imide and chloroform mixtures. Journal of Molecular Liquids, 2019, 283, 748-755.	2.3	9
3985	Rotational spectrum and structure of 2-chlorothiophene and its complex with argon. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 218, 136-141.	2.0	6
3986	Why electrostatically enhanced thiourea is better than Schreiner's thiourea in both catalytic activity and regioselectivity?. Organic Chemistry Frontiers, 2019, 6, 1821-1831.	2.3	7
3987	DFT and Thermal Decomposition Studies on Gemcitabine. Zeitschrift Fur Physikalische Chemie, 2019, 233, 1503-1527.	1.4	10
3988	Mercapto-benzothiazolyl based ruthenium borate complexes: synthesis and reactivity towards various phosphines. Dalton Transactions, 2019, 48, 7413-7424.	1.6	11

#	ARTICLE	IF	CITATIONS
3989	Structural, bonding, and superhalogen properties of Au ₄ X ₄ O (X = F, Cl, Br, and I) clusters. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	5
3990	MD/QM modeling of the modified gold nanoparticles and investigation of their sensing ability for selective detection of melamine. <i>Journal of Molecular Liquids</i> , 2019, 284, 454-461.	2.3	6
3991	Synthesis, PXRD structural determination, Hirshfeld surface analysis and DFT/TD-DFT investigation of 3N-ethyl-2N TM -(2-ethylphenylimino) thiazolidin-4-one. <i>Journal of Molecular Structure</i> , 2019, 1189, 8-20.	1.8	28
3992	Competition/Cooperation between Humic Acid and Graphene Oxide in Uranyl Adsorption Implicated by Molecular Dynamics Simulations. <i>Environmental Science & Technology</i> , 2019, 53, 5102-5110.	4.6	53
3993	A theoretical insight into several common anion recognitions based on double π -dentate hydrogen bond and anion π coexistence. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3959.	0.9	5
3994	The theoretical investigation on the properties of fluorine-substituted uracil. <i>Computational and Theoretical Chemistry</i> , 2019, 1156, 43-51.	1.1	1
3995	Design of apolar chitosan-type adsorbent for removal of Cu(II) and Pb(II): An experimental and DFT viewpoint of the complexation process. <i>Journal of Environmental Chemical Engineering</i> , 2019, 7, 103070.	3.3	23
3996	Extensive theoretical study of corrosion inhibition efficiency of some pyrimidine derivatives on iron and the proposal of new inhibitor. <i>Journal of Molecular Liquids</i> , 2019, 284, 225-231.	2.3	32
3997	Structurally diverse diterpenoids from <i>Isodon ternifolius</i> collected from three regions. <i>Tetrahedron</i> , 2019, 75, 2797-2806.	1.0	6
3998	Interaction of epitaxial graphene with heavy metals: towards novel sensing platform. <i>Nanotechnology</i> , 2019, 30, 294002.	1.3	13
3999	Intriguing electric field effect on magnetic spin couplings in dielectron clathrate hydrates. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25916.	1.0	4
4000	Furthering the Diverse Hydrogen Atom Transfer and Carbon Bond Dissociation of Amino Acids under Vacuum Ultraviolet. <i>ChemistrySelect</i> , 2019, 4, 2129-2134.	0.7	1
4001	Experimental and quantum chemical study on nano-copper immobilized on magnetic graphitic carbon nitride core shell particles; a reusable heterogeneous catalyst toward reduction of nitro arenes. <i>Journal of Molecular Structure</i> , 2019, 1185, 38-49.	1.8	12
4002	Copper(π)-catalyzed asymmetric aza Diels π -Alder reactions of azoalkenes toward fulvenes: a molecular electron density theory study. <i>New Journal of Chemistry</i> , 2019, 43, 4765-4776.	1.4	21
4003	Differential Binding of Tetrel-Bonding Bipodal Receptors to Monatomic and Polyatomic Anions. <i>Molecules</i> , 2019, 24, 227.	1.7	21
4004	Dicyanamide-interlaced assembly of Zn(II)-schiff-base complexes derived from salicylaldimino type compartmental ligands: Syntheses, crystal structures, FMO, ESP, TD-DFT, fluorescence lifetime, in vitro antibacterial and anti-biofilm properties. <i>Inorganica Chimica Acta</i> , 2019, 489, 244-254.	1.2	49
4005	Dithiolation of [70]Fullerene with Aliphatic Primary Thiols in the Presence of n-Butylamine via Aerobic Oxidation Reaction. <i>Journal of Organic Chemistry</i> , 2019, 84, 3045-3054.	1.7	7
4006	Ab initio calculations and reduced density gradient analyses of the structure and energetics of hydrated calcium fluoride and calcium carbonate. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5744-5758.	1.3	5

#	ARTICLE	IF	CITATIONS
4007	A Straightforward Route to Aromatic Excited States in Molecular Motors that Improves Photochemical Efficiency. <i>ChemPhotoChem</i> , 2019, 3, 450-460.	1.5	13
4008	Terminal Modulation in Search of a Balance between Hole Transport and Electron Transfer at the Interface for BODIPY-Based Organic Solar Cells. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6407-6415.	1.5	10
4009	Localized Surface Plasmon Resonance in Free Silver Nanoclusters Ag _n , <i>n</i> = 20–147. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6205-6212.	1.5	20
4010	CO ₂ Adsorption on the B ₁₂ N ₁₂ Nanocage Encapsulated with Alkali Metals: A Density Functional Study. <i>Nano</i> , 2019, 14, 1950034.	0.5	5
4011	Investigation of Conversion and Decay Processes in Thermally Activated Delayed Fluorescence Copper(I) Molecular Crystal: Theoretical Estimations from an ONIOM Approach Combined with the Tuned Range-Separated Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2080-2090.	1.1	13
4012	Chiral phosphoric acid-catalyzed asymmetric C(sp ³)–H functionalization of biomass-derived 2,5-dimethylfuran <i>via</i> two sequential Cope-type rearrangements. <i>Organic Chemistry Frontiers</i> , 2019, 6, 1162-1167.	2.3	21
4013	Theoretical study on photophysical properties of a series of functional pyrimidine-based organic light-emitting diodes emitters presenting thermally activated delayed fluorescence. <i>Journal of Computational Chemistry</i> , 2019, 40, 1578-1585.	1.5	16
4014	Sulfuric acid and aromatic carboxylate clusters H ₂ SO ₄ –ArCOO [–] : Structures, properties, and their relevance to the initial aerosol nucleation. <i>International Journal of Mass Spectrometry</i> , 2019, 439, 27-33.	0.7	8
4015	Strategy to modulate the singlet-triplet energy gap for spiro-based thermally activated delayed fluorescence molecules. <i>Journal of Luminescence</i> , 2019, 209, 372-378.	1.5	18
4016	A combined MD/QM study on the sensing mechanism of Pb ²⁺ by glutathione functionalized gold nanoparticles. <i>Journal of Molecular Liquids</i> , 2019, 280, 120-127.	2.3	13
4017	A mononuclear cobalt(II) salophen-type complex: Synthesis, theoretical and experimental electronic absorption and infrared spectra, crystal structure, and predicting of second- and third-order nonlinear optical properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 215, 225-232.	2.0	3
4018	Origin of Selectivity of a Triazinyl Ligand for Americium(III) over Neodymium(III). <i>Chemistry - A European Journal</i> , 2019, 25, 3248-3252.	1.7	33
4019	A sky-blue thermally activated delayed fluorescence emitter based on multimodified carbazole donor for efficient organic light-emitting diodes. <i>Organic Electronics</i> , 2019, 68, 113-120.	1.4	20
4020	How intermolecular interactions influence electronic absorption spectra: insights from the molecular packing of uracil in condensed phases. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4072-4081.	1.3	19
4021	A Novel Electrochemical Sensor Based on Silsesquioxane/Nickel (II) Phthalocyanine for the Determination of Sulfanilamide in Clinical and Drug Samples. <i>Electroanalysis</i> , 2019, 31, 867-875.	1.5	29
4022	Effect of external electric field on C–X···Y halogen bonds. <i>Journal of Molecular Modeling</i> , 2019, 25, 57.	0.8	11
4023	D-A- π -A based organic dyes for efficient DSSCs: A theoretical study on the role of π -spacer. <i>Computational Materials Science</i> , 2019, 161, 163-176.	1.4	65
4024	Heterobimetallic copper(<i>scp</i>) complexes bearing both 1,1-bis(diphenylphosphino)ferrocene and functionalized 3-(2-pyridyl)-1,2,4-triazole. <i>New Journal of Chemistry</i> , 2019, 43, 4261-4271.	1.4	12

#	ARTICLE	IF	CITATIONS
4025	Multi-Residue Method for the Analysis of Stilbene Estrogens in Milk. <i>International Journal of Molecular Sciences</i> , 2019, 20, 744.	1.8	9
4026	A probe into underlying factors affecting ultrafast charge transfer at Donor/IDIC interface of all-small-molecule nonfullerene organic solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 375, 1-8.	2.0	11
4027	State-specific electrostatic potential descriptors for estimating solvatochromic effects. <i>Journal of Molecular Modeling</i> , 2019, 25, 60.	0.8	2
4028	Structure, stability, and electronic structure properties of quasi-fullerenes. <i>Computational and Theoretical Chemistry</i> , 2019, 1152, 7-18.	1.3	13
4029	Hydrogen sulfide interaction with pristine, defected and M-decorated black phosphorous (M= B, Co, V,) <i>Tj ETQq0 0,0rgBT /Ov</i>	1.3	13
4030	Icosahedral transition metal clusters (M ₁₃ , M = Fe, Ni, and Cu) adsorbed on graphene quantum dots, a DFT study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 110, 52-58.	1.3	25
4031	Thermally Induced trans \rightarrow cis Isomerization and Its Photoinduced Reversal Monitored using Absorption and Luminescence: Cooperative Effect of Metal Coordination and Steric Substituent. <i>Chemistry - A European Journal</i> , 2019, 25, 5177-5185.	1.7	8
4032	Theoretical study on organic dyes with tunable π -spacers for dye-sensitized solar cells: Inspired by the organic polymer photovoltaics. <i>Chemical Physics Letters</i> , 2019, 719, 39-44.	1.2	13
4033	Psychiatric Disorders and Oxidative Injury: Antioxidant Effects of Zolpidem Therapy disclosed In Silico. <i>Computational and Structural Biotechnology Journal</i> , 2019, 17, 311-318.	1.9	22
4034	Effect of (super)alkali doping on the electronic and second-order nonlinear optical properties of graphitic C ₃ N ₄ . <i>Optik</i> , 2019, 183, 455-462.	1.4	18
4035	Adsorption of ibuprofen on silicon decorated fullerenes and single walled carbon nanotubes: A comparative DFT study. <i>Journal of Molecular Structure</i> , 2019, 1184, 110-113.	1.8	33
4036	DFT characterization of the mechanism for Staudinger/aza-Wittig tandem organocatalysis. <i>Tetrahedron</i> , 2019, 75, 1852-1859.	1.0	10
4037	Micro Solid Phase Extraction Surface-Enhanced Raman Spectroscopy (μ -SPE/SERS) Screening Test for the Detection of the Synthetic Cannabinoid JWH-018 in Oral Fluid. <i>Analytical Chemistry</i> , 2019, 91, 4780-4789.	3.2	38
4038	Redox Trimetallic Nanozyme with Neutral Environment Preference for Brain Injury. <i>ACS Nano</i> , 2019, 13, 1870-1884.	7.3	90
4039	<i>In situ</i> nitroso formation induced structural diversity of uranyl coordination polymers. <i>Inorganic Chemistry Frontiers</i> , 2019, 6, 775-785.	3.0	19
4040	Structural and electronic properties of chemically modified fullerenes. <i>Molecular Simulation</i> , 2019, 45, 623-635.	0.9	1
4041	Organic Compounds of Actinyls: Systematic Computational Assessment of Structural and Topological Properties in [AnO ₂ (C ₂ O ₄) ₂] _n (An = Th, U, Pu, Am) <i>Tj ETQq0 0,0rgBT /Ov</i>	1.9	11
4042	Impact of confinement in multimolecular inclusion compounds of melamine and cyanuric acid. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8205-8214.	1.3	5

#	ARTICLE	IF	CITATIONS
4043	Influence of nanopore density on ethylene/acetylene separation by monolayer graphene. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6126-6132.	1.3	15
4044	N ⁺ Sn coordination in the complexes of tin halides with pyridine: A comparison between Sn(II) and Sn(IV). <i>Applied Organometallic Chemistry</i> , 2019, 33, e4811.	1.7	15
4045	Effect of Ligands on the Lewis Acidity of the Metal and the Binding of N-Bases to Iridium Pincer Complexes. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1389-1397.	1.0	5
4046	Synthesis and physico-chemical properties of a novel chromate compound with potential biological applications, bis(2-phenylethylammonium) chromate(VI). <i>Journal of Molecular Structure</i> , 2019, 1185, 168-182.	1.8	57
4047	Structural and Electronic Properties of Medium-Sized Aluminum-Doped Boron Clusters AlB _n and Their Anions. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6276-6283.	1.5	59
4048	Tetrel bonds and conformational equilibria in the formamide-CO ₂ complex: a rotational study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7016-7020.	1.3	24
4049	Feasibility of Pristine and Decorated AlN and SiC Nanotubes in Sensing of Noble Gases: A DFT study. <i>ChemistrySelect</i> , 2019, 4, 2453-2462.	0.7	23
4050	Computational insight into the contribution of para-substituents on the reduction potential, proton affinity, and electronic properties of nitrobenzene compounds. <i>Journal of Molecular Modeling</i> , 2019, 25, 78.	0.8	12
4051	Studies on predicting reactive sites of 3,9-diazatetraasteranes by conceptual density functional theory and experiment. <i>Structural Chemistry</i> , 2019, 30, 1707-1714.	1.0	4
4052	Possible lower energy isomer of carbon clusters C _n (n = 11, 12) via particle swarm optimization algorithm: Ab initio investigation. <i>Chemical Physics Letters</i> , 2019, 721, 74-85.	1.2	7
4053	Supramolecular polymers derived from the PtII and PdII schiff base complexes via C(sp ²)-H...Hal hydrogen bonding: Combined experimental and theoretical study. <i>Journal of Organometallic Chemistry</i> , 2019, 886, 71-75.	0.8	36
4054	Synthesis, molecular structure and DFT studies of two heteroleptic nickel(II) s-triazine pincer type complexes. <i>Journal of Molecular Structure</i> , 2019, 1185, 461-468.	1.8	10
4055	Two triphenylamine-based luminescent metal-organic frameworks as a dual-functional sensor for the detection of nitroaromatic compounds and ofloxacin antibiotic. <i>CrystEngComm</i> , 2019, 21, 2559-2570.	1.3	53
4056	Chalcogen stabilized trimetallic clusters: synthesis, structures, and bonding of [(Cp* ₃ M)(E) _{6+m} (BH) _n] (M = Nb or Ta; E = S or Se; n = 0 or 1) <i>Tetrahedron Letters</i> , 2019, 50, 1078-1081.	1.4	14
4057	Catalytic Mechanism for 2,3-Dihydroxybiphenyl Ring Cleavage by Nonheme Extradiol Dioxygenases BphC: Insights from QM/MM Analysis. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2244-2253.	1.2	5
4058	Room-Temperature Phosphorescence from Metal-Free Organic Materials in Solution: Origin and Molecular Design. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1037-1042.	2.1	34
4059	Photoresponsive sulfone-based molecules: photoinduced electron transfer and heat/air-stable radicals in the solid state. <i>New Journal of Chemistry</i> , 2019, 43, 4506-4510.	1.4	3
4060	Identification of an Overlooked Halogen-Bond Synthone and Its Application in Designing Fluorescent Materials. <i>Chemistry - A European Journal</i> , 2019, 25, 6584-6590.	1.7	11

#	ARTICLE	IF	CITATIONS
4061	Origin of the π -stacking induced shifts in absorption spectral bands of the green fluorescent protein chromophore. <i>Chemical Physics</i> , 2019, 522, 32-38.	0.9	15
4062	Conversion mechanism and isomeric preferences of the cis and trans isomers of anti-cancer medicine carmustine; A double hybrid DFT calculation. <i>Chemical Physics</i> , 2019, 522, 39-43.	0.9	6
4063	Fine-tuned dual fluorescence behavior of N-substituted aniline-imidazopyridine based switches: Mechanistic understanding, substituent and solvent effects. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 214, 407-428.	2.0	6
4064	Deciphering the Impact of Surface Defects and Functionalization on the Binding Strength and Electronic Properties of Graphene-Polypyrrole Nanocomposites: A First-Principles Approach. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5447-5459.	1.5	3
4065	Application of an inverse-design method to optimizing porphyrins in dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5834-5844.	1.3	8
4066	Strong influence of weak hydrogen bonding on actinide-phosphonate complexation: accurate predictions from DFT followed by experimental validation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5566-5577.	1.3	6
4067	Insight into Structural Characteristics of Protein-Substrate Interaction in Pimaricin Thioesterase. <i>International Journal of Molecular Sciences</i> , 2019, 20, 877.	1.8	2
4068	Manifestation of exo-cyclic aromaticity in triangular heterocyclic B_2F_2X systems ($X = O, S, Se, NH$). <i>Bulletin of Materials Science</i> , 2019, 42, 1.	0.8	2
4069	A new method to analyze and understand molecular linear and nonlinear optical responses via field-induced functions: a straightforward alternative to sum-over-states (SOS) analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6274-6286.	1.3	13
4070	Hexacoordinated Tetrel-Bonded Complexes between TF_4 ($T=Si, Ge, Sn, Pb$) and NCH : Competition between σ - and π -Holes. <i>ChemPhysChem</i> , 2019, 20, 959-966.	1.0	25
4071	Atomic pseudopotentials for reproducing π -orbital electron behavior in sp^2 carbon atoms. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25914.	1.0	3
4072	Conformational landscape of the weakly bound difluoromethane-1,1-difluoroethane dimer explored by rotational spectroscopy and quantum chemical calculations. <i>Journal of Molecular Spectroscopy</i> , 2019, 357, 32-37.	0.4	3
4073	Comparison of σ -hole and π -hole tetrel bonds in complexes of borazine with TH_3F and F_2TO/H_2TO ($T=C, Si, Ge$). <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25910.	1.0	19
4074	Computational study of the hydrogen peroxide scavenging mechanism of allyl methyl disulfide, an antioxidant compound from garlic. <i>Molecular Diversity</i> , 2019, 23, 985-995.	2.1	12
4075	Accurate Prediction for Dynamic Hybrid Local and Charge Transfer Excited States from Optimally Tuned Range-Separated Density Functionals. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5616-5625.	1.5	19
4076	Aminonitro Groups Surrounding a Fused Pyrazolotriazine Ring: A Superior Thermally Stable and Insensitive Energetic Material. <i>ACS Applied Energy Materials</i> , 2019, 2, 2263-2267.	2.5	111
4077	Structure and non-covalent interactions of 1,3-difluoropropane and its complex with water explored by rotational spectroscopy and quantum chemical calculations. <i>Journal of Chemical Physics</i> , 2019, 150, 064305.	1.2	5
4078	Experimental and theoretical studies of palladium(II) and platinum(II) complexes derived from di-(2-pyridyl)methyl-N,N'-dibenzylthiocarbamate. <i>Polyhedron</i> , 2019, 162, 177-185.	1.0	1

#	ARTICLE	IF	CITATIONS
4079	A DFT-based study of the hydrogen-bonding interactions between myricetin and ethanol/water. <i>Journal of Molecular Modeling</i> , 2019, 25, 67.	0.8	11
4080	Simultaneous Formation of <i>cis</i> - and <i>trans</i> -CH ₃ OCu(OH) Intermediates in Methane Activation by Cu in Solid Ar. <i>Inorganic Chemistry</i> , 2019, 58, 3237-3246.	1.9	1
4081	Vibrational Optical Activity of Intermolecular, Overtone, and Combination Bands: 2-Chloropropionitrile and \pm -Pinene. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2147-2156.	1.2	23
4082	Theoretical Determination of Total Electron-impact Ionization Cross Sections of Dichlorodifluoromethane (R12) and Tetrafluoroethane (R134). , 2019, , .		0
4083	DFT Investigation of a Charge-Transfer Complex Formation Between <i>p</i> -Phenylenediamine and 3,5-Dinitrosalicylic Acid. <i>Journal of Structural Chemistry</i> , 2019, 60, 1906-1916.	0.3	9
4084	Spectral Calculation of Cucurbituril[n] Molecule Based on Density Functional Theory. <i>IOP Conference Series: Earth and Environmental Science</i> , 2019, 384, 012034.	0.2	0
4085	QTAIM Analysis of Mono-Hydroxy Derivatives of <i>cis</i> -Borate Anions [BnHnâ€“ 1OH]2â€“ (n = 6, 10, 12). <i>Russian Journal of Inorganic Chemistry</i> , 2019, 64, 1825-1828.	0.3	6
4086	Catalyst-Dependent Chemoselectivity in the Dirhodium-Catalyzed Cyclization Reactions Between Enodiazacetamide and Nitrosoarene: A Theoretical Study. <i>Frontiers in Chemistry</i> , 2019, 7, 586.	1.8	6
4087	First-principles study on the singletâ€“triplet energy gap of thermally activated delayed fluorescence molecules. <i>Molecular Crystals and Liquid Crystals</i> , 2019, 690, 84-94.	0.4	0
4088	Experimental and theoretical charge-density analysis of hippuric acid: insight into its binding with human serum albumin. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 750-762.	0.5	3
4089	Insulation Properties of Liquid C6F12O for the Use in Eco-Friendly Transmission Equipment. , 2019, , .		0
4090	Unravelling the mechanism and the origin of the selectivity of the [3â€“+â€“2] cycloaddition reaction between electrophilic nitrene and nucleophilic alkene. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	11
4091	Probing the molecular structure and properties of neutral and anionic ground states of SO2 and CO2. <i>European Physical Journal D</i> , 2019, 73, 1.	0.6	5
4092	Insight into Two-Dimensional Borophene: Five-Center Bond and Phonon-Mediated Superconductivity. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 47279-47288.	4.0	14
4093	Laboratory Evolution of GH11 Endoxylanase Through DNA Shuffling: Effects of Distal Residue Substitution on Catalytic Activity and Active Site Architecture. <i>Frontiers in Bioengineering and Biotechnology</i> , 2019, 7, 350.	2.0	20
4094	Impact of Functional Group Methylation on the Disaggregation Trend of Asphaltene: A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 29543-29555.	1.5	25
4095	The influence of the grafted aryl groups on the solvation properties of the graphyne and graphdiyne - a MD study. <i>Open Chemistry</i> , 2019, 17, 703-710.	1.0	40
4096	Theoretical insight of alpha amino acid phenylalanine adsorption on pristine and decorated fullerenes. <i>Main Group Metal Chemistry</i> , 2019, 42, 135-142.	0.6	2

#	ARTICLE	IF	CITATIONS
4097	Removal of platinum (IV) from hydrochloric acid medium with OMImT: Theoretical and experimental evidences for a neutral complexing mechanism. <i>Journal of Molecular Liquids</i> , 2019, 293, 111529.	2.3	2
4098	Orbital-Weighted Dual Descriptor for the Study of Local Reactivity of Systems with (Quasi-) Degenerate States. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10556-10562.	1.1	89
4099	Fishbone-Like Polymer from Green Cationic Polymerization of Methyl Eleostearate as Biobased Nontoxic PVC Plasticizer. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 18976-18984.	3.2	24
4100	Vibrational frequencies and electronic structures of 2-amino-1, 9-dihydro-9-[(2-hydroxyethoxy)methyl]-6H-purin-6-one using density functional theory method. <i>AIP Conference Proceedings</i> , 2019, , .	0.3	0
4101	Influence of CO ₂ ; Molecules Adsorption on the Electronic Properties of Zigzag and Armchair ZnO Nanotubes. <i>Journal of Nano Research</i> , 0, 60, 51-62.	0.8	2
4102	Modulating intramolecular chalcogen bonds in aromatic (thio)(seleno)phene-based derivatives. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23645-23650.	1.3	20
4103	Rotational characterization of Sâˆ™F chalcogen bonds in the complex of 2,2,4,4-tetrafluoro-1,3-dithietane and difluoromethane. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24659-24665.	1.3	7
4104	Cooperative nature of the sulfur centered hydrogen bond: investigation of (H ₂ S) _n (n = 2â€“4) clusters using an affordable yet accurate level of theory. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 25439-25448.	1.3	15
4105	Unraveling the regioselectivity of odd electron halogen bond formation using electrophilicity index and chemical hardness parameters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 26580-26590.	1.3	15
4106	The control effects of different scaffolds in chiral phosphoric acids: a case study of enantioselective asymmetric arylation. <i>Catalysis Science and Technology</i> , 2019, 9, 6482-6491.	2.1	7
4107	Molecular modeling of cytotoxic activity of a new terpenoid-like bischalcone. <i>New Journal of Chemistry</i> , 2019, 43, 18451-18460.	1.4	6
4108	Aminonitrones as highly reactive bifunctional synthons. An expedient one-pot route to 5-amino-1,2,4-triazoles and 5-amino-1,2,4-oxadiazoles â€“ potential antimicrobials targeting multi-drug resistant bacteria. <i>New Journal of Chemistry</i> , 2019, 43, 17358-17366.	1.4	9
4109	Cooperation and competition of hydrogen and halogen bonds in 2D self-assembled nanostructures based on bromine substituted coumarins. <i>New Journal of Chemistry</i> , 2019, 43, 17182-17187.	1.4	16
4110	Extraordinary solution-processability of lignin in phenolâ€“maleic anhydride and dielectric films with controllable properties. <i>Journal of Materials Chemistry A</i> , 2019, 7, 23162-23172.	5.2	16
4111	Revealing the role of different nitrogen functionalities in the drug delivery performance of graphene quantum dots: a combined density functional theory and molecular dynamics approach. <i>Journal of Materials Chemistry B</i> , 2019, 7, 6156-6171.	2.9	70
4112	Structures and bonding properties of CPt ²⁺ /O and CPt ²⁺ H ⁺ /O: Anion photoelectron spectroscopy and quantum chemical calculations. <i>Journal of Chemical Physics</i> , 2019, 151, 224303.	1.2	7
4113	The mutual noncovalent interactions based on metallophilic cluster and anions: A theoretical investigation of the molecular structure and spectroscopic properties of Hostâ€“Guest complexes. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950028.	1.8	1
4114	Computational study of regiodivergent pathways in the copper-catalyzed borocyanation of 1,3-dienes: Mechanism and origin of regioselectivity. <i>Journal of Organometallic Chemistry</i> , 2019, 904, 121014.	0.8	12

#	ARTICLE	IF	CITATIONS
4115	Conformational preference determined by inequivalent n-pairs: rotational studies on acetophenone and its monohydrate. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22888-22894.	1.3	18
4116	Matrix infrared spectroscopy of F ₂ BMF and FBiWF ₂ (M = Cr, Mo and W) complexes and quantum chemistry calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 25577-25583.	1.3	5
4117	OBCN isomerization and noble gas insertion compounds of identical valence electron number species: stability and bonding. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 26311-26323.	1.3	4
4118	Transition from exohedral to endohedral geometries of anionic and neutral B ₄ Si _n (n = 4–15) clusters: quantum chemical calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 26154-26165.	1.3	7
4119	Magnesium oxide clusters as promising candidates for hydrogen storage. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23102-23110.	1.3	19
4120	The axial/equatorial conformational landscape and intramolecular dispersion: new insights from the rotational spectra of monoterpenoids. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 26111-26116.	1.3	14
4121	The first coordination polymers with an [O] ₂ [N]P(S)-Hg segment: a combined experimental, theoretical and database study. <i>Dalton Transactions</i> , 2019, 48, 17908-17918.	1.6	3
4122	Nitramino-furazan-functionalized fused high-nitrogen backbones as energetic materials with high detonation performance and good molecular stabilities. <i>New Journal of Chemistry</i> , 2019, 43, 16300-16304.	1.4	4
4123	One-pot synthesis of benzotripyrrole derivatives from 1H-pyrroles. <i>New Journal of Chemistry</i> , 2019, 43, 18437-18441.	1.4	2
4124	Polymeric tungsten carbide nanoclusters: structural evolution, ligand modulation, and assembled nanomaterials. <i>Nanoscale</i> , 2019, 11, 19903-19911.	2.8	20
4125	Regio- and chemo-selective cyclization of allenic-Ugi products for the synthesis of 3-pyrroline skeletons. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 8858-8870.	1.5	10
4126	A high-mobility, high-luminescence and low-threshold pentacene-doped cyano-substituted distyrylbenzene crystal. <i>Journal of Materials Chemistry C</i> , 2019, 7, 13447-13453.	2.7	9
4127	Triphenylpyrazine: methyl substitution to achieve deep blue AIE emitters. <i>Journal of Materials Chemistry C</i> , 2019, 7, 13047-13051.	2.7	17
4128	DFT Study on Photosensitizer-Free Visible-Light-Mediated Au-Catalyzed <i>cis</i> -Difunctionalization of Alkynes: Mechanism and Selectivities as Compared to Rh Catalysis. <i>Journal of Organic Chemistry</i> , 2019, 84, 16171-16182.	1.7	10
4129	Synergistic and antagonistic interplay between tetrel bond and pnictogen bond in complexes involving ring compounds. <i>Journal of Molecular Modeling</i> , 2019, 25, 351.	0.8	11
4130	Valine adsorption on pristine and N-doped graphenes: DFT, AIM, and IGM study. <i>Materials Research Express</i> , 2019, 6, 125061.	0.8	6
4131	Structural and electronic properties of nanosize semiconductor CeSiO ₄ (n = 4–20) material: A double-hybrid density functional theory investigation. <i>Computational and Theoretical Chemistry</i> , 2019, 1170, 112635.	1.1	7
4132	A comparative study to predict regioselectivity, electrophilicity and nucleophilicity with Fukui function and Hirshfeld charge. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	138

#	ARTICLE	IF	CITATIONS
4133	Acetone Dimer Hydrogenation under Vacuum Ultraviolet: An Intracluster Trimolecular Dissociation Mechanism. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10739-10745.	1.1	2
4134	Unraveling the Structure-Dependent Radiative and Nonradiative Decays in (CdSe) ₁₃ Clusters through First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 30714-30722.	1.5	11
4135	Donor-Acceptor vs Electron-Shared Bonding: Triatomic Si ₃ C ₃ (≈ 3) Clusters Stabilized by Cyclic Alkyl(amino) Carbene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10764-10771.	1.1	5
4136	Anti-inflammatory diterpenoids from the Brazilian alga <i>Dictyota menstrualis</i> . <i>Algal Research</i> , 2019, 44, 101695.	2.4	4
4137	Asymmetric Total Synthesis of (â ⁺)-Pavidolide B via a Thiyl-Radical-Mediated [3 + 2] Annulation Reaction. <i>Journal of Organic Chemistry</i> , 2019, 84, 15958-15971.	1.7	14
4138	Recovery of Au(III) from Acidic Chloride Media by Homogenous Liquid-Liquid Extraction with UCST-Type Ionic Liquids. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 19975-19983.	3.2	29
4139	RgnBe ₃ B ₃ ⁺ : theoretical investigation of Be ₃ B ₃ ⁺ and its rare gas capability. <i>Journal of Molecular Modeling</i> , 2019, 25, 349.	0.8	0
4140	Nature-Derived Sodium-Ion Battery: Mechanistic Insights into Na-Ion Coordination within Sustainable Molecular Cathode Materials. <i>ACS Applied Energy Materials</i> , 2019, 2, 8596-8604.	2.5	14
4141	UV-Visible Lysine-Glutamate Dimer Excitations in Protein Charge Transfer Spectra: TDDFT Descriptions Using an Optimally Tuned CAM-B3LYP Functional. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10967-10979.	1.2	14
4142	Well-Defined Scandacyclopropenes: Synthesis, Structure, and Reactivity. <i>Journal of the American Chemical Society</i> , 2019, 141, 20547-20555.	6.6	40
4143	Probing the Fluxional Bonding Nature of Rapid Cope rearrangements in Bullvalene C ₁₀ H ₁₀ and Its Analogs C ₈ H ₈ , C ₉ H ₁₀ , and C ₈ BH ₉ . <i>Scientific Reports</i> , 2019, 9, 17074.	1.6	12
4144	Synthesis, spectroscopic (FT-IR and UV-Vis), crystallographic and theoretical studies, and a molecular docking simulation of an imatinib-like template. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 1681-1689.	0.2	2
4145	A Ferrocenophane-Based Diaminophosphenium Ion. <i>Organometallics</i> , 2019, 38, 4717-4725.	1.1	8
4146	Molecular Modeling on Morphology of 3,4-Bis(3-nitrofurazan-4-yl)furoxan Crystals in Dichloroethane or Benzene Mixture Solvents. <i>Journal of Molecular Modeling</i> , 2019, 25, 373.	0.8	6
4147	Chemical bonding in Period 2 homonuclear diatomic molecules: a comprehensive relook. <i>Journal of Chemical Sciences</i> , 2019, 131, 1.	0.7	6
4148	Synthesis, Structure, and Luminescence Properties of Boron Complex with 4-Bromo-2-(1H-imidazo[4,5-f][1,10]phenanthrolin-2-yl)phenoxide Ligand. <i>Russian Journal of General Chemistry</i> , 2019, 89, 2246-2250.	0.3	0
4149	Radiative and non-radiative exciton recombination rate constants in ZnSe clusters. <i>European Physical Journal B</i> , 2019, 92, 1.	0.6	7
4150	Synthesis, X-ray Crystal Structure and Antimicrobial Activity of Unexpected Trinuclear Cu(II) Complex from s-Triazine-Based Di-Compartmental Ligand via Self-Assembly. <i>Crystals</i> , 2019, 9, 661.	1.0	1

#	ARTICLE	IF	CITATIONS
4151	Relativistic Effects on NMR Parameters of Halogen-Bonded Complexes. <i>Molecules</i> , 2019, 24, 4399.	1.7	11
4152	Synthesis and Structure of Methylsulfanyl Derivatives of Nickel Bis(Dicarbollide). <i>Molecules</i> , 2019, 24, 4449.	1.7	9
4153	Comparative Analysis of Hydrogen, van der Waals, and Halogen Bonds in Ammonia Complexes with HCl and ClF Molecules. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 2394-2406.	0.1	3
4154	Theoretical Investigation on the Structural and Spectroscopic Properties of σ -Crossed [Anthraquinone-Diamine/Diimine-Pt] Complexes. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 2570-2574.	0.1	0
4155	Mechanism of Catalytic Effect of Water Clusters on the Oxidation of Phosphine Gas. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 2373-2382.	0.1	1
4156	Molecular Doping of PCPDTBT Copolymers: Comparison of Molecular Complexes with and without Integer Charge Transfer. <i>Journal of Physical Chemistry C</i> , 2019, 123, 30863-30870.	1.5	14
4157	CLiAl_2E and CLi_2AlE (E = P, As, Sb, Bi): Planar Tetracoordinate Carbon Clusters with 16 and 14 Valence Electrons. <i>ACS Omega</i> , 2019, 4, 21311-21318.	1.6	8
4158	Reaction mechanisms of iron(III) catalyzed carbonyl-olefin metatheses in 2,5- and 3,5-hexadienals: significant substituent and aromaticity effects. <i>Organic Chemistry Frontiers</i> , 2019, 6, 3917-3924.	2.3	15
4159	Conformation Transition of Intracellular Part of Glucagon Receptor in Complex With Agonist Glucagon by Conventional and Accelerated Molecular Dynamics Simulations. <i>Frontiers in Chemistry</i> , 2019, 7, 851.	1.8	5
4160	A Comprehensive Topological Analysis of a Novel Flavonoid Extracted from Brazilian Cerrado Plants. <i>ChemistrySelect</i> , 2019, 4, 14012-14020.	0.7	3
4161	Toward High-Efficient Chiral Separation Using Hierarchically Porous HROP@Silica-Gel-Sheet Composite. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 48402-48411.	4.0	14
4162	Hyperconjugative aromaticity and protodeauration reactivity of polyaurated indoliums. <i>Nature Communications</i> , 2019, 10, 5639.	5.8	28
4163	Actinide Endohedral and Exohedral Cubic Siloxanes: $\text{An(IV)}@(\text{HSiO}_{1.5})_8$ and $\text{An(IV)}\&\text{(RSiO}_{1.5})_8$ (An = U, Np, Pu; R = H, Cl, OH). <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 4660-4667.	1.0	2
4164	The energy frameworks of aufbau synthon modules in 4-cyanopyridine co-crystals. <i>CrystEngComm</i> , 2019, 21, 7057-7068.	1.3	25
4165	Effect of the charge state on bare monoicosahedral $[\text{Au}_{13}]^{z+}$ and diphosphine-protected Au_{13} clusters $[\text{Au}_{13}(\text{dmpe})_5\text{Cl}_2]^{z+}$: structural, electronic and vibrational DFT studies. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23855-23864.	1.3	7
4166	Unexpectedly strong Xe binding by host-guest interaction. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 26232-26236.	1.3	5
4167	Direct synthesis of acetic acid from carbon dioxide and methane over Cu-modulated BEA, MFI, MOR and TON zeolites: a density functional theory study. <i>Catalysis Science and Technology</i> , 2019, 9, 6613-6626.	2.1	26
4168	Insight into the structure and bonding of copper(I) iodide clusters and a cluster-based coordination polymer. <i>New Journal of Chemistry</i> , 2019, 43, 16176-16187.	1.4	4

#	ARTICLE	IF	CITATIONS
4169	Ionic liquid-assisted catalysis for glycosidation of two triterpenoid sapogenins. <i>New Journal of Chemistry</i> , 2019, 43, 16881-16888.	1.4	6
4170	Predicting lanthanide boride inverse sandwich tubular molecular rotors with the smallest core-shell structure. <i>Nanoscale</i> , 2019, 11, 21311-21316.	2.8	19
4171	The directions of an external electric field control the catalysis of the hydroboration of C=C-O unsaturated compounds. <i>RSC Advances</i> , 2019, 9, 29331-29336.	1.7	4
4172	Theoretical study on the excited state decay properties of iron(II) polypyridine complexes substituted by bromine and chlorine. <i>RSC Advances</i> , 2019, 9, 31621-31627.	1.7	15
4173	Unraveling mechanisms of the uncoordinated nucleophiles: theoretical elucidations of the cleavage of bis(<i>p</i> -nitrophenyl) phosphate mediated by zinc-complexes with apical nucleophiles. <i>RSC Advances</i> , 2019, 9, 37696-37704.	1.7	2
4174	Retention of strong intramolecular hydrogen bonds in high polarity solvents in binaphthalene-benzamide derivatives: extensive NMR studies. <i>RSC Advances</i> , 2019, 9, 32759-32770.	1.7	8
4175	Aggregation-induced emission enhancement (AIEE)-active boron-difluoride dyes with reversible mechanochromic fluorescence. <i>RSC Advances</i> , 2019, 9, 35872-35877.	1.7	19
4176	Strategic tuning of excited-state properties of electroluminescent materials with enhanced hot exciton mixing. <i>RSC Advances</i> , 2019, 9, 33693-33709.	1.7	5
4177	Comparative investigation of interactions of hydrogen, halogen and tetrel bond donors with electron-rich and electron-deficient π -systems. <i>RSC Advances</i> , 2019, 9, 32811-32820.	1.7	22
4178	Theoretical study of substituent effects on electride characteristics and the nonlinear optical properties of Li@calix[4]pyrrole. <i>RSC Advances</i> , 2019, 9, 37919-37925.	1.7	5
4179	Predicting viable isomers of [X,C,N] and [H,X,C,N] (X = Sn, Pb). <i>RSC Advances</i> , 2019, 9, 40772-40780.	1.7	2
4180	Are there analogues of the indenyl effect in larger ring systems: a DFT study of hydride attack on [Mn(CO) ₃ (naphthalene)] ⁺ and [Cr(CO) ₃ (benzotropylium)] ⁺ . <i>Structural Chemistry</i> , 2019, 30, 107-114.	1.0	2
4181	Synthesis, photoluminescence and electroluminescence of triphenylphosphine functionalized cyclometalated iridium(III) complexes. <i>Dyes and Pigments</i> , 2019, 160, 717-725.	2.0	8
4182	Magnetic interaction in a 2D solid through hydrogen bonds and π - π stacking. <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 471, 70-76.	1.0	18
4183	Spectroscopic, antimicrobial and computational study of novel benzoxazole derivative. <i>Journal of Molecular Structure</i> , 2019, 1176, 881-894.	1.8	17
4184	Density functional theory study on the adsorption of alkali metal ions with pristine and defected graphene sheet. <i>Molecular Physics</i> , 2019, 117, 462-473.	0.8	22
4185	Theoretical studies on 4H-cyclopenta[2,1-b:3,4-b']dithiophene-based Windmill-shaped nanogrids with low reorganization energies. <i>Chemical Physics</i> , 2019, 516, 191-198.	0.9	7
4186	Effects of nitro- and amino-group on the antioxidant activity of genistein: A theoretical study. <i>Food Chemistry</i> , 2019, 275, 339-345.	4.2	49

#	ARTICLE	IF	CITATIONS
4187	Catalytic oxidation mechanisms of carbon monoxide over single and double vacancy Cr-embedded graphene. <i>Journal of Materials Science</i> , 2019, 54, 1395-1408.	1.7	11
4188	Structural diversity of metallacycle intermediates for ethylene dimerization on heterogeneous NiMCM-41 catalyst: a quantum chemical perspective. <i>Structural Chemistry</i> , 2019, 30, 137-150.	1.0	36
4189	Structures, stabilities and electronic properties of boron-doped silicon clusters B_3Si_n ($n=1-17$) and their anions. <i>Molecular Physics</i> , 2019, 117, 382-394.	0.8	9
4190	Enhancement of the excited-state intramolecular proton transfer process to produce all-powerful DSE molecules for bridging the gap between ACQ and AIE. <i>Dyes and Pigments</i> , 2019, 160, 839-847.	2.0	29
4191	$Ln-Pt$ electron polarization effects on the magnetic relaxation of heterometallic $Ho-Pt$ and $Er-Pt$ complexes. <i>Dalton Transactions</i> , 2019, 48, 7144-7149.	1.6	10
4192	Aminonitrone-iminohydroxamic acid tautomerism: Theoretical and spectroscopic study. <i>Journal of Molecular Structure</i> , 2019, 1176, 759-765.	1.8	7
4193	Electron-hole interactions in choline-phosphotungstic acid boosting molecular oxygen activation for fuel desulfurization. <i>Applied Catalysis B: Environmental</i> , 2019, 248, 573-586.	10.8	88
4194	Tetrachloromethane as halogen bond donor toward metal-bound halides. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2019, 234, 9-17.	0.4	24
4195	DFT study on the selective complexation of meso-2,3-dimercaptosuccinic acid with toxic metal ions (Cd^{2+} , Hg^{2+} and Pb^{2+}) for pharmaceutical and biological applications. <i>Journal of Molecular Structure</i> , 2019, 1176, 901-907.	1.8	36
4196	Hydrogen bond interactions of dopamine hydrochloride with urea. <i>Physics and Chemistry of Liquids</i> , 2019, 57, 746-754.	0.4	4
4197	Tris(3,5-dimethylpyrazolyl)methane copper(I) complexes featuring one disubstituted cyanamide ligand. <i>Inorganica Chimica Acta</i> , 2019, 484, 69-74.	1.2	9
4198	Noble Gas-Tungsten Peroxide Complexes in Noble Gas Matrixes: Infrared Spectroscopy and Density Functional Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 556-564.	1.1	3
4199	Molecular Origins of the Nonlinear Optical Responses of a Series of \hat{I}^\pm -(X-2-Pyridylamino)-cresol Chromophores from Concerted X-ray Diffraction, Hyper-Rayleigh Scattering, and $Ab Initio$ Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 665-676.	1.5	7
4200	Theoretical/experimental investigation and antimutagenic effect of the oxidovanadium(IV) baicalin coordination complex. <i>Inorganica Chimica Acta</i> , 2019, 487, 369-378.	1.2	8
4201	$Ab initio$ calculations of the NO_2 fission for CL-20 conformers. <i>Journal of Energetic Materials</i> , 2019, 37, 154-161.	1.0	5
4202	Mechanistic insight into \hat{I}^2O^4 linkage cleavage of lignin model compound catalyzed by a SO_3H -functionalized imidazolium ionic liquid: An unconventional $E1$ elimination. <i>Molecular Catalysis</i> , 2019, 463, 140-149.	1.0	8
4203	Understanding the Nature of Transition States in the Confined Nanospace of Different Acidic Zeolites on the Desulfurization Mechanism of Thiophene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1260-1278.	1.5	5
4204	Substitution Effect on the Charge Transfer Processes in Organo-Imido Lindqvist-Polyoxomolybdate. <i>Molecules</i> , 2019, 24, 44.	1.7	3

#	ARTICLE	IF	CITATIONS
4205	Standard enthalpies of formation of dicyclopropyldinitromethane and tricyclopropylmethane. <i>Journal of Chemical Thermodynamics</i> , 2019, 132, 316-321.	1.0	6
4206	M@C ₅₀ as Higher Intermediates towards Large Endohedral Metallofullerenes: Theoretical Characterization, Aromatic and Bonding Properties from Relativistic DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1429-1443.	1.5	15
4207	Study of the reaction mechanism of aluminum based composite fuel and chlorine trifluoride oxide. <i>Energy</i> , 2019, 168, 393-399.	4.5	6
4208	A combined experimental and theoretical study on gas adsorption performance of amine and amide porous polymers. <i>Microporous and Mesoporous Materials</i> , 2019, 279, 61-72.	2.2	15
4209	Spectroscopic and electronic structure characterization of hydrogen bonding in 2-Bromohydroquinone. <i>Journal of Molecular Structure</i> , 2019, 1181, 71-82.	1.8	8
4210	Effects of Noncovalent Interactions on the Impact Sensitivity of HNS-Based Cocrystals: A DFT Study. <i>Crystal Growth and Design</i> , 2019, 19, 756-767.	1.4	30
4211	Rational selection of the monomer for molecularly imprinted polymer preparation for selective and sensitive detection of 3-methylindole in water. <i>Journal of Electroanalytical Chemistry</i> , 2019, 832, 129-136.	1.9	18
4212	Synthesis, physicochemical and quantum chemical studies on a new organic NLO crystal: Cinnamoylproline. <i>Journal of Molecular Structure</i> , 2019, 1180, 826-838.	1.8	12
4213	Substituted Aromatic-Facilitated Dissemination of Mobile Antibiotic Resistance Genes via an Antihydrolysis Mechanism Across an Extracellular Polymeric Substance Permeable Barrier. <i>Environmental Science & Technology</i> , 2019, 53, 604-613.	4.6	18
4214	Theoretical design of bistetrazole diolate derivatives as novel non-nitro energetic salts with low sensitivity. <i>Structural Chemistry</i> , 2019, 30, 1015-1022.	1.0	7
4215	Intramolecular and intermolecular bifurcated hydrogen bonds in 2-(pyrrolyl-7-yl)hydroxy-2-methylidene-3,3-dihydro-1 <i>H</i> -indena-1-one. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3924.	0.9	5
4216	C-H...O hydrogen bonding interactions for sterically hindered phenols and their phenoxyl radicals. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3927.	0.9	5
4217	Mechanistic insights into the efficient intramolecular chemiexcitation of dioxetanones from TDFT and multireference calculations. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25881.	1.0	14
4218	Shedding light on the electronic structure of [Ru(η -6-C ₁₆ H ₁₆)(NH ₃) ₃] ²⁺ complex: a computational insight. <i>Journal of Molecular Modeling</i> , 2019, 25, 11.	0.8	5
4219	Electrochemiluminescence sensor based on upconversion nanoparticles and oligoaniline-crosslinked gold nanoparticles imprinting recognition sites for the determination of dopamine. <i>Biosensors and Bioelectronics</i> , 2019, 128, 129-136.	5.3	58
4220	The interaction between chitosan and tannic acid calculated based on the density functional theory. <i>Chemical Physics</i> , 2019, 520, 100-107.	0.9	56
4221	On the negative cooperativity of argon clusters containing one lithium cation or fluorine anion. <i>Chemical Physics Letters</i> , 2019, 716, 192-198.	1.2	25
4222	Nickel-catalyzed carboxylation of aryl zinc reagent with CO ₂ : A theoretical and experimental study. <i>Journal of CO₂ Utilization</i> , 2019, 29, 262-270.	3.3	3

#	ARTICLE	IF	CITATIONS
4223	Design, two-directional synthesis, DFT study of new pyrimido[5,4-d]pyrimidine-2,8-dione derivatives. <i>Tetrahedron</i> , 2019, 75, 749-756.	1.0	7
4224	Interaction between Acetic Acid and Glycerol: A Model for Secondary Reactions during Holocellulose Pyrolysis. <i>Journal of Physical Chemistry A</i> , 2019, 123, 674-681.	1.1	12
4225	Nature of Defect States within Amorphous NPB Investigated through Drive-Level Capacitance Profiling. <i>Journal of Physical Chemistry C</i> , 2019, 123, 165-174.	1.5	8
4226	Modulation of Electron-Donating Ability in D ^π A Small Molecules for Application in Organic Solar Cells. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1069-1081.	1.5	16
4227	Conformational Preferences of Isolated Glycylglycine (Gly-Gly) Investigated with IRMPD-VUV Action Spectroscopy and Advanced Computational Approaches. <i>Journal of Physical Chemistry A</i> , 2019, 123, 862-872.	1.1	10
4228	Placing Metal in the Bowl: Does Rim Alkylation Matter?. <i>Organometallics</i> , 2019, 38, 552-566.	1.1	11
4229	Investigating the Effect of NO on the Capture of CO ₂ Using Superbase Ionic Liquids for Flue Gas Applications. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 3567-3574.	3.2	29
4230	All-Optical Poling and Two-Photon Absorption in Heterocyclic Azo Dyes with Different Side Groups. <i>Journal of Physical Chemistry C</i> , 2019, 123, 725-734.	1.5	37
4231	Evaluating Computational and Structural Approaches to Predict Transformation Products of Polycyclic Aromatic Hydrocarbons. <i>Environmental Science & Technology</i> , 2019, 53, 1595-1607.	4.6	15
4232	Strong Fluorescent Lanthanide Salen Complexes: Photophysical Properties, Excited-State Dynamics, and Bioimaging. <i>Inorganic Chemistry</i> , 2019, 58, 1806-1814.	1.9	39
4233	Backbone Conformation Tuning of Carboxylate-Functionalized Wide Band Gap Polymers for Efficient Non-Fullerene Organic Solar Cells. <i>Macromolecules</i> , 2019, 52, 341-353.	2.2	37
4234	Substituent effects on the photophysical properties of amino-aurone-derivatives. <i>Molecular Physics</i> , 2019, 117, 1451-1458.	0.8	6
4235	Mechanisms and regioselectivities of DABCO/DMAP-catalyzed [2+4] annulation reactions of allenolate with β,γ -unsaturated cyclic ketimine: A DFT study. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3914.	0.9	5
4236	Insights into the non-covalent interaction between modified nucleobases and graphene nanoflake from first-principles. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 107, 73-79.	1.3	19
4237	Efficient remediation of 2,4-dichlorophenol from aqueous solution using β -cyclodextrin-based submicron polymeric particles. <i>Chemical Engineering Journal</i> , 2019, 360, 531-541.	6.6	30
4238	A combination of FTIR and DFT methods to study the structure and interaction properties of TSILs and DMSO mixtures. <i>Journal of Chemical Thermodynamics</i> , 2019, 131, 441-448.	1.0	13
4239	Theoretical investigation on the low-energy isomer identification, structural evolution, stability, and electronic properties of Al ₁₀ -Be ($x = 1-9$) nanoalloys. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 87, 56-67.	1.3	0
4240	Deciphering the nature of interactions in nandrolone/testosterone encapsulated cucurbituril complexes: a computational study. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2019, 93, 183-192.	0.9	3

#	ARTICLE	IF	CITATIONS
4241	Theoretical insights into the excited state process of 4-tert-butyl-5-(tert-butylmethoxyphenyl)thiazolo[5,4-d]thiazole-2-yl)phenol. Journal of the Chinese Chemical Society, 2019, 66, 385-390.		8
4242	Solvent dependent linear and nonlinear optical properties of triphenylamine unit incorporated difluoroboron β -diketonate complexes. Dyes and Pigments, 2019, 162, 776-785.	2.0	26
4243	Imidazolium-based ionic liquids with inorganic anions in the extraction of salidroside and tyrosol from Rhodiola: The role of cations and anions on the extraction mechanism. Journal of Molecular Liquids, 2019, 275, 136-145.	2.3	23
4244	The nature of photoinduced intermolecular charge transfer in fluorescence resonance energy transfer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 209, 228-233.	2.0	19
4245	Cu ₂ O modified g-C ₃ N ₄ as an effective catalyst for the synthesis of propargylamines: experimental, quantum mechanical mechanistic and kinetic study. Reaction Kinetics, Mechanisms and Catalysis, 2019, 126, 265-282.	0.8	11
4246	Experimental enthalpies of formation and sublimation of urea compounds: An accuracy assessment. Journal of Chemical Thermodynamics, 2019, 131, 254-261.	1.0	9
4247	Crystallographic, spectroscopic and theoretical investigations on Ni(II) complexes of a tridentate NNS donor thiosemicarbazone. Polyhedron, 2019, 158, 398-407.	1.0	14
4248	Are solvent effects important for intramolecular C-H...O hydrogen bonding interactions?. Journal of Physical Organic Chemistry, 2019, 32, e3912.	0.9	2
4249	Study of the Geometric Structures, Electronic and Magnetic Properties of Aluminium-Antimony Alloy Clusters. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2019, 74, 109-120.	0.7	1
4250	How to screen a promising anchoring group from heterocyclic components in dye sensitized solar cell: A theoretical investigation. Electrochimica Acta, 2019, 296, 545-554.	2.6	10
4251	A combination of FTIR and DFT to study the structure and interaction properties of TSILs and water mixture. Journal of Molecular Liquids, 2019, 275, 49-56.	2.3	11
4252	Partially Covalent Two-Electron/Multicentric Bonding between Semiquinone Radicals. Crystal Growth and Design, 2019, 19, 391-402.	1.4	29
4253	Inclusion complexes of β -cyclodextrin and polymorphs of mebendazole: Physicochemical characterization. European Journal of Pharmaceutical Sciences, 2019, 127, 330-338.	1.9	13
4254	Hydrogen Bond Interaction of Ascorbic Acid with Urea: Experimental and Theoretical Study. Zeitschrift Fur Physikalische Chemie, 2019, 233, 1061-1072.	1.4	8
4255	Combined spectroscopic, molecular docking and quantum mechanics study of β -casein and ferulic acid interactions following UHT-like treatment. Food Hydrocolloids, 2019, 89, 351-359.	5.6	50
4256	Thermal Stability of Polymer Additives: Comparison of Decomposition Models Including Oxidative Pyrolysis. Journal of Vinyl and Additive Technology, 2019, 25, E12.	1.8	10
4257	Nonlinear optical properties of donor-acceptor dyads formed between phthalocyanine and fullerene. Journal of Computational Methods in Sciences and Engineering, 2019, 19, 427-439.	0.1	1
4258	Molecular docking studies, charge transfer excitation and wave function analyses (ESP, ELF, LOL) on valacyclovir : A potential antiviral drug. Computational Biology and Chemistry, 2019, 78, 9-17.	1.1	159

#	ARTICLE	IF	CITATIONS
4259	Enthalpies of formation of diamantanes in the gas and crystalline phase: comparison of theory and experiment. <i>Structural Chemistry</i> , 2019, 30, 615-621.	1.0	3
4260	Construct 3D Pd@MoS ₂ -conjugated polypyrrole frameworks Heterojunction with unprecedented photocatalytic activity for Tsuji-Trost reaction under visible light. <i>Applied Catalysis B: Environmental</i> , 2019, 244, 356-366.	10.8	20
4261	Unusual self-assembly of chloroaluminium phthalocyanine on graphite. <i>Surface Science</i> , 2019, 681, 104-110.	0.8	3
4262	Exceptionally Long C-C Single Bonds in Diamino-carborane as Induced by Negative Hyperconjugation. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1397-1401.	7.2	62
4263	Comparative study of the chemiluminescence of coelenterazine, coelenterazine-e and Cypridina luciferin with an experimental and theoretical approach. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2019, 190, 21-31.	1.7	23
4264	Syntheses, crystal structures and photo physical aspects of azido-bridged tetranuclear cadmium (II) complexes: DFT/TD-DFT, thermal, antibacterial and anti-biofilm properties. <i>Journal of Molecular Structure</i> , 2019, 1179, 694-708.	1.8	27
4265	Impact of electronically excited state hydrogen bonding on luminescent covalent organic framework: a TD-DFT investigation. <i>Molecular Physics</i> , 2019, 117, 823-830.	0.8	7
4266	A Density Functional Theory Study on Nonlinear Optical Properties of Double Cage Excess Electron Compounds: Theoretically Design M[Cu(Ag)@ (NH ₃) _n] (M = Be, Mg and Ca; n = 1-3). <i>Journal of Computational Chemistry</i> , 2019, 40, 971-979.		18
4267	Computational study of new 1,2,3-triazole derivative of lithocholic acid: Structural aspects, non-linear optical properties and molecular docking studies as potential PTP 1B enzyme inhibitor. <i>Computational Biology and Chemistry</i> , 2019, 78, 144-152.	1.1	4
4268	Understanding Solid-State Solvation-Enhanced Thermally Activated Delayed Fluorescence Using a Descriptor-Tuned Screened Range-Separated Functional. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4407-4416.	1.5	36
4269	Hydralazine derivative of aldehyde: A new type of [M ⁺ ·H] ⁺ ion formed in electrospray ionization mass spectrometry. <i>Journal of Mass Spectrometry</i> , 2019, 54, 239-249.	0.7	2
4270	Lin@Tetracyanoethylene (n ⁻ =1-4) systems: Lithium salt vs lithium electride. <i>Computational and Theoretical Chemistry</i> , 2019, 1149, 17-23.	1.1	7
4271	Synthesis, photophysical properties and DFT studies of the pyridine-imidazole (Pylm) Cu(I) complexes: Impact of the pyridine ring functionalized by different substituents. <i>Inorganica Chimica Acta</i> , 2019, 488, 34-40.	1.2	9
4272	Synthesis and structure diversity of high coordination number Cd(II) complexes of large s-triazine bis-Schiff base pincer chelate. <i>Inorganica Chimica Acta</i> , 2019, 488, 131-140.	1.2	15
4273	Experimental X-ray Electron Density Study of Atomic Charges, Oxidation States, and Inverted Ligand Field in Cu(CF ₃) ₃ (CF ₃) ₄ ⁺ . <i>Inorganic Chemistry</i> , 2019, 58, 2133-2139.	1.9	28
4274	Theoretical and conceptual DFT study of pnictogen- and halogen-bonded complexes of PH ₂ X-BrCl. <i>Journal of Molecular Modeling</i> , 2019, 25, 28.	0.8	16
4275	Achieving excellent electro-optic activity of chromophores by introducing a stronger electron donor and modifying the π-bridge. <i>Dyes and Pigments</i> , 2019, 163, 740-748.	2.0	11
4276	Heterobimetallic Uranium-Nickel/Palladium/Platinum Complexes of Phosphinoaryl Oxide Ligands: A Theoretical Probe for Metal-Metal Bonding and Electronic Spectroscopy. <i>Inorganic Chemistry</i> , 2019, 58, 1290-1300.	1.9	13

#	ARTICLE	IF	CITATIONS
4277	Effect of reduced sulfur group on the formation of CX3R-type disinfection by-products during chlor(am)ination of reduced sulfur compounds. <i>Chemical Engineering Journal</i> , 2019, 361, 227-234.	6.6	10
4278	Tuning the physicochemical properties of the single-walled boron nitride nanotube by covalent grafting of triazolium-based [MTZ][X ⁺ 3] (X ⁺ 3= NTf ₂ ⁻ , TfO ⁻ and BF ₄ ⁻) ionic liquids in the gas phase and solvent media: A quantum chemical approach. <i>Journal of Molecular Liquids</i> , 2019, 277, 726-737.	2.3	2
4279	Geometric Structures and Electronic Properties of Al _n VO ⁺ (n = 5-14) Clusters: Photoelectron Spectroscopy and Theoretical Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1931-1938.	1.5	12
4280	Synthesis and Properties of Novel Fluorescence Probe Based on 1,8-Naphthalimide for Detection of Hydrogen Sulfide. <i>Chemical Research in Chinese Universities</i> , 2019, 35, 5-11.	1.3	13
4281	Molecular-level insights into furfural hydrogenation intermediates over single-atomic Cu catalysts on magnesia and silica nanoclusters. <i>Molecular Simulation</i> , 2019, 45, 154-163.	0.9	30
4282	Reducible Inverse CeO _x -Based Catalyst as a Potential Candidate for Electroreduction. <i>Catalysts</i> , 2019, 9, 22.	1.6	4
4283	Theoretical study of the reactions between arsenic and nitrogen oxides during coal combustion. <i>Journal of Molecular Modeling</i> , 2019, 25, 30.	0.8	4
4284	DFT/TD-DFT study of novel T shaped phenothiazine-based organic dyes for dye-sensitized solar cells applications. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 212, 272-280.	2.0	51
4285	Improved Transistor Performance by Modulating Molecular Packing with Donor and Acceptor Moieties. <i>Chemistry - an Asian Journal</i> , 2019, 14, 1686-1691.	1.7	6
4286	Computational study of structural, vibrational and electronic properties of the highly symmetric molecules M ₄ S ₆ (M ⁻ =P, As, Sb, Bi). <i>Computational and Theoretical Chemistry</i> , 2019, 1149, 41-48.	1.1	1
4287	Capturing methanol and dimethoxymethane gases with ionic liquids. <i>Fuel</i> , 2019, 241, 704-714.	3.4	19
4288	Size Effect on Au _n Cl _{n+1} ⁺ (2 ≤ n ≤ 7). <i>ACS Omega</i> , 2019, 4, 650-654.	1.6	9
4289	Enhanced light-harvesting of benzodithiophene conjugated porphyrin electron donors in organic solar cells. <i>Journal of Materials Chemistry C</i> , 2019, 7, 380-386.	2.7	11
4290	Rational Design of Organic Probes for Turn-On Two-Photon Excited Fluorescence Imaging and Photodynamic Therapy. <i>CheM</i> , 2019, 5, 600-616.	5.8	48
4291	Theoretical evaluation of microscopic structural and macroscopic thermo-physical properties of molten AF-ThF ₄ systems (A ⁺ =Li ⁺ , Na ⁺ and K ⁺). <i>Journal of Molecular Liquids</i> , 2019, 277, 409-417.	2.3	16
4292	Cycloartane triterpenoids from <i>Actaea vaginata</i> with anti-inflammatory effects in LPS-stimulated RAW264.7 macrophages. <i>Phytochemistry</i> , 2019, 160, 1-10.	1.4	30
4293	The nature of chirality induced by molecular aggregation and self-assembly. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 212, 188-198.	2.0	26
4294	Synthesis, Structure, Electrochemical, and Spectroscopic Properties of Hetero-Bimetallic Ru(II)/Fe(II)-Alkynyl Organometallic Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 1155-1166.	1.9	21

#	ARTICLE	IF	CITATIONS
4295	Functionalization of Endohedral Metallofullerenes toward Improving Barrier Height for the Relaxation of Magnetization for Dy ₂ @C ₈₀ -X (X = CF ₃), Tj ETQq0 0 0 rgBT / Overlock 10 Tf 50 73	1.7	35
4296	Atomic Charges in Describing Properties of Aromatic Molecules. <i>Journal of Organic Chemistry</i> , 2019, 84, 1908-1915.	1.7	35
4297	Chemical Kinetics of H-Atom Abstraction from Ethanol by HÈ [•] : Implication for Combustion Modeling. <i>Journal of Physical Chemistry A</i> , 2019, 123, 971-982.	1.1	20
4298	O ₂ Activation and Oxidative Dehydrogenation of Propane on Hexagonal Boron Nitride: Mechanism Revisited. <i>Journal of Physical Chemistry C</i> , 2019, 123, 2256-2266.	1.5	42
4299	Thermodynamic Properties of Hydrogen-Producing Cobaloxime Catalysts: A Density Functional Theory Analysis. <i>ACS Omega</i> , 2019, 4, 582-592.	1.6	9
4300	Crystallization-Induced Red Phosphorescence and Grinding-Induced Blue-Shifted Emission of a Benzobis(1,2,5-thiadiazole)â€“Thiophene Conjugate. <i>ACS Omega</i> , 2019, 4, 344-351.	1.6	39
4301	Significance of hydrogen bonding and other noncovalent interactions in determining octahedral tilting in the CH ₃ NH ₃ PbI ₃ hybrid organic-inorganic halide perovskite solar cell semiconductor. <i>Scientific Reports</i> , 2019, 9, 50.	1.6	95
4302	Infrared Spectra of the HAnX and H ₂ AnX ₂ Molecules (An=Th and U, X=Cl and Tj ETQq1 1 0.784314 rgBT / Overlock 10 Tf 50 73 <i>Journal</i> , 2019, 25, 1795-1805.	1.7	3
4303	Assembly of Tetrazolylfuroxan Organic Salts: Multipurpose Green Energetic Materials with High Enthalpies of Formation and Excellent Detonation Performance. <i>Chemistry - A European Journal</i> , 2019, 25, 4225-4233.	1.7	60
4304	Enhanced nonlinear optical properties of porphyrin with an extended Ï€-conjugated bridge. <i>Structural Chemistry</i> , 2019, 30, 1211-1219.	1.0	8
4305	Biochar-induced Fe(III) reduction for persulfate activation in sulfamethoxazole degradation: Insight into the electron transfer, radical oxidation and degradation pathways. <i>Chemical Engineering Journal</i> , 2019, 362, 561-569.	6.6	220
4306	The role of the polarity on the mechanism and selectivity in the [3+2] cycloaddition reaction between CF ₃ -ynone ylide and azide group: A quantum chemical investigation. <i>Journal of Fluorine Chemistry</i> , 2019, 219, 79-91.	0.9	9
4307	Fluoroborylene Complexes FBMF ₂ (M = Sc, Y, La, Ce): Matrix Infrared Spectra and Quantum Chemical Calculations. <i>Inorganic Chemistry</i> , 2019, 58, 2363-2371.	1.9	6
4308	Sustainable Metallocavitand for Flue Gas-Selective Sorption: A Multiscale Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 3188-3202.	1.5	5
4309	Citrinin Monomer and Dimer Derivatives with Antibacterial and Cytotoxic Activities Isolated from the Deep Sea-Derived Fungus <i>Penicillium citrinum</i> NLG-S01-P1. <i>Marine Drugs</i> , 2019, 17, 46.	2.2	36
4310	A detecting Al ³⁺ ion luminophor 2-(Anthracen-1-yliminomethyl)-phenol: Theoretical investigation on the fluorescence properties and ESIPT mechanism. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 208, 309-314.	2.0	22
4311	Adsorption sensitivity of pristine and Al- or Si-doped boron nitride nanoflake to COCl ₂ : a DFT study. <i>Molecular Physics</i> , 2019, 117, 626-634.	0.8	13
4312	Theoretical insights on the rigidified dithiophene effects on the performance of near-infrared cis-squaraine-based dye-sensitized solar cells with panchromatic absorption. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 369, 150-158.	2.0	13

#	ARTICLE	IF	CITATIONS
4313	Interactions of promazine with selected biomolecules: Photophysical and computational investigation. <i>Chemical Physics</i> , 2019, 517, 161-176.	0.9	5
4314	Photo-transformation of atrazine in aqueous solution in the presence of Fe ³⁺ -montmorillonite clay and humic substances. <i>Science of the Total Environment</i> , 2019, 652, 224-233.	3.9	17
4315	Water soluble Eu(III) complexes of macrocyclic triamide ligands: Structure, stability, luminescence and redox properties. <i>Inorganica Chimica Acta</i> , 2019, 486, 252-260.	1.2	11
4316	Me ₃ SiBr/InCl ₃ catalyzed allylation of alcohols: Identifying the combined Lewis structure and investigating the reaction mechanism. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3902.	0.9	5
4317	GPUs as boosters to analyze scalar and vector fields in quantum chemistry. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25671.	1.0	28
4318	An insight into intramolecular blue-shifting C-H... hydrogen bonds in 1,3-hexadien-5-yne and its halogen-substituted derivatives. <i>Chemical Physics</i> , 2019, 518, 58-68.	0.9	7
4319	A theoretical investigation on the selective extraction of Cu(II) from Ni(II) by 2-aminomethylpyridine derivatives: A DFT study. <i>Polyhedron</i> , 2019, 157, 200-207.	1.0	6
4320	Computational prediction on photophysical properties of two excited state intramolecular proton transfer (ESIPT) fluorophores bearing the benzothiazole group. <i>Molecular Physics</i> , 2019, 117, 804-812.	0.8	14
4321	Effect of intermolecular interaction on excited-state properties of thermally activated delayed fluorescence molecules in solid phase: A QM/MM study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 209, 248-255.	2.0	12
4322	Experimental and theoretical study on the interactions between dopamine hydrochloride and nicotinamide. <i>Journal of Molecular Structure</i> , 2019, 1178, 599-605.	1.8	3
4323	Triicosahedral Au ₃₇ cluster as a carrier/detector for anti-cancer cisplatin drug. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 52-62.	1.2	9
4324	Synthesis, Elucidation, Hirshfeld surface analysis, and DFT calculations of 4-chloro-N-[2-(2-1H-indol-3-yl-acetyl-amino)-phenyl]-benzamide. <i>Journal of Molecular Structure</i> , 2019, 1178, 384-393.	1.8	25
4325	Deep-blue thermally activated delayed fluorescence materials with high glass transition temperature. <i>Journal of Luminescence</i> , 2019, 206, 146-153.	1.5	9
4326	Cd(II) enhanced fluorescence and Zn(II) quenched fluorescence with phenylenevinylene terpyridine: A theoretical investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 209, 40-48.	2.0	11
4327	The theoretical study about the ESIPT mechanism for 2,4-bis(benzooxazol-2-yl)hydroquinone: Single or double?. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3903.	0.9	7
4328	Effect of the external electric field on the electronic structure, spectroscopic features, NLO properties, and interionic interactions in ionic liquids: A DFT approach. <i>Journal of Molecular Liquids</i> , 2019, 273, 314-325.	2.3	23
4329	Design and synthesis of stable cuprous complexes bearing P ⁺ N-type ligands for vapor-deposited organic light-emitting device. <i>Organic Electronics</i> , 2019, 64, 158-165.	1.4	14
4330	Under different solvents excited-state intramolecular proton transfer mechanism and solvatochromic effect of 2-(2-hydroxyphenyl) benzothiazole molecule. <i>Journal of Luminescence</i> , 2019, 206, 326-334.	1.5	48

#	ARTICLE	IF	CITATIONS
4331	DFT study of adenine–cytosine mismatch in quaternary systems involving DNA bases. <i>Structural Chemistry</i> , 2019, 30, 1023-1031.	1.0	3
4332	Aluminum cluster for CO and O ₂ adsorption. <i>Journal of Molecular Modeling</i> , 2019, 25, 2.	0.8	6
4333	Halogen bonds and metal bonds involving superalkalies M ₂ OCN/M ₂ NCO (M = Li, Na) complexes. <i>Structural Chemistry</i> , 2019, 30, 965-977.	1.0	13
4334	Influence of substituents on the reduction potential and pK _a values of 1,2-diketones tautomers: A theoretical study. <i>Electrochimica Acta</i> , 2019, 297, 947-960.	2.6	19
4335	Understanding the role of noncovalent interactions on the rate of some Diels–Alder reactions in different solvents. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25878.	1.0	7
4336	Mechanical Insights into Aggregation-Induced Delayed Fluorescence Materials with Anti-Kasha Behavior. <i>Advanced Science</i> , 2019, 6, 1801629.	5.6	111
4337	Multiple Ether-Functionalized Phosphonium Ionic Liquids as Highly Fluid Electrolytes. <i>ChemPhysChem</i> , 2019, 20, 443-455.	1.0	22
4338	Reductive transformation of nitroaromatic compounds by Pd nanoparticles on nitrogen-doped carbon (Pd@NC) biosynthesized using <i>Pantoea</i> sp. IMH. <i>Journal of Hazardous Materials</i> , 2019, 366, 338-345.	6.5	21
4339	Odd-even effect of the number of free valence electrons on the electronic structure properties of gold-thiolate clusters. <i>Molecular Physics</i> , 2019, 117, 1442-1450.	0.8	5
4340	Theoretical study of the mechanism of the manganese catalase KatB. <i>Journal of Biological Inorganic Chemistry</i> , 2019, 24, 103-115.	1.1	4
4341	Origin and evolution of the initial hydrocarbon pool intermediates in the transition period for the conversion of methanol to olefins over H-ZSM-5 zeolite. <i>Journal of Catalysis</i> , 2019, 369, 382-395.	3.1	72
4342	Dinuclear Cu ^I and Ag ^I Pyrazolates Supported with Tertiary Phosphines: Synthesis, Structures, and Photophysical Properties. <i>European Journal of Inorganic Chemistry</i> , 2019, 821-827.	1.0	20
4343	Accessibility of Uranyl–Plutonium Complex Supported by a Polypyrrrolic Macrocyclic: An Implication for Experimental Synthesis. <i>Inorganic Chemistry</i> , 2019, 58, 950-959.	1.9	5
4344	Metal-Involving Bifurcated Halogen Bonding Câ–Br–Â–Î ² (Cl–Pt). <i>Crystal Growth and Design</i> , 2019, 19, 1364-1376.	1.4	51
4345	Lanthanides with Unusually Low Oxidation States in the PrB ₃ and PrB ₄ Boride Clusters. <i>Inorganic Chemistry</i> , 2019, 58, 411-418.	1.9	39
4346	Not All Bis[2-(4,6-difluorophenyl)pyridyl- <i>N</i> , <i>C</i>]-iridium(III) Picolinate (Flrpic) Isomers Are Unsuitable for Developing Long-Lifetime Blue Phosphorescent Organic Light-Emitting Diodes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 227-232.	1.5	6
4347	Structure and Interaction of Ionic Liquid Monolayer on Graphite from First-Principles. <i>Journal of Physical Chemistry C</i> , 2019, 123, 618-624.	1.5	8
4348	Hydrogen bonding networks in gabapentin protic pharmaceutical salts: NMR and in silico studies. <i>Magnetic Resonance in Chemistry</i> , 2019, 57, 243-255.	1.1	2

#	ARTICLE	IF	CITATIONS
4349	Enhanced Zintl anions by carbon doping in Al ₆ Na clusters and new magic structure Al ₆ Na ₄ C. International Journal of Quantum Chemistry, 2019, 119, e25871.	1.0	2
4350	Effect of fluorination on bandgap, first and second order hyperpolarizabilities in lithium substituted adamantane: A time dependent density functional theory. Chemical Physics Letters, 2019, 715, 310-316.	1.2	11
4351	Unraveling the sequence of the electronic flow along the water-assisted ring-opening reaction in mutagen MX. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	5
4352	Single-point Attack of Two H ₂ O Molecules towards a Lewis Acid Site on the GaAl ₁₂ Clusters for Hydrogen Evolution. ChemPhysChem, 2019, 20, 499-505.	1.0	22
4353	Theoretical investigation of the gas-phase reaction of NiO ⁺ with ethane. Structural Chemistry, 2019, 30, 937-944.	1.0	0
4354	Theoretical study on the atmospheric reaction of CH ₃ SH with O ₂ . International Journal of Quantum Chemistry, 2019, 119, e25822.	1.0	6
4355	Intermolecular hydrogen bonding H ⁺ ⋯Cl in crystal structure of palladium(II)-bis(diaminocarbene) complex. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 155-164.	0.4	8
4356	Synthesis, crystal structure, DFT calculations and molecular docking of l-pyroglutamic acid. Journal of Molecular Structure, 2019, 1178, 436-449.	1.8	31
4357	Comparison of radical scavenging behavior of chromones dihydrogenistein and demethyltaxasin ^a a DFT approach. Structural Chemistry, 2019, 30, 167-173.	1.0	2
4358	Ab initio investigation of possible lower-energy candidate structure for cationic water cluster (H ₂ O) ₁₂₊ via particle swarm optimization method. Structural Chemistry, 2019, 30, 151-165.	1.0	3
4359	Drug-DNA interaction, a joint DFT-D3/MD study on safranal as an anticancer and DNA nanostructure model. Canadian Journal of Chemistry, 2019, 97, 120-130.	0.6	5
4360	Robust metal-pentagon interactions in the Th ⁺ -based endohedral metallofullerenes revealed by DFT calculations. International Journal of Quantum Chemistry, 2019, 119, e25826.	1.0	8
4361	Directional affinity of a spherical Gold nanoparticle for the adsorption of DNA bases. Colloids and Surfaces B: Biointerfaces, 2019, 173, 493-503.	2.5	7
4362	Theoretical insights into co-sensitization mechanism in Zn-porphyrin and Y123 co-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 369, 25-33.	2.0	16
4363	Antioxidant and spectral properties of chalcones and analogous aurones: Theoretical insights. International Journal of Quantum Chemistry, 2019, 119, e25808.	1.0	25
4364	Dependence of characteristic interlayer vibration modes on interlayer spin arrangement in stacked graphene nanofragments. Carbon, 2019, 141, 339-347.	5.4	2
4365	Tuning the electronic and optical properties of graphene quantum dots by selective boronization. Journal of Materials Chemistry C, 2019, 7, 237-246.	2.7	54
4366	Modulation of photophysical properties of copper(I) complexes containing pyridyl-imidazole (Pylm) ligands functionalized by naphthyl, phenanthryl, and anthryl groups. Inorganica Chimica Acta, 2019, 484, 237-244.	1.2	12

#	ARTICLE	IF	CITATIONS
4367	Non-covalent interactions observed in nevirapinium pentaiodide hydrate which include the rare I ₄ ⋯I ⁺ ⋯I⋯O=C halogen bonding. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2019, 234, 101-108.	0.4	5
4368	Stability, Electronic and Magnetic Properties of Mn-Doped Copper Clusters: A Meta-GGA Functional Investigation. <i>Journal of Cluster Science</i> , 2019, 30, 31-44.	1.7	11
4369	Interactions of B ₁₂ N ₁₂ fullerenes on graphene and boron nitride nanosheets: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 86, 27-34.	1.3	62
4370	Solvatochromism and azo-hydrazo tautomerism of novel arylazo pyridone dyes: Experimental and quantum chemical study. <i>Arabian Journal of Chemistry</i> , 2019, 12, 3463-3478.	2.3	4
4371	The influence of 5-fluorouracil anticancer drug on the DNA base pairs; a quantum chemical study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 1-19.	2.0	16
4372	New substituted aminopyrimidine derivatives as BACE1 inhibitors: in silico design, synthesis and biological assays. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 229-246.	2.0	7
4373	Experimental and Theoretical Study on the Interaction of P-Aminophenol Hydrochloride with H ₂ O. <i>Zeitschrift Fur Physikalische Chemie</i> , 2019, 233, 303-313.	1.4	2
4374	Exploring enhanced hydrogen adsorption on Ti doped Al nanoclusters: A DFT study. <i>Chemical Physics</i> , 2019, 518, 123-133.	0.9	9
4375	A detailed experimental and computational study of monocarbohydrazones. <i>Arabian Journal of Chemistry</i> , 2020, 13, 932-953.	2.3	6
4376	Quinoline derivatives as possible lead compounds for anti-malarial drugs: Spectroscopic, DFT and MD study. <i>Arabian Journal of Chemistry</i> , 2020, 13, 632-648.	2.3	97
4377	Baецкеins L and M, two novel C-methylated triflavonoids from the roots of <i>Baецkea frutescens</i> L.. <i>Natural Product Research</i> , 2020, 34, 278-283.	1.0	1
4378	Removal of bisphenol A using Mg-Al-layer double hydroxide and Mg-Al calined layer double hydroxide. <i>Separation Science and Technology</i> , 2020, 55, 501-512.	1.3	9
4379	The influence of CH⋯I interaction on coupling constants across N⋯H⋯F hydrogen bond in a substituted T-shaped configuration: a theoretical study. <i>Molecular Physics</i> , 2020, 118, e1580393.	0.8	1
4380	Theoretical evaluation to improve the performance of composite wax powder: cooperativity effects involving the strong Na ⁺ ⋯I ⁻ and weak hydrogen-bonding interactions in the complex of graphene oxide with Na ⁺ and CH ₄ . <i>Molecular Physics</i> , 2020, 118, e1612106.	0.8	3
4381	Interaction of different types of nanocages (Al ₁₂ N ₁₂), Tj ETQqO O 0 rgBT /Overlock 10 Tf 50 192 Td (Al _{sub}) ClCN: DFT, TD-DFT, QTAIM, and NBO calculations. <i>Molecular Physics</i> , 2020, 118, 1626506.	0.8	29
4382	Palladium(II) and platinum(II) pyrrolate-quinoline-imine chloro-complexes by metal-assisted condensation reactions. <i>Chemical Papers</i> , 2020, 74, 3673-3682.	1.0	2
4383	A mechanism study for trace phoxim in water extracted by DLLME with composite extractant containing ionic liquids. <i>Journal of Dispersion Science and Technology</i> , 2020, 41, 441-449.	1.3	4
4384	Density functional theory study towards investigating the adsorption properties of the $\hat{1}^3$ -Fe ₂ O ₃ nanoparticles as a nanocarrier for delivery of Flutamide anticancer drug. <i>Adsorption</i> , 2020, 26, 925-939.	1.4	12

#	ARTICLE	IF	CITATIONS
4385	Superatomic properties of transition-metal-doped tetrahedral lithium clusters: TM@Li ₁₄ . <i>Molecular Physics</i> , 2020, 118, e1592256.	0.8	9
4386	B ₁₂ N ₁₂ cluster as a collector of noble gases: A quantum chemical study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 115, 113697.	1.3	32
4387	Interaction of (G ₄) ₂ and (X ₄) ₂ DNA quadruplexes with Cu ⁺ , Ag ⁺ and Au ⁺ metal cations: a quantum chemical calculation on structural, energetic and electronic properties. <i>Structural Chemistry</i> , 2020, 31, 465-484.	1.0	4
4388	Inhibition and interfacial behaviour of novel amidine inhibitors against brass corrosion in 1 M HNO ₃ under flow conditions. <i>Journal of Adhesion Science and Technology</i> , 2020, 34, 25-47.	1.4	6
4389	Polydopamine-induced growth of mineralized ⁵⁶ Fe-FeOOH nanorods for construction of silk fabric with excellent superhydrophobicity, flame retardancy and UV resistance. <i>Chemical Engineering Journal</i> , 2020, 382, 122988.	6.6	65
4390	Self-assembly, protonation-dependent morphology, and photophysical properties of perylene bisimide with tertiary amine groups. <i>Dyes and Pigments</i> , 2020, 173, 107896.	2.0	10
4391	Hydrogen adsorption on pristine and platinum decorated graphene quantum dot: A first principle study. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 23977-23987.	3.8	34
4392	Manipulation of epitaxial graphene towards novel properties and applications. <i>Materials Today: Proceedings</i> , 2020, 20, 37-45.	0.9	2
4393	Synthesis, crystal structure, and non-covalent interactions in 4-hydrazinobenzoic acid hydrochloride. <i>Journal of Molecular Structure</i> , 2020, 1201, 127154.	1.8	1
4394	A photo-switch for peroxydisulfate non-radical/radical activation over layered CuFe oxide: Rational degradation pathway choice for pollutants. <i>Applied Catalysis B: Environmental</i> , 2020, 261, 118232.	10.8	89
4395	Theoretical study of the 1,3-DC reaction between fluorinated alkynes and azides: Reactivity indices, transition structures, IGM and ELF analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 94, 107458.	1.3	20
4396	A mild and sequentially Pd/Cu-catalyzed domino synthesis of acidochromic Indolo[3,2-a]carbazoles and Free bases of apocyanine dyes. <i>Dyes and Pigments</i> , 2020, 173, 107890.	2.0	2
4397	A theoretical study on spectroscopic properties and quantum yields of chiral-at-metal cyclometalated Pt(II) complexes. <i>Journal of Molecular Structure</i> , 2020, 1199, 126975.	1.8	1
4398	Design of novel superalkali doped silicon carbide nanocages with giant nonlinear optical response. <i>Optics and Laser Technology</i> , 2020, 122, 105855.	2.2	73
4399	Non-covalent interactions and spectroscopic study of chalcone derivative 1-(4-chlorophenyl)-3-(5-methylfuran-2-yl) prop-2-en-1-one. <i>Journal of Molecular Structure</i> , 2020, 1201, 127145.	1.8	12
4400	Existence of Al ₂ F ₇ ³⁻ in molten MF ₃ (M ⁺ = K, Cs) systems as determined by Raman spectroscopy and structural simulation. <i>Journal of Energy Chemistry</i> , 2020, 44, 19-23.	7.1	13
4401	Intermolecular interactions-photophysical properties relationships in phenanthrene-9,10-dicarbonitrile assemblies. <i>Journal of Molecular Structure</i> , 2020, 1199, 126789.	1.8	8
4402	Synthesis, crystal structure, antioxidant activity and dft study of 2-aryl-2,3-dihydro-4H-[1,3]thiazino[3,2-a]benzimidazol-4-One. <i>Journal of Molecular Structure</i> , 2020, 1199, 127036.	1.8	17

#	ARTICLE	IF	CITATIONS
4403	DFT studies on the reaction mechanism and kinetics of dibutyl phthalate initiated by hydroxyl and sulfate radicals: Prediction of the most reactive sites. <i>Chemical Engineering Journal</i> , 2020, 381, 122680.	6.6	56
4404	Degradation mechanisms of ofloxacin and cefazolin using peroxymonosulfate activated by reduced graphene oxide-CoFe ₂ O ₄ composites. <i>Chemical Engineering Journal</i> , 2020, 383, 123056.	6.6	63
4405	Vibrational spectra, hydrogen bonding analysis and herbicidal activity study of mefenacet: A DFT approach. <i>Journal of Molecular Structure</i> , 2020, 1201, 127203.	1.8	12
4406	Comprehensive study on the topological properties of 5-Amino-2-Methyl Benzene Sulfonamide involving inter and intra molecular hydrogen bonds. <i>Journal of Molecular Structure</i> , 2020, 1201, 127208.	1.8	6
4407	An effective strategy for simply varying relative position of two carbazole groups in the thermally activated delayed fluorescence emitters to achieve deep-blue emission. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 226, 117564.	2.0	10
4408	Construction of multi-channel fluorescence sensor array and its application for accurate identification and sensitive quantification of multiple metal ions. <i>Sensors and Actuators B: Chemical</i> , 2020, 303, 127277.	4.0	28
4409	Few-layered metal-organic framework nanosheets as a highly selective and efficient scavenger for heavy metal pollution treatment. <i>Chemical Engineering Journal</i> , 2020, 383, 123189.	6.6	38
4410	Quantum chemical investigations on spectral and dissociation properties of L-glutamic acid. <i>Chemical Physics Letters</i> , 2020, 738, 136865.	1.2	3
4411	Ultrasonic and DFT studies of aliphatic amine π -Cyclic ether interactions in n-hexane solvent at 303.15K. <i>Journal of Molecular Liquids</i> , 2020, 297, 111906.	2.3	4
4412	Electronic structure, vibrational spectra and ¹ H NMR chemical shifts of the ion pair composites within imidazolium functionalized geminal dicationic ionic liquids from density functional theory. <i>Journal of Molecular Structure</i> , 2020, 1201, 127112.	1.8	2
4413	Mechanism and origin of diastereoselectivity of N-heterocyclic carbene-catalyzed cross-benzoin reaction: A DFT study. <i>Chinese Chemical Letters</i> , 2020, 31, 736-738.	4.8	34
4414	A combined DFT and FT-IR study on the surface interactions in alumina supported ionic liquid [H ⁺ Pyr] ⁺ [HSO ₄] ⁻ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 226, 117545.	2.0	7
4415	The mechanism of negative and positive hydrogen ions production on the Ni surface. <i>Vacuum</i> , 2020, 171, 108982.	1.6	1
4416	Comparative study of multi-functional luminogens with 1,3,5-triazine as the core and phenothiazine or phenoxy donors as the peripheral moieties for non-doped/doped fluorescent and red phosphorescent OLEDs. <i>Dyes and Pigments</i> , 2020, 173, 107793.	2.0	16
4417	DFT, spectroscopic, DSC/TGA, electronic, biological and molecular docking investigation of 2,5-thiophenedicarboxylic acid: A promising anticancer agent. <i>Journal of Molecular Structure</i> , 2020, 1200, 127099.	1.8	14
4418	Molecular design of a new family of bridged bis(multinitro π -triazole) with outstanding oxygen balance as high-density energy compounds. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26056.	1.0	5
4419	Structural stability and evolution of terbium-doped silicon clusters and influence of 4f ⁿ electronic transition mechanism on magnetism and appearance of photoelectron spectroscopy for TbSi _n ⁺ (<i>n</i> = 6-18) clusters. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26087.	1.0	9
4420	Theoretical insights into sensing of hexavalent chromium on buckled and planar polymeric carbon nitride nanosheets of heptazine and triazine structures. <i>Molecular Simulation</i> , 2020, 46, 54-61.	0.9	28

#	ARTICLE	IF	CITATIONS
4421	Photocatalytic difference of amoxicillin and cefotaxime under visible light by mesoporous g-C ₃ N ₄ : Mechanism, degradation pathway and DFT calculation. <i>Chemical Engineering Journal</i> , 2020, 383, 123134.	6.6	156
4422	Mechanistic insights into the origin of substituent-directed product Zê selectivity for gold-catalyzed [4+1]-annulations of 1,4-diyne-3-ols with isoxazoles: A DFT study. <i>Molecular Catalysis</i> , 2020, 480, 110647.	1.0	5
4423	Zn(II) complex derived from bidentate Schiff base ligand: Synthesis, characterization, DFT studies and evaluation of anti-inflammatory activity. <i>Journal of Molecular Structure</i> , 2020, 1201, 127177.	1.8	28
4424	A combination of FTIR and DFT to study the microscopic structure and hydrogen-bonding interaction properties of the [BMIM][BF ₄] and water. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 226, 117624.	2.0	21
4425	As(III) adsorption onto different-sized polystyrene microplastic particles and its mechanism. <i>Chemosphere</i> , 2020, 239, 124792.	4.2	177
4426	Recyclable menthol-based deep eutectic solvent micellar system for extracting phytochemicals from <i>Ginkgo biloba</i> leaves. <i>Journal of Cleaner Production</i> , 2020, 244, 118648.	4.6	42
4427	Thermophysical and molecular modelling insights into glycerol + alcohol liquid mixtures. <i>Journal of Molecular Liquids</i> , 2020, 297, 111811.	2.3	8
4428	A theoretical study of the absorption spectra of electron-deficient pentacene derivatives using DFT and TDDFT. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 225, 117480.	2.0	6
4429	DFT characterization and design of anthracene-based molecules for improving spectra and charge transfer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 227, 117627.	2.0	5
4430	The structure and interaction properties of two task-specific ionic liquids and acetonitrile mixtures: A combined FTIR and DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 226, 117641.	2.0	25
4431	B ₃ Ge ₁₂ : a aromatic molecular sandwich-shaped structure with short B-B single bonds coordinated by a Ge ₁₂ hexagonal prism and reinforced by f double delocalised bonding patterns. <i>Molecular Physics</i> , 2020, 118, e1676476.	0.8	1
4432	Tuning opto-electronic properties of alkoxy-induced based electron acceptors in infrared region for high performance organic solar cells. <i>Journal of Molecular Liquids</i> , 2020, 298, 111963.	2.3	58
4433	Design-based synthesis, molecular docking analysis of an anti-inflammatory drug, and geometrical optimization and interaction energy studies of an indole acetamide derivative. <i>Journal of Molecular Structure</i> , 2020, 1202, 127244.	1.8	27
4434	Molecular designing of naphthalene diimide based fullerene-free small organic solar cell - Acceptors with high photovoltaic performance by density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117685.	2.0	14
4435	Effects of defects in g-C ₃ N ₄ on excited-state charge distribution and transfer: Potential for improved photocatalysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 227, 117687.	2.0	26
4436	Evoking non-bonding S interaction by aryl phosphine sulfide for selectively enhanced electronic property of organic semiconductors. <i>Chemical Engineering Journal</i> , 2020, 380, 122562.	6.6	14
4437	Theoretical prediction of structures and inclusion properties of heteroatom-bridged pillar[n]arenes. <i>Structural Chemistry</i> , 2020, 31, 329-337.	1.0	9
4438	A sensitive sensing platform for acetaminophen based on palladium and multi-walled carbon nanotube composites and electrochemical detection mechanism. <i>Materials Chemistry and Physics</i> , 2020, 239, 121977.	2.0	27

#	ARTICLE	IF	CITATIONS
4439	Adsorption and dissociation of H ₂ on Al ₄ Si _m (m = 2, 3, and 4) clusters. <i>Environmental Progress and Sustainable Energy</i> , 2020, 39, e13337.	1.3	3
4440	Carbon quantum dots modified tubular g-C ₃ N ₄ with enhanced photocatalytic activity for carbamazepine elimination: Mechanisms, degradation pathway and DFT calculation. <i>Journal of Hazardous Materials</i> , 2020, 381, 120957.	6.5	134
4441	Halogen bond between hypervalent halogens YF ₃ /YF ₅ (Y=Cl, Br, I) and H ₂ X (X= O, S, Se). <i>Molecular Physics</i> , 2020, 118, e1656834.	0.8	2
4442	C/N/O centred metal clusters: super valence bonding and magic structure with 26 valence electrons. <i>Molecular Physics</i> , 2020, 118, .	0.8	0
4443	Photodegradation mechanism and genetic toxicity of bezafibrate by Pd/g-C ₃ N ₄ catalysts under simulated solar light irradiation: The role of active species. <i>Chemical Engineering Journal</i> , 2020, 379, 122294.	6.6	36
4444	A theoretical investigation of the fragment interaction and nonlinear optical and electronic properties of tris(β ² -diketonato)iron(III) complexes. <i>Structural Chemistry</i> , 2020, 31, 215-232.	1.0	0
4445	A new interpretation of the ESIPT mechanism of 2-(benzimidazol-2-yl)-3-hydroxychromone derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117359.	2.0	34
4446	Understanding co-loading of doxorubicin and camptothecin on graphene and folic acid-conjugated graphene for targeting drug delivery: classical MD simulation and DFT calculation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 2737-2745.	2.0	36
4447	Enhanced photovoltaic performances of C219-based dye sensitizers by introducing electron-withdrawing substituents: a density functional theory study. <i>Molecular Physics</i> , 2020, 118, e1636151.	0.8	2
4448	Stability and electronic properties of Rh-doped ruthenium clusters and their interaction with NH ₃ molecule. <i>Molecular Physics</i> , 2020, 118, .	0.8	13
4449	Understanding the origin of the enantioselectivity and the mechanism of the asymmetric reduction of ketimine generated from acetophenone with oxazaborolidine catalyst. <i>Structural Chemistry</i> , 2020, 31, 253-261.	1.0	7
4450	Excited state intramolecular proton transfer (ESIPT) luminescence mechanism for 4-N,N-diethylamino-3-hydroxyflavone in propylene carbonate, acetonitrile and the mixed solvents. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117416.	2.0	10
4451	TD-DFT insights into the sensing potential of the luminescent covalent organic framework for indoor pollutant formaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117432.	2.0	7
4452	Exploring the detailed spectroscopic characteristics, chemical and biological activity of two cyanopyrazine-2-carboxamide derivatives using experimental and theoretical tools. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117414.	2.0	69
4453	The investigation of the G-quadruplex aptamer selectivity to Pb ²⁺ ion: a joint molecular dynamics simulation and density functional theory study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 3659-3675.	2.0	11
4454	Ab initio study of aerogen-bonds between some heterocyclic compounds of benzene with the noble gas elements (Ne, Ar, and Kr). <i>Structural Chemistry</i> , 2020, 31, 435-445.	1.0	4
4455	DFT studies on the interactions of pristine, Al and Ga-doped boron nitride nanosheets with CH ₃ X (X=F, Cl, Br, I). <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 3676-3687.	1.8	37
4456	Quantum chemical calculation studies of Pd _n Si ₁₂ (n = 1, 2, 3) clusters: effects of doping Pd atoms on the structural and electronic properties. <i>Molecular Physics</i> , 2020, 118, e1656350.	0.8	2

#	ARTICLE	IF	CITATIONS
4457	Chromate(VI)-induced homogeneous oxidation and photolysis of aqueous tetracycline: Kinetics and mechanism. <i>Chemical Engineering Journal</i> , 2020, 379, 122276.	6.6	25
4458	Absorption properties of a BODIPY-curved graphene nanoflake system: A theoretical investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117465.	2.0	3
4459	A new look on the electric spark sensitivity of nitramines. <i>Defence Technology</i> , 2020, 16, 10-17.	2.1	6
4460	New insight on the combined effects of hydrothermal treatment and FeSO ₄ /Ca(ClO) ₂ oxidation for sludge dewaterability improvement: From experimental to theoretical investigation. <i>Fuel Processing Technology</i> , 2020, 197, 106196.	3.7	22
4461	A pyrimidine derivative as a high efficiency inhibitor for the corrosion of carbon steel in oilfield produced water under supercritical CO ₂ conditions. <i>Corrosion Science</i> , 2020, 164, 108334.	3.0	51
4462	Regioselectivity in nonsymmetric methyl pentyl Pillar[5]arene bound to non-symmetric axles. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 94, 107460.	1.3	0
4463	Red, green and blue phosphorescent organic light-emitting diodes with ITO-free anode material. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 389, 112229.	2.0	7
4464	Porphyrim/Quinoidal π -Bithiophene π -Based Macrocycles and Their Dications: Template-Free Synthesis and Global Aromaticity. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 2230-2234.	7.2	18
4465	A DFT study on Pt doped (4,0) SWCNT: CO adsorption and sensing. <i>Applied Surface Science</i> , 2020, 504, 144141.	3.1	73
4466	Hydrolysis mechanism of double six-membered ring pentaborate anion. <i>Chemical Physics Letters</i> , 2020, 739, 136930.	1.2	4
4467	Simulated solar light driven Fe(III)/Fe(II) redox cycle for roxarsone degradation and simultaneous arsenate immobilization. <i>Journal of Hazardous Materials</i> , 2020, 394, 121635.	6.5	29
4468	Mechanism and enantioselectivity of the asymmetric [3+2]-annulation between N-methylindole and enoldiazoacetamide catalyzed by prolinato-coordinated dirhodium: A theoretical study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 94, 107489.	1.3	2
4469	Structural, docking and spectroscopic studies of a new piperazine derivative, 1-Phenylpiperazine-1,4-dium bis(hydrogen sulfate). <i>Journal of Molecular Structure</i> , 2020, 1202, 127351.	1.8	63
4470	DFT study of adsorption of ions on doped and defective graphene. <i>Materials Today Communications</i> , 2020, 22, 100714.	0.9	17
4471	Optical properties of S ₂ and S ₃ excited states of protonated schiff-base retinal chromophores in TPA, ECD and ROA. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117532.	2.0	3
4472	Multicomponent supramolecular assemblies of 1(2H)-Phthalazinone and Tetrafluoroterephthalic acid: Understanding the role of hydrogen bonding on the structure and properties using experimental and computational analyses. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117689.	2.0	6
4473	Construction of a metallic silver nanoparticle-decorated bismuth oxybromide-based composite material as a readily recyclable photocatalyst. <i>Journal of Cleaner Production</i> , 2020, 246, 119007.	4.6	24
4474	Bridging Small Molecules to Conjugated Polymers: Efficient Thermally Activated Delayed Fluorescence with a Methyl-Substituted Phenylene Linker. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 1320-1326.	7.2	66

#	ARTICLE	IF	CITATIONS
4475	Theoretical Study on Factors Influencing the Efficiency of Dye-Sensitized Solar Cells. Journal of Electronic Materials, 2020, 49, 318-332.	1.0	11
4476	Insight into the optoelectronic characteristics of diimide-based acceptors in organic solar cells by performing DFT calculation and molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2020, 94, 107488.	1.3	4
4477	Synthesis and structural studies of hexafluorophosphate-based organic salts: A combined experimental and computational analysis. Journal of Molecular Structure, 2020, 1202, 127337.	1.8	1
4478	The one-pot synthesis of homoleptic phenylphthalazine iridium(III) complexes and their application in high efficiency OLEDs. Journal of Luminescence, 2020, 219, 116846.	1.5	10
4479	Insight into the oxidative desulfurization mechanism of aromatic sulfur compounds over Ti-MWW zeolite: A computational study. Microporous and Mesoporous Materials, 2020, 294, 109837.	2.2	14
4480	Extremely large nonlinear optical response and excellent electronic stability of true alkaline earthides based on hexaammine complexant. Journal of Molecular Liquids, 2020, 297, 111899.	2.3	54
4481	Mono-silicon isoelectronic replacement in CAI 4 : van't hoff/le bel carbon or not?. Journal of Computational Chemistry, 2020, 41, 119-128.	1.5	2
4482	Axial chiral binaphthalene-diketopyrrolopyrrole dyads as efficient far-red to near-infrared circularly polarized luminescent emitters. Dyes and Pigments, 2020, 173, 107998.	2.0	14
4483	The effects of amino group meta- and para-substitution on ESIPT mechanisms of amino 2-(2-hydroxyphenyl) benzazole derivatives. Journal of Luminescence, 2020, 218, 116836.	1.5	59
4484	Palladium-Catalyzed [3+2] Annulation of Naphthalimide Acceptors and Thiophene Donors. Journal of Organic Chemistry, 2020, 85, 142-149.	1.7	8
4485	Enhanced anaerobic digestion performance of corn stalk pretreated with freezing-thawing and ammonia: An experimental and theoretical study. Journal of Cleaner Production, 2020, 247, 119112.	4.6	23
4486	Dynamical fluxionality, multiplicity of geometrical forms, and electronic properties of anionic, neutral, and cationic Ta _n Si ₁₂ (n=1-3) clusters: quantum chemical calculations. Molecular Physics, 2020, 118, e1682209.	0.8	6
4487	Porphyrin/Quinoidal-Bithiophene-Based Macrocycles and Their Dications: Template-Free Synthesis and Global Aromaticity. Angewandte Chemie, 2020, 132, 2250-2254.	1.6	3
4488	Exploring odd-even effects of simple oligomer-like DRCNnT series: a study based on density functional theory/time-dependent density functional theory calculations. International Journal of Quantum Chemistry, 2020, 120, e26066.	1.0	2
4489	Experimental and theoretical probing of the physicochemical properties of ionic liquids composed of [Bn-DBU] ⁺ cation and various anions. Journal of Molecular Structure, 2020, 1202, 127226.	1.8	12
4490	Quercetin@ZIF-90 as a novel antioxidant for label-free colorimetric ATP sensing at neutral pH. Sensors and Actuators B: Chemical, 2020, 304, 127324.	4.0	19
4491	Molecular knot with nine crossings: Structure and electronic properties from density functional theory computation. Journal of Molecular Graphics and Modelling, 2020, 94, 107481.	1.3	1
4492	Analysis of hydrogen bonding and weak interactions in the crystal structure of (E)-N-(4-ethylphenyl)-2-(4-hydroxybenzylidene)thiosemicarbazone: experimental and theoretical studies. Molecular Physics, 2020, 118, e1670878.	0.8	1

#	ARTICLE	IF	CITATIONS
4493	Molecular dynamics simulation of a lignite structure simplified model absorbing water. <i>Molecular Simulation</i> , 2020, 46, 71-81.	0.9	20
4494	The finding of transition-metal-doped binary superatoms: TM@Li ₁₅ . <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2020, 53, 015101.	0.6	1
4495	Efficient Intersystem Crossing in the Tröger's Base Derived From 4-Amino-1,8-Naphthalimide and Application as a Potent Photodynamic Therapy Reagent. <i>Chemistry - A European Journal</i> , 2020, 26, 3591-3599.	1.7	32
4496	Spectroscopic, quantum chemical, QTAIM analysis, molecular dynamics simulation, docking studies and solvent effect of pyridin-2-yl oxyacetic acid herbicide and its derivatives. <i>Journal of Molecular Structure</i> , 2020, 1206, 127677.	1.8	12
4497	Poly(1,3,5-tris(4-ethynylphenyl)-benzene) Conjugated Polymers as Electrochemical Sensors for Hydrogen Peroxide Detection. <i>ACS Applied Polymer Materials</i> , 2020, 2, 685-690.	2.0	7
4498	Exploring the mechanism of olfactory recognition in the initial stage by modeling the emission spectrum of electron transfer. <i>PLoS ONE</i> , 2020, 15, e0217665.	1.1	2
4499	Effects of Hydroxyl Group on the Interaction of Carboxylated Flavonoid Derivatives with <i>S. Cerevisiae</i> β -Glucosidase. <i>Current Computer-Aided Drug Design</i> , 2020, 16, 31-44.	0.8	10
4500	Theoretical and experimental investigation of the spectroscopic features of and interionic interactions in 1-hexyl-3-methylimidazolium chloride, 1-hexyl-3-methylimidazolium tetrafluoroborate and 1-hexyl-3-methylimidazolium hexafluorophosphate ionic liquids. <i>Journal of Molecular Liquids</i> , 2020, 301, 112468.	2.3	18
4501	Synergistic Catalytic Synthesis of Gemini Lipoamino Acids Based on Multiple Hydrogen-Bonding Interactions in Natural Deep Eutectic Solvents-Enzyme System. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 989-997.	2.4	5
4502	Diastereoselective Synthesis of Steroid-[60]Fullerene Hybrids and Theoretical Underpinning. <i>Journal of Organic Chemistry</i> , 2020, 85, 2426-2437.	1.7	11
4503	Active centre and reactivity descriptor of a green single component imidazole catalyst for acetylene hydrochlorination. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2849-2857.	1.3	12
4504	Revisiting van der Waals Radii: From Comprehensive Structural Analysis to Knowledge-Based Classification of Interatomic Contacts. <i>ChemPhysChem</i> , 2020, 21, 370-376.	1.0	39
4505	Engineering the excited state of graphitic carbon nitride nanostructures by covalently bonding with graphene quantum dots. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	13
4506	Antimicrobial finish of cotton fabrics treated by sophorolipids combined with 1,2,3,4-butanetetracarboxylic acid. <i>Cellulose</i> , 2020, 27, 2859-2872.	2.4	13
4507	Atmospheric implications of hydration on the formation of methanesulfonic acid and methylamine clusters: A theoretical study. <i>Chemosphere</i> , 2020, 244, 125538.	4.2	18
4508	Influence of corrosion products on the inhibition effect of pyrimidine derivative for the corrosion of carbon steel under supercritical CO ₂ conditions. <i>Corrosion Science</i> , 2020, 166, 108442.	3.0	32
4509	Assessment of adsorption behavior of 5-fluorouracil and pyrazinamide on carbon nitride and folic acid-conjugated carbon nitride nanosheets for targeting drug delivery. <i>Journal of Molecular Liquids</i> , 2020, 301, 112435.	2.3	42
4510	External Electric Field-Dependent Photoinduced Charge Transfer in a Donor-Acceptor System in Two-Photon Absorption. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2319-2332.	1.5	38

#	ARTICLE	IF	CITATIONS
4511	Understanding the singletâ€“triplet energy splittings in transition metal-capped carbon chains. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2858-2869.	1.3	0
4512	Tuning the near infrared II emitting wavelength of small molecule dyes by single atom alteration. <i>Chemical Communications</i> , 2020, 56, 523-526.	2.2	20
4513	<i>cis</i> alkenes stabilized by intramolecular sulphurâ€“I interactions. <i>Chemical Communications</i> , 2020, 56, 814-817.	2.2	5
4514	Thermally activated delayed fluorescence emitters with dual conformations for white organic light-emitting diodes: mechanism and molecular design. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1313-1323.	1.3	20
4515	Deeply coloured and highly fluorescent dipolar merocyanines based on tricyanofuran. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2748-2762.	1.3	19
4516	Mechanistic insights into Cu-catalyzed enantioselective Friedelâ€“Crafts reaction between indoles and 2-aryl-N-sulfonylaziridines. <i>Catalysis Science and Technology</i> , 2020, 10, 1117-1124.	2.1	2
4517	Behavior, mechanism and equilibrium studies of Au(<i>iii</i>) extraction with an ionic liquid [C ₄ -6-C ₄ Blm]Br ₂ . <i>Dalton Transactions</i> , 2020, 49, 504-510.	1.6	5
4518	Isolation of the novel example of a monomeric organotellurinic acid. <i>Dalton Transactions</i> , 2020, 49, 1173-1180.	1.6	10
4519	Hexaiododiplatinate(<i>ii</i>) as a useful supramolecular synthon for halogen bond involving crystal engineering. <i>Dalton Transactions</i> , 2020, 49, 356-367.	1.6	49
4520	Unravelling the mechanism of cobalt-catalysed remote Câ€“H nitration of 8-aminoquinolinamides and expansion of substrate scope towards 1-naphthylpicolinamide. <i>Chemical Science</i> , 2020, 11, 534-542.	3.7	1
4521	A new hypervalent iodine(<i>iii</i>)/(<i>v</i>) oxidant and its application to the synthesis of 2 <i>H</i> -azirines. <i>Chemical Science</i> , 2020, 11, 947-953.	3.7	21
4522	Behaviors of hydrogen bonds formed by lignite and aromatic solvents in direct coal liquefaction: Combination analysis of density functional theory and experimental methods. <i>Fuel</i> , 2020, 265, 117011.	3.4	15
4523	Isolation of Homoleptic Dicationic Tellurium and Monocationic Bismuth Analogues of Non-N-Heterocyclic Carbene Derivatives. <i>Organometallics</i> , 2020, 39, 334-343.	1.1	15
4524	Regular/abnormal variation in the strength and nature of the halogen bond between H ₂ Te and the dihalogens: Prominent effect of methyl substituents. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5468.	1.7	3
4525	DFT study of the effect of Ca on NO heterogeneous reduction by char. <i>Fuel</i> , 2020, 265, 116995.	3.4	52
4526	Effects of solvents on the excited state intramolecular proton transfer and hydrogen bond mechanisms of alizarin and its isomers. <i>Journal of Molecular Liquids</i> , 2020, 301, 112415.	2.3	56
4527	The Feâ€“Nâ€“C oxidase-like nanozyme used for catalytic oxidation of NOM in surface water. <i>Water Research</i> , 2020, 171, 115491.	5.3	29
4528	Donorâ€“Acceptor-Appended Triarylboron Lewis Acids: Ratiometric or Time-Resolved Turn-On Fluorescence Response toward Fluoride Binding. <i>Inorganic Chemistry</i> , 2020, 59, 1414-1423.	1.9	11

#	ARTICLE	IF	CITATIONS
4529	Degradation mechanism of biphenyl and 4,4-dichlorobiphenyl cis-dihydroxylation by non-heme 2,3 dioxygenases BphA: A QM/MM approach. <i>Chemosphere</i> , 2020, 247, 125844.	4.2	9
4530	Pressure-dependent kinetics on benzoyl radical + O ₂ and its implications for low temperature oxidation of benzaldehyde. <i>Combustion and Flame</i> , 2020, 214, 139-151.	2.8	7
4531	Luminescent probe based on photochromic cyclometalated iridium(III) complex for high selectivity detection of thiophenol. <i>Dyes and Pigments</i> , 2020, 175, 108191.	2.0	11
4532	Probing the adsorption and release mechanisms of cytarabine anticancer drug on/from dopamine functionalized graphene oxide as a highly efficient drug delivery system. <i>Journal of Molecular Liquids</i> , 2020, 301, 112458.	2.3	26
4533	Innovative Organic Electroluminescent Materials with a Doublet Ground State: A Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2020, 124, 662-673.	1.1	4
4534	Does gold behaves as hydrogen? A joint theoretical and experimental study. <i>Nanoscale Advances</i> , 2020, 2, 844-850.	2.2	3
4535	Effect of diphenylamine substitution on color tuning and charge transfer of a series of Pt(II) complexes for red emitters: A Theoretical study. <i>Chemical Physics Letters</i> , 2020, 740, 137077.	1.2	1
4536	A self-calibrating dual responsive platform for the sensitive detection of sulfite and sulfonic derivatives based on a robust Hf(IV) metal-organic framework. <i>Chemical Communications</i> , 2020, 56, 631-634.	2.2	16
4537	Halogen bonding (HaB) in E-X-M systems: influence of the halogen donor on the HaB nature. <i>CrystEngComm</i> , 2020, 22, 870-877.	1.3	9
4538	Metal-involving halogen bond Ar-[Pt(II)] in a platinum acetylacetonate complex. <i>CrystEngComm</i> , 2020, 22, 554-563.	1.3	34
4539	Ordering self-assembly structures via intermolecular Br ⁻ S interactions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1437-1443.	1.3	6
4540	Unveiling the effect of electron tunneling on the plasmonic resonance of closely spaced gold particles. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1747-1755.	1.3	1
4541	Time-dependent DFT study of the K-edge spectra of vanadium and titanium complexes: effects of chloride ligands on pre-edge features. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 674-682.	1.3	16
4542	Spin modification of iron(II) complexes via covalent (dative) and dispersion guided non-covalent bonding with N-heterocyclic carbenes: DFT, DLPNO-CCSD(T) and MCSCF studies. <i>Dalton Transactions</i> , 2020, 49, 164-170.	1.6	5
4543	3-Amino-1-propanol and N-methylaminoethanol: coordination to zinc(II) vs. decomposition to ammonia. <i>New Journal of Chemistry</i> , 2020, 44, 387-400.	1.4	7
4544	A one-pot route to N-acyl ureas: a formal four-component hydrolytic reaction involving aminonitrones and isocyanide dibromides. <i>New Journal of Chemistry</i> , 2020, 44, 1253-1262.	1.4	7
4545	A BPt ₄ S ₄ cluster: a planar tetracoordinate boron system with three charges all at their global energy minima. <i>New Journal of Chemistry</i> , 2020, 44, 767-772.	1.4	8
4546	Light-induced disruption of an acyl hydrazone link as a novel strategy for drug release and activation: isoniazid as a proof-of-concept case. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 859-870.	3.0	12

#	ARTICLE	IF	CITATIONS
4547	Theoretical insights into the effect of pristine, doped and hole graphene on the overall performance of dye-sensitized solar cells. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 157-168.	3.0	9
4548	Combined NMR, DFT and X-ray studies highlight structural and hydration changes of [Ln(AAZTA)] ³⁺ complexes across the series. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 795-803.	3.0	16
4549	Theoretical perspective for luminescent mechanism of thermally activated delayed fluorescence emitter with excited-state intramolecular proton transfer. <i>Journal of Materials Chemistry C</i> , 2020, 8, 98-108.	2.7	27
4550	Accurate estimation of the photoelectric conversion efficiency of a series of anthracene-based organic dyes for dye-sensitized solar cells. <i>Journal of Materials Chemistry C</i> , 2020, 8, 2388-2399.	2.7	47
4551	All-metallic Zn=Zn Double-bonded Octahedral Zn ₂ M ₄ (M=Li, Na) Clusters with Negative Oxidation State of Zinc. <i>ChemPhysChem</i> , 2020, 21, 459-463.	1.0	11
4552	Theoretical study on alkaloid encapsulating via cyclopentano-curbit[n]uril (n=8, 10)/graphene oxide heterojunction. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26155.	1.0	0
4553	Ligand stabilized transient MNC and its influence on MNC→MCN isomerization process: a computational study (M=Cu, Ag, and Au). <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	3
4554	Perethylated pillar[n]arenes versus pillar[n]arenes: theoretical perspectives. <i>Journal of Molecular Modeling</i> , 2020, 26, 3.	0.8	3
4555	Effect of solvent mixture on the formation of CL-20/HMX cocrystal explosives. <i>Journal of Molecular Modeling</i> , 2020, 26, 8.	0.8	14
4556	Pnictogen, chalcogen, and halogen bonds in catalytic systems: theoretical study and detailed comparison. <i>Journal of Molecular Modeling</i> , 2020, 26, 16.	0.8	18
4557	The conformational search, the stability, fragment interaction and resistance to acidic attack of epoxy-polyurethanes in different solvent media. <i>Structural Chemistry</i> , 2020, 31, 861-875.	1.0	2
4558	Enhanced photocatalytic removal of amoxicillin with Ag/TiO ₂ /mesoporous g-C ₃ N ₄ under visible light: property and mechanistic studies. <i>Environmental Science and Pollution Research</i> , 2020, 27, 7025-7039.	2.7	35
4559	Substituent effects on the halogen and pnictogen bonds characteristics in ternary complexes 4-YPhNH ₂ -PH ₂ F ₂ -ClX (Y=H, F, CN, CHO, NH ₂ , CH ₃ , NO ₂ and OCH ₃ , and X=F, OH, CN, NC, FCC and NO ₂): theoretical study. <i>Journal of Chemical Sciences</i> , 2020, 132, 1.		
4560	A novel concept for the biodegradation mechanism of dianionic catechol with homoprotocatechuate 2,3-dioxygenase: A non-proton-assisted process. <i>Chemosphere</i> , 2020, 246, 125796.	4.2	1
4561	A computational study of the interaction of C ₂ hydrocarbons with CuBTC. <i>Computational Materials Science</i> , 2020, 173, 109438.	1.4	5
4562	The abnormal solvatochromism, high-contrast mechanochromism and internal mechanism of two AIEE-active 1 ² -diketones. <i>Dyes and Pigments</i> , 2020, 175, 108149.	2.0	16
4563	Synthesis, crystal structure, evaluation of urease inhibition potential and the docking studies of cobalt(III) complex based on barbituric acid Schiff base ligand. <i>Inorganica Chimica Acta</i> , 2020, 503, 119405.	1.2	18
4564	A theoretical research of dihydrogen storage in Sc _x N _y (x+y=4) compounds. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 4693-4702.	3.8	0

#	ARTICLE	IF	CITATIONS
4565	Theoretical insight into the degradation of p-nitrophenol by OH radicals synergized with other active oxidants in aqueous solution. <i>Journal of Hazardous Materials</i> , 2020, 389, 121901.	6.5	62
4566	Solvent dependence of the stereoselectivity in bipyridine N,N'-dioxide catalyzed allylation of aromatic aldehydes: A computational perspective. <i>Molecular Catalysis</i> , 2020, 483, 110712.	1.0	2
4567	Salt-with-Salt, a novel strategy to design the flexible solid electrolyte membrane for highly safe lithium metal batteries. <i>Journal of Membrane Science</i> , 2020, 597, 117768.	4.1	25
4568	Theoretical study of hydrogen bonding in complex alcohol liquid mixtures. <i>Journal of Molecular Liquids</i> , 2020, 300, 112331.	2.3	3
4569	Visualization of vibrational-resolution charge transfer enhanced resonance Raman scattering spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 229, 117945.	2.0	4
4570	Substitution effect on luminescent property of thermally activated delayed fluorescence molecule with aggregation induced emission: A QM/MM study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 229, 117964.	2.0	15
4571	A diketopyrrolopyrrole-based hybrid organic nanoprobe for ratiometric imaging of endogenous hypochlorite in live cells. <i>Sensors and Actuators B: Chemical</i> , 2020, 307, 127632.	4.0	9
4572	Combined Experimental and Theoretical Study on Hampered Phosphine Dissociation in Heteroleptic Ni/Zn Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 514-522.	1.9	6
4573	Computational Study of Encapsulation of Polyaromatic Hydrocarbons by Endo-Functionalized Receptors in Nonpolar Medium. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 212-225.	2.5	10
4574	Effect of a Hydrogen Bond on Molecular Probing Properties in the Solvent. <i>Journal of Physical Chemistry A</i> , 2020, 124, 520-528.	1.1	7
4575	Au ₄₂ N ₂₀ : A Stable Aromatic Deltoidal Hexecontahedron Molecule. <i>Journal of Physical Chemistry C</i> , 2020, 124, 425-429.	1.5	0
4576	Systematical Investigation of Chain Length Effect on the Melting Point of a Series of Bifunctional Anthraquinone Derivatives via X-ray Diffraction and Scanning Tunneling Microscopy. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1646-1654.	1.5	14
4577	Regulation of the Molecular Architectures on Second-Order Nonlinear Optical Response and Thermally Activated Delayed Fluorescence Property: Homoconjugation and Twisted Donor-Acceptor. <i>Journal of Physical Chemistry C</i> , 2020, 124, 921-931.	1.5	19
4578	Silicon Promoted Cationic Polymerization of Phenylacetylenes. <i>Macromolecules</i> , 2020, 53, 240-248.	2.2	6
4579	Topological Analysis of the Electron Density in the Carbonyl Complexes M(CO) ₈ (M = Ca, Tj ETQq0 0 0 rgBT /Overlock 10	1.1	21
4580	Theoretical investigation of excited-state proton transfer (ESPT) for 2,5-bis(2-benzothiazolyl)hydroquinone: single or double?. <i>Molecular Physics</i> , 2020, 118, e1705413.	0.8	4
4581	Redox-Active Ligand Assisted Catalytic Water Oxidation by a Ru IV =O Intermediate. <i>Angewandte Chemie</i> , 2020, 132, 4029-4037.	1.6	11
4582	Redox-Active Ligand Assisted Catalytic Water Oxidation by a Ru ^{IV} =O Intermediate. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 4000-4008.	7.2	40

#	ARTICLE	IF	CITATIONS
4583	Spherical Aromaticity of All-metal [Bi ₈ Bi ₁₂] ^{3+/5+} Clusters. <i>Chemistry - A European Journal</i> , 2020, 26, 2073-2079.	1.7	21
4584	The capability of the pristine and (Sc, Ti) doped Be ₁₂ O ₁₂ nanocluster to detect and adsorb of Mercaptopyridine molecule: A first principle study. <i>Journal of Molecular Structure</i> , 2020, 1205, 127593.	1.8	19
4585	Alkaline earth metal decorated phosphide nanoclusters for potential applications as high performance NLO materials; A first principle study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 118, 113906.	1.3	38
4586	Rationalizing the Activity of an Artificial Diels-Alderase: Establishing Efficient and Accurate Protocols for Calculating Supramolecular Catalysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 1300-1310.	6.6	68
4587	Unveiling the Relationship between Energy Transfer and the Triplet Energy Level by Tuning Diarylethene within Europium(III) Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 661-668.	1.9	9
4588	Bridging Small Molecules to Conjugated Polymers: Efficient Thermally Activated Delayed Fluorescence with a Methyl-Substituted Phenylene Linker. <i>Angewandte Chemie</i> , 2020, 132, 1336-1342.	1.6	14
4589	Design of new quinolin-2-one-pyrimidine hybrids as sphingosine kinases inhibitors. <i>Bioorganic Chemistry</i> , 2020, 94, 103414.	2.0	19
4590	Structures and energetics of clusters surrounding diatomic anions stabilized by hydrogen, halogen, and other noncovalent bonds. <i>Chemical Physics</i> , 2020, 530, 110590.	0.9	15
4591	Five new Sb(V) bromide complexes and their polybromide derivatives with pyridinium-type cations: Structures, thermal stability and features of halogen-halogen contacts in solid state. <i>Inorganica Chimica Acta</i> , 2020, 502, 119278.	1.2	5
4592	The substituent effects on the [3+2] cycloaddition of nitrile oxides generated by photooxidation of arylazides to acetonitrile. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 95, 107491.	1.3	2
4593	Study of the mechanisms of dialkyl carbonates directly formed from carbon dioxide and alcohols: New insights from kinetic and thermodynamic processes. <i>Molecular Catalysis</i> , 2020, 482, 110699.	1.0	2
4594	<i>ab initio</i> calculation of electrostatic potentials for C ₆₀ and C ₈₀ . <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2020, 53, 035102.	0.6	10
4595	On Silylated Oxonium and Sulfonium Ions and Their Interaction with Weakly Coordinating Borate Anions. <i>Chemistry - A European Journal</i> , 2020, 26, 1640-1652.	1.7	20
4596	Role of glycine on sulfuric acid-ammonia clusters formation: Transporter or participator. <i>Journal of Environmental Sciences</i> , 2020, 89, 125-135.	3.2	9
4597	Importance of the interaction adsorbent-adsorbate in the dyes adsorption process and DFT modeling. <i>Journal of Molecular Structure</i> , 2020, 1203, 127398.	1.8	25
4598	Four-coordinate N-heterocyclic carbene (NHC) copper(I) complexes bearing functionalized 3-benzyl-1-(pyridyl)-1H-imidazolylidene ligands: Synthesis, photophysical properties and computational study. <i>Polyhedron</i> , 2020, 175, 114240.	1.0	7
4599	Synergistic Effect of Nitrogen Dopants on Carbon Nanotubes on the Catalytic Selective Epoxidation of Styrene. <i>ACS Catalysis</i> , 2020, 10, 129-137.	5.5	55
4600	Photophysical properties and immobilisation of fluorescent pH responsive aminated benzimidazo[1,2-a]quinoline-6-carbonitriles. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 227, 117588.	2.0	5

#	ARTICLE	IF	CITATIONS
4601	Boosting Efficiency of Near-Infrared Organic Light-Emitting Diodes with Os(II)-Based Pyrazinyl Azolate Emitters. <i>Advanced Functional Materials</i> , 2020, 30, 1906738.	7.8	57
4602	Theoretical study of the desorption of neutral and ionic alkali metal atoms from the excited Li + (H ₂) Tj ETQq1 1 0.784314 rgBT /Over to Journal of Quantum Chemistry, 2020, 120, e26104.	1.0	3
4603	Chromate separation by selective crystallization. <i>Chinese Chemical Letters</i> , 2020, 31, 1974-1977.	4.8	9
4604	The aromatic character of the transition state structures (TSs) involved in pseudocyclic reactions of fluorinated compounds. <i>Journal of Fluorine Chemistry</i> , 2020, 229, 109421.	0.9	2
4605	Suppression of aggregation caused quenching in U-shaped thermally activated delayed fluorescence molecules: Tert-butyl effect. <i>Journal of Luminescence</i> , 2020, 219, 116899.	1.5	20
4606	One-pot synthesis, spectroscopic characterizations, quantum chemical calculations, docking and cytotoxicity of 1-((dibenzylamino)methyl)pyrrolidine-2,5-dione. <i>Journal of Molecular Structure</i> , 2020, 1203, 127403.	1.8	8
4607	Novel cyclic and linearizing cyclic Pd(II) nano-hoop-based coordination complexes achieving nonlinear optical activity transparency trade-off optimization. <i>Organic Electronics</i> , 2020, 78, 105564.	1.4	5
4608	Increasing Photothermal Efficacy by Simultaneous Intra- and Intermolecular Fluorescence Quenching. <i>Advanced Functional Materials</i> , 2020, 30, 1908073.	7.8	49
4609	Construction and mechanism of a novel Z-scheme photocatalyst $\text{Fe}_2\text{O}_3/\text{P3HT}$ with O-Ti-O for organic pollutant degradation under visible light. <i>Applied Surface Science</i> , 2020, 505, 144639.	3.1	18
4610	Probing impacts of π -conjugation and multiarm on the performance of two-dimensionally expanded small molecule hole-transporting materials: A theoretical investigation. <i>Synthetic Metals</i> , 2020, 259, 116219.	2.1	13
4611	Salt Formation: Route To Improve Energetic Performance and Molecular Stability Simultaneously. <i>Crystal Growth and Design</i> , 2020, 20, 197-205.	1.4	13
4612	Insight into the reaction mechanism of CH ₂ SH with HO ₂ : A density functional theory study. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26146.	1.0	2
4613	A DFT study on mechanisms of CO ₂ coupling with propargylic alcohols using alkali carbonates. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26150.	1.0	2
4614	Adsorption of iron(II, III) cations on pristine heptazine and triazine polymeric carbon nitride quantum dots of buckled and planar structures: theoretical insights. <i>Adsorption</i> , 2020, 26, 429-442.	1.4	32
4615	The effect of adsorption and grafting on the acidity of $[(\text{HSO}_3)\text{C}_3\text{C}_1\text{im}]^+[\text{Cl}]^{\ominus}$ on the surface of (SiO ₂) ₄₀ H ₄ clusters. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 96, 107528.	1.3	4
4616	Thermodynamics and Kinetics of Click Reaction between Benzyl Azide and Different Alkynes by Microcalorimetry. <i>Organic Process Research and Development</i> , 2020, 24, 163-171.	1.3	2
4617	Possible pre-phase transition of the HMX crystal observed by the variation of hydrogen-bonding network under high pressures. <i>CrystEngComm</i> , 2020, 22, 330-348.	1.3	13
4618	Evaluation and understanding the performances of various derivatives of carbonyl-stabilized phosphonium ylides in CO ₂ transformation to cyclic carbonates. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 223-237.	1.3	21

#	ARTICLE	IF	CITATIONS
4619	Influence of nonmetal dopants on charge separation of graphitic carbon nitride by time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 647-657.	1.3	16
4620	Two-step phosphorescent mechanochromism due to intramolecular deformation. <i>Journal of Materials Chemistry C</i> , 2020, 8, 715-720.	2.7	33
4621	Water dimer isomers: interaction energies and electronic structure. <i>Journal of Molecular Modeling</i> , 2020, 26, 20.	0.8	15
4622	Copigmentation evidence of oenin with phenolic compounds: A comparative study of spectrographic, thermodynamic and theoretical data. <i>Food Chemistry</i> , 2020, 313, 126163.	4.2	19
4623	Investigating the stability of icosahedral Ni ₁₃ –xCu _x (x = 1–12) bimetallic nanoclusters supported on defective graphene: Insights from first-principles calculations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 118, 113880.	1.3	9
4624	Corrections of Molecular Morphology and Hydrogen Bond for Improved Crystal Density Prediction. <i>Molecules</i> , 2020, 25, 161.	1.7	11
4625	Interaction mechanism of flavonoids and bovine β -lactoglobulin: Experimental and molecular modelling studies. <i>Food Chemistry</i> , 2020, 312, 126066.	4.2	38
4626	Generation of molybdenum hydride species via addition of molecular hydrogen across metal-oxygen bond at monolayer oxide/metal composite interface. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 2975-2988.	3.8	10
4627	Crystal Structure and Computational Study on Methyl-3-Aminothiophene-2-Carboxylate. <i>Crystals</i> , 2020, 10, 19.	1.0	8
4628	Naphthyl-fused Phosphepines: Luminescent Contorted Polycyclic Heterocycles. <i>Chemistry - A European Journal</i> , 2020, 26, 1856-1863.	1.7	17
4629	Molecular structure, FT-IR and NMR analyses of dihydrogen-bonded B ₃ N ₃ H ₆ -HM complexes: a DFT and MP2 approach. <i>Chemical Papers</i> , 2020, 74, 1609-1619.	1.0	6
4630	Strain-controlled carbon nitride: A continuously tunable membrane for gas separation. <i>Applied Surface Science</i> , 2020, 506, 144675.	3.1	29
4631	Preparation and properties of anion exchange membranes with exceptional alkaline stable polymer backbone and cation groups. <i>Journal of Membrane Science</i> , 2020, 596, 117720.	4.1	84
4632	Characterization of the Ground States of BeC ₂ and BeC ₂ ⁺ via Photoelectron Velocity Map Imaging Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 88-92.	2.1	1
4633	Role of hydrogen bonding interactions within of the conformational preferences of calix[n = 4,6,8]arene: DFT and QTAIM analysis. <i>Journal of Molecular Modeling</i> , 2020, 26, 12.	0.8	7
4634	¹ H Functionalization of Hydrogen-Rich [(Cp*V) ₂ (B ₂ H ₆) ₂]: Synthesis and Structures of [(Cp*V) ₂ (B ₂ X ₂) ₂ (H ₈) ₂] (X = Cl, SePh; Cp* =) Tj ETQq1 1 0.784314 rgBT	1.1	15
4635	Urease inhibition studies of six Ni(II), Co(II) and Cu(II) complexes with two sexidentate N ₂ O ₄ -donor bis-Schiff base ligands: An experimental and DFT computational study. <i>Journal of Inorganic Biochemistry</i> , 2020, 204, 110959.	1.5	9
4636	Theoretical screening of high-efficiency sensitizers with D- π -A framework for DSSCs by altering promising donor group. <i>Solar Energy</i> , 2020, 196, 146-156.	2.9	35

#	ARTICLE	IF	CITATIONS
4637	Nucleophilicity versus Brønsted Basicity Controlled Chemoselectivity: Mechanistic Insight into Silver- or Scandium-Catalyzed Diazo Functionalization. <i>ACS Catalysis</i> , 2020, 10, 1256-1263.	5.5	31
4638	DFT/TDDFT investigation on the π -A type molecule probes 4-(5-R-thiophen-2-yl)-2-isobutyl-2H-[1,2,3]triazolo[4,5-e][1,2,4] triazolo[1,5-a]pyrimidines: fluorescence sensing mechanism and roles of weak interactions. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	6
4639	Photomechanical Luminescence from Through-Space Conjugated AIEgens. <i>Angewandte Chemie</i> , 2020, 132, 8913-8917.	1.6	12
4640	The thermodynamic, quantum, AIM and NBO study of the interaction of pyrazinamide drug with the pristine and transition metal-doped B12P12. <i>Adsorption</i> , 2020, 26, 955-970.	1.4	12
4641	Rapid removal of toxic metals Cu ²⁺ and Pb ²⁺ by amino trimethylene phosphonic acid intercalated layered double hydroxide: A combined experimental and DFT study. <i>Chemical Engineering Journal</i> , 2020, 392, 123711.	6.6	147
4642	Synthesis, crystal structure, TD/DFT calculations and Hirshfeld surface analysis of 1-(4-((Benzo)dioxol-5-ylmethyleneamino)phenyl)ethanone oxime. <i>Journal of Molecular Structure</i> , 2020, 1204, 127552.	1.8	28
4643	Degradation mechanism for Zearalenone ring-cleavage by Zearalenone hydrolase RmZHD: A QM/MM study. <i>Science of the Total Environment</i> , 2020, 709, 135897.	3.9	43
4644	Tunable linear and nonlinear optical properties of chromophores containing 3,7-(di)vinylquinoxalinone core by modification of receptors moieties. <i>Optical Materials</i> , 2020, 99, 109580.	1.7	19
4645	Integrated probing the influence of dye acceptor with several electron withdrawing groups for dye-sensitized solar cells. <i>Solar Energy</i> , 2020, 195, 491-498.	2.9	7
4646	Halogen bond in separation science: A critical analysis across experimental and theoretical results. <i>Journal of Chromatography A</i> , 2020, 1616, 460788.	1.8	23
4647	Lasagna-like supramolecular polymers derived from the PdII osazone complexes via C(sp ²) \cdots H \cdots Hal hydrogen bonding. <i>Inorganica Chimica Acta</i> , 2020, 502, 119378.	1.2	23
4648	A combined study on the skeletal vibration of aminopyrine by terahertz time-domain spectroscopy and DFT simulation. <i>Optik</i> , 2020, 208, 163913.	1.4	4
4649	Rational design of SM315-based porphyrin sensitizers for highly efficient dye-sensitized solar cells: A theoretical study. <i>Journal of Molecular Structure</i> , 2020, 1205, 127567.	1.8	5
4650	Experimental and computational analysis of 1-(4-chloro-3-nitrophenyl)-3-(3,4-dichlorophenyl)thiourea. <i>Journal of Molecular Structure</i> , 2020, 1205, 127587.	1.8	53
4651	Efficiency enhancement of pyridinium ylide dye-sensitized solar cells by introduction of benzothiadiazolyl chromophore: A computational study. <i>Materials Today Communications</i> , 2020, 22, 100839.	0.9	2
4652	Reverse Sandwich Structures from Interplay between Lone Pair \cdots Hole Atom-Directed C \cdots A \cdots d ⁺ [M] and Halogen Bond Interactions. <i>Crystal Growth and Design</i> , 2020, 20, 995-1008.	1.4	35
4653	Dehydration of 1-Butanol with a Deep Eutectic Solvent by Liquid-Liquid Extraction. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 846-855.	1.8	26
4654	Controllable Photophysical and Nonlinear Properties in Conformation Isomerization of Macrocyclic [32]Octaphyrin(1.0.1.0.1.0.1.0) Involving H \cdots ackel and M \cdots qbius Topologies. <i>Journal of Physical Chemistry C</i> , 2020, 124, 845-853.	1.5	30

#	ARTICLE	IF	CITATIONS
4655	Zintl phase crystal assembled by magic Al_6CNa_4 cluster. <i>Chemical Physics Letters</i> , 2020, 739, 137026.	1.2	0
4656	Remarkable Stabilities of Trimetallic Nitride Clusterfullerenes $MSc_2N@C_{70}$ (M = Sc, Y, Dy) with Three Pentagon Adjacencies: A Theoretical Survey. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1135-1145.	1.5	4
4657	Tuning the optoelectronic properties of oligothiophenes for solar cell applications by varying the number of cyano and fluoro substituents for solar cell applications: A theoretical study. <i>Journal of Chemical Research</i> , 2020, 44, 235-242.	0.6	3
4658	Symmetric C \cdots H \cdots C Hydrogen Bonds Predicted by Quantum Chemical Calculations. <i>Journal of Organic Chemistry</i> , 2020, 85, 397-402.	1.7	3
4659	Theoretical Study of the Mechanism of Catalytic Enantioselective N-H and O-H Insertion Reactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2-11.	1.1	8
4660	Theoretical study on cyclophane amide molecular receptors and its complexation behavior with TCNQ. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2020, 203, 111735.	1.7	11
4661	A DFT/EDA study of ethanol decomposition over Pt, Cu and Rh metal clusters. <i>Molecular Catalysis</i> , 2020, 482, 110694.	1.0	9
4662	Co-effects of the electron transfer and intersystem crossing on the photophysics of a phenothiazine based Hg ²⁺ sensor. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 229, 117939.	2.0	4
4663	Shedding light on the energetics, regioselectivity, stereoselectivity, and mechanistic aspects of [3 + 2] cycloaddition reaction between azomethine imines and 2-sulfolene through molecular electron density theory. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4042.	0.9	3
4664	Coordination behavior of uranyl with PDAM derivatives in solution: Combined study with ESI-MS and DFT. <i>Journal of Molecular Liquids</i> , 2020, 300, 112287.	2.3	12
4665	Contributions of metalloporphyrin linkers and Zr ₆ nodes in gas adsorption on a series of bioinspired zirconium-based metal-organic frameworks: A computational study. <i>Journal of Molecular Structure</i> , 2020, 1204, 127559.	1.8	3
4666	Impact of Approximate DFT Density Delocalization Error on Potential Energy Surfaces in Transition Metal Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 264-277.	2.3	22
4667	The influence of driving force on intramolecular electron transfer: A theoretical study of subphthalocyanine-AzaBODIPY supramolecular triad. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26131.	1.0	4
4668	Coordination bonding in dicopper and dichromium tetrakis(1/4-acetato)diaqua complexes: Nature, strength, length, and topology. <i>Journal of Computational Chemistry</i> , 2020, 41, 698-714.	1.5	7
4669	Photomechanical Luminescence from Through-Space Conjugated AIEgens. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 8828-8832.	7.2	67
4670	Molecular Hydrogen-Induced Carbon Chain Rearrangement in Cyclopentadienyl-Tethered Titanium(III) Permethyltitanocene Complexes. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 128-136.	1.0	2
4671	Physicochemical properties of the imidazolium-based dicationic ionic liquids (DILs) composed of ethylene spacer by changing the anions: a quantum chemical approach. <i>Ionics</i> , 2020, 26, 1963-1988.	1.2	9
4672	Methionine-montmorillonite composite – A novel material for efficient adsorption of lead ions. <i>Advanced Powder Technology</i> , 2020, 31, 708-717.	2.0	27

#	ARTICLE	IF	CITATIONS
4673	COSMO-RS based ionic liquid screening for the separation of acetonitrile and ethanol azeotropic mixture. <i>Journal of Chemical Technology and Biotechnology</i> , 2020, 95, 1191-1202.	1.6	14
4674	Theoretical investigation of the self-association of antitumor drug imexon. <i>Chemical Papers</i> , 2020, 74, 1597-1608.	1.0	0
4675	AlEgens with bright mechanoluminescence and thermally activated delayed fluorescence derived from (9H-carbazol-9-yl)(phenyl)methanone. <i>Dyes and Pigments</i> , 2020, 174, 108093.	2.0	8
4676	Theoretical investigation of a cation-controllable molecular shuttle of tetracationic cyclophane. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4036.	0.9	0
4677	Design of novel inorganic alkaline earth metal doped aluminum nitride complexes (AEM@Al ₁₂ N ₁₂) with high chemical stability, improved electronic properties and large nonlinear optical response. <i>Optik</i> , 2020, 207, 163792.	1.4	27
4678	Vibrational spectroscopy, reactive site analysis and molecular docking studies on 2-[(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)methoxy]-3-hydroxypropyl (2S)-2-amino-3-methylbutanoate. <i>Journal of Molecular Structure</i> , 2020, 1202, 127274.	1.8	25
4679	Theoretical studies of photovoltaic properties of five new silol dithiophene based D ₂ -A ₁ -D ₂ donors. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26047.	1.0	2
4680	Theoretical investigations of spin-orbit coupling and intersystem crossing in reaction carbon dioxide activated by [Re(CO) ₂] ⁺ . <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26109.	1.0	1
4681	Boron nitride B ₁₁ N ₁₂ M ⁺ (M = B, Al, Ga, and In) nanocages as a catalyst for CO oxidation by N ₂ O: A density functional study. <i>Computational and Theoretical Chemistry</i> , 2020, 1171, 112660.	1.1	7
4682	Study on electronic structure and excitation characteristics of cyclo[18]carbon. <i>Chemical Physics Letters</i> , 2020, 741, 136975.	1.2	29
4683	Theoretically exploring the luminescence mechanism tuned by intermolecular weak interactions of a mechanochromic 9-anthryl gold(I) isocyanide complex. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 388, 112195.	2.0	3
4684	Dissolution behavior of microcrystalline cellulose in DBU-based deep eutectic solvents: Insights from spectroscopic investigation and quantum chemical calculations. <i>Journal of Molecular Liquids</i> , 2020, 299, 112140.	2.3	31
4685	The interactions between polar solvents (methanol, acetonitrile, dimethylsulfoxide) and the ionic liquid 1-ethyl-3-methylimidazolium bis(fluorosulfonyl)imide. <i>Journal of Molecular Liquids</i> , 2020, 299, 112159.	2.3	48
4686	Molecular docking and quantum chemical calculations of 4-methoxy-2-[3-(4-chlorophenyl)-5-(4-(propane-2-yl)PHENYL)-4,5-dihydro-1H-pyrazol-1-yl]-1,3-thiazol-4-yl}phenol. <i>Journal of Molecular Structure</i> , 2020, 1203, 127452.	1.8	20
4687	A novel approach for the selective extraction of Li ⁺ from the leaching solution of spent lithium-ion batteries using benzo-15-crown-5 ether as extractant. <i>Separation and Purification Technology</i> , 2020, 237, 116325.	3.9	54
4688	Computational insight into energetic cage derivatives based on hexahydro-1,3,5-trinitro-1,3,5-triazine. <i>Journal of the Chinese Chemical Society</i> , 2020, 67, 961-968.	0.8	1
4689	Formation mechanism of methanesulfonic acid and ammonia clusters: A kinetics simulation study. <i>Atmospheric Environment</i> , 2020, 222, 117161.	1.9	24
4690	Theoretical studies on the noncovalent interaction of fructose and functionalized ionic liquids. <i>Carbohydrate Research</i> , 2020, 487, 107882.	1.1	13

#	ARTICLE	IF	CITATIONS
4691	Quantum chemical studies of selective back-extraction of Am(III) from Eu(III) and Cm(III) with two hydrophilic 1,10-phenanthroline-2,9-bis-triazolyl ligands. <i>Radiochimica Acta</i> , 2020, 108, 517-526.	0.5	11
4692	Origin of Regio- and Stereoselectivity in the NHC-catalyzed Reaction of Alkyl Pyridinium with Aliphatic Enal. <i>ChemCatChem</i> , 2020, 12, 1068-1074.	1.8	27
4693	Investigation of structural stability, electronic properties of S-doped CdSe using ab initio calculations. <i>Structural Chemistry</i> , 2020, 31, 701-708.	1.0	3
4694	Understanding how specific functional groups in humic acid affect the sorption mechanisms of different calcinated layered double hydroxides. <i>Chemical Engineering Journal</i> , 2020, 392, 123633.	6.6	11
4695	A novel strategy for synthesizing Fe, N, and S tridoped graphene-supported Pt nanodendrites toward highly efficient methanol oxidation. <i>Journal of Catalysis</i> , 2020, 381, 275-284.	3.1	92
4696	Prediction of photoelectric properties, especially power conversion efficiency of cells, of IQ1 and derivative dyes in high-efficiency dye-sensitized solar cells. <i>Solar Energy</i> , 2020, 195, 82-88.	2.9	25
4697	Interplay between thin silver films and epitaxial graphene. <i>Surface and Coatings Technology</i> , 2020, 381, 125200.	2.2	6
4698	Designing new donor materials based on functionalized DCCnT with different electron-donating groups: A density functional theory (DFT) and time dependent density functional theory (TDDFT)-based study. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26112.	1.0	5
4699	Theoretical study of electronic and nonlinear optical properties of Janus all-cis-1,2,3,4,5,6-hexafluorocyclohexane derivative with an extended π conjugation. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	3
4700	Photoninduced charge redistribution of graphene determined by edge structures in the infrared region. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 229, 117858.	2.0	8
4701	Au ₂ Si ₂ O: a honeycomb-shaped structure with short Au~Au single bond at the centre coordinated by twelve Si ₅ pentagons and reinforced by strong Au~Si interactions and aromaticity. <i>Molecular Physics</i> , 2020, 118, e1692152.	0.8	4
4702	Comparative study of the effects of ortho-, meta- and para-carboranes (C ₂ B ₁₀ H ₁₂) on the physicochemical properties, cytotoxicity and antiviral activity of uridine and 2 α -deoxyuridine boron cluster conjugates. <i>Bioorganic Chemistry</i> , 2020, 94, 103466.	2.0	7
4703	Performance optimization of CdS precipitated graphene oxide/polyacrylic acid composite for efficient photodegradation of chlortetracycline. <i>Journal of Hazardous Materials</i> , 2020, 388, 121780.	6.5	37
4704	Importance of the iron-sulfur component and of the siroheme modification in the resting state of sulfite reductase. <i>Journal of Inorganic Biochemistry</i> , 2020, 203, 110928.	1.5	4
4705	Degradation behaviors of Isopropylphenazone and Aminopyrine and their genetic toxicity variations during UV/chloramine treatment. <i>Water Research</i> , 2020, 170, 115339.	5.3	36
4706	Mechanism for hydrolysis of double six-membered ring tetraborate anion. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26118.	1.0	3
4707	First-principles study of the reaction mechanism governing the SNAr of the dimethylamine on 2-methoxy-5-nitrothiophenes. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	5
4708	Effect of nitrogen substitution and π -conjugation on photophysical properties and excited state intramolecular proton transfer reactions of methyl salicylate derivatives: Theoretical investigation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 389, 112267.	2.0	13

#	ARTICLE	IF	CITATIONS
4709	Complexation of trivalent lanthanides and actinides with diethylenetriaminepentaacetic acid: Theoretical unraveling of bond covalency. <i>Journal of Molecular Liquids</i> , 2020, 299, 112174.	2.3	18
4710	Metal-π-Halogen Bonding Seen through the Eyes of Vibrational Spectroscopy. <i>Materials</i> , 2020, 13, 55.	1.3	26
4711	Regioselective Hydroalkylation and Arylalkylation of Alkynes by Photoredox/Nickel Dual Catalysis: Application and Mechanism. <i>Angewandte Chemie</i> , 2020, 132, 5787-5795.	1.6	14
4712	Regioselective Hydroalkylation and Arylalkylation of Alkynes by Photoredox/Nickel Dual Catalysis: Application and Mechanism. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 5738-5746.	7.2	81
4713	A phenyl-rich β-cyclodextrin porous crosslinked polymer for efficient removal of aromatic pollutants: Insight into adsorption performance and mechanism. <i>Chemical Engineering Journal</i> , 2020, 387, 124020.	6.6	88
4714	A theoretical study on electronic spectra of a novel series of metal substituted boron subphthalocyanine chloride. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 229, 118018.	2.0	7
4715	Probing the Aromaticity and Stability of Metallatricycles by DFT Calculations: Toward Clar Structure in Organometallic Chemistry. <i>Organometallics</i> , 2020, 39, 80-86.	1.1	7
4716	Graphene and silicene quantum dots for nanomedical diagnostics. <i>RSC Advances</i> , 2020, 10, 801-811.	1.7	16
4717	Theoretical Prediction of Properties of Cyclopenta[b]pyrrol-2-one Derivatives. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 2072-2076.	0.1	0
4718	Asymmetric Cyanation of Activated Olefins with Ethyl Cyanofornate Catalyzed by Ti(IV)-Catalyst: A Theoretical Study. <i>Catalysts</i> , 2020, 10, 1079.	1.6	2
4719	Water-Soluble Bismuth(III) Polynuclear Tyrosinehydroxamate Metallamacrocyclic Complex: Structural Parallels to Lanthanide Metallacrowns. <i>Molecules</i> , 2020, 25, 4379.	1.7	9
4720	Factors Impacting π- and σ-Hole Regions as Revealed by the Electrostatic Potential and Its Source Function Reconstruction: The Case of 4,4'-Bipyridine Derivatives. <i>Molecules</i> , 2020, 25, 4409.	1.7	15
4721	Effects of alkali additives in saturated LiNO ₃ aqueous electrolyte for improvement in cycling stability of polyimide anode. <i>Journal of Power Sources</i> , 2020, 477, 229040.	4.0	3
4722	Quantum computational, spectroscopic and molecular docking studies of 5,5-dimethylhydantoin and its bromine and chlorine derivatives. <i>Chemical Data Collections</i> , 2020, 29, 100461.	1.1	0
4723	Computational assessment on wave function (ELF, LOL) analysis, molecular confirmation and molecular docking explores on 2-(5-Amino-2-Methylanylino)-4-(3-pyridyl) pyrimidine. <i>Chemical Data Collections</i> , 2020, 29, 100525.	1.1	31
4724	Minimizing aromatics entrainment in dephenolization of coal-based liquids by deep eutectic solvents. <i>Chemical Engineering Science: X</i> , 2020, 8, 100070.	1.5	2
4725	Computational study of metal ions adsorption on pristine and heteroatom doped peritetracene. <i>Computational and Theoretical Chemistry</i> , 2020, 1191, 113006.	1.1	0
4726	Hirshfeld surface, charge density and site selectivity studies of 1-(2-Methyl-5-nitro-1H-imidazol-1-yl)-acetone. <i>Computational and Theoretical Chemistry</i> , 2020, 1191, 113044.	1.1	3

#	ARTICLE	IF	CITATIONS
4727	A new triazine-based conjugated polymer from simple monomers with stable photocatalytic hydrogen evolution under visible light. <i>Polymer</i> , 2020, 211, 123079.	1.8	12
4728	Porous Membrane with High Selectivity for Alkaline Quinone-Based Flow Batteries. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 48533-48541.	4.0	18
4729	Cyclodextrin Porous Liquid Materials for Efficient Chiral Recognition and Separation of Nucleosides. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 45916-45928.	4.0	50
4730	Electrically conductive Cu(scp)-based 1D coordination polymer with theoretical insight. <i>Dalton Transactions</i> , 2020, 49, 15323-15331.	1.6	8
4731	Effects of structural variations on π -dimer formation: long-distance multicenter bonding of cation-radicals of tetrathiafulvalene analogues. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25054-25065.	1.3	8
4732	Theoretical study on functionalized acrylonitrile compounds with a large second-order nonlinear optical response. <i>New Journal of Chemistry</i> , 2020, 44, 19623-19629.	1.4	7
4733	Intermolecular C-H \cdots M dihydrogen bonds in five-membered heterocyclic complexes: a DFT and ab-initio study. <i>Monatshefte für Chemie</i> , 2020, 151, 1569-1579.	0.9	6
4734	Synthesis, physicochemical properties and computational study of donor-acceptor polymer for optical limiting application. <i>SN Applied Sciences</i> , 2020, 2, 1.	1.5	2
4735	Atomistic Structures, Stabilities, Electronic Properties, and Chemical Bonding of Boron-Aluminum Mixed Clusters B_3AlO_n ($n = 2-6$). <i>Journal of Cluster Science</i> , 2021, 32, 1261-1276.	1.7	4
4736	Theoretical Research on Excited States: Ultraviolet and Fluorescence Spectra of Aromatic Amino Acids. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2020, 12, 530-536.	2.2	7
4737	The effect of the degree of substitution on the solubility of cellulose acetoacetates in water: A molecular dynamics simulation and density functional theory study. <i>Carbohydrate Research</i> , 2020, 496, 108134.	1.1	9
4738	On the stabilization of $Sc_3C@I(31924)$ -C80 by functionalization of fluorine. <i>Chemical Physics Letters</i> , 2020, 759, 137969.	1.2	2
4739	A theoretical exploration of charge transfer dynamics in PTB7Ir/PC71BM triplet-material-based organic photovoltaics. <i>Organic Electronics</i> , 2020, 87, 105956.	1.4	3
4740	Distinctive Characteristics of Al_7Li : A Superatom Counterpart of Group IVA Elements. <i>Inorganic Chemistry</i> , 2020, 59, 14093-14100.	1.9	7
4741	Charge-Inverted Hydrogen-Bridged Bond in HCa_3E ($E = Si, Ge, \text{ and } Sn$): Matrix Isolation Infrared Spectroscopic and Theoretical Studies. <i>Inorganic Chemistry</i> , 2020, 59, 14355-14366.	1.9	3
4742	Perturbation of Pyridinium CVP Spectra by N_2 and H_2 Tags: An Experimental and BOMD Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8519-8528.	1.1	5
4743	Evaluation of Single-Reference DFT-Based Approaches for the Calculation of Spectroscopic Signatures of Excited States Involved in Singlet Fission. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8446-8460.	1.1	10
4744	Y-shaped potential third-order nonlinear optical material β -3-(2-amino-2-oxoethyl)-5-methyl hexanoic acid: an analysis of structural, spectroscopic and docking studies. <i>New Journal of Chemistry</i> , 2020, 44, 18185-18198.	1.4	7

#	ARTICLE	IF	CITATIONS
4745	Upgrading crude bio-oil by in situ and ex situ catalytic pyrolysis through ZSM-5, Ni ₂ Fe ₃ , and Ni ₂ Fe ₃ /ZSM-5: Yield, component, and quantum mechanism. <i>Journal of Renewable and Sustainable Energy</i> , 2020, 12, 053101.	0.8	2
4746	Insight into 6-aminopenicillanic acid structure and study of the quantum mechanical calculations of the acid-base site on $\text{Fe}_2\text{O}_3/\text{SiO}_2$ core-shell nanocomposites and as efficient catalysts in multicomponent reactions. <i>New Journal of Chemistry</i> , 2020, 44, 20688-20696.	1.4	4
4747	DFT Study on Interaction of Estrone and Imidazolium-Based Hydrophobic Ionic Liquids. , 2020, , .		1
4748	Effect of Dodecyl Trimethyl Ammonium Bromide on the Migration of Water Molecules in the Pores of Lignite: An Experimental and Molecular Simulation Study. <i>ACS Omega</i> , 2020, 5, 25456-25466.	1.6	12
4749	Degradation Mechanism of Benzo[<i>a</i>]pyrene Initiated by the OH Radical and H_2O_2 : An Insight from Density Functional Theory Calculations. <i>ACS Omega</i> , 2020, 5, 25552-25560.	1.6	9
4750	Comparison of Vitamin C and Its Derivative Antioxidant Activity: Evaluated by Using Density Functional Theory. <i>ACS Omega</i> , 2020, 5, 25467-25475.	1.6	38
4751	S_2N_2 as a σ -Donor and π -Acceptor Property. <i>ChemistrySelect</i> , 2020, 5, 12176-12189.	0.7	3
4752	Tuning of Structure Evolution and Electronic Properties through Palladium-Doped Boron Clusters: PdB_{16} as a Motif for Boron-Based Nanotubes. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9187-9193.	1.1	11
4753	Pyridine-Based Bipolar Hosts for Solution-Processed Bluish-Green Thermally Activated Delayed Fluorescence Devices: A Subtle Regulation of Chemical Stability and Carrier Transportation. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 49905-49914.	4.0	24
4754	Theoretical Study on Neutral Molecules with Square Planar Tetracoordinate Oxygen O(B) ₄ Arrangements. <i>ACS Omega</i> , 2020, 5, 24513-24519.	1.6	2
4755	Multicenter electron-sharing π -bonding in the $\text{AgFe}(\text{CO})_4^+$ complex. <i>Dalton Transactions</i> , 2020, 49, 15256-15266.	1.6	5
4756	Rivalry between Regium and Hydrogen Bonds Established within Diatomic Coinage Molecules and Lewis Acids/Bases. <i>ChemPhysChem</i> , 2020, 21, 2557-2563.	1.0	11
4757	Discrimination of enzyme-substrate complexes by reactivity using the electron density analysis: peptide bond hydrolysis by the matrix metalloproteinase-2. <i>Mendeleev Communications</i> , 2020, 30, 583-585.	0.6	10
4758	Two dimensional porous frameworks of graphyne family as therapeutic delivery vehicles for Idarubicin biomolecule in silico: Density functional theory and molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , 2020, 319, 114334.	2.3	8
4759	Kinetic and mechanistic insights into the abatement of clofibric acid by integrated UV/ozone/peroxydisulfate process: A modeling and theoretical study. <i>Water Research</i> , 2020, 186, 116336.	5.3	37
4760	Synthesis, Structural Characterization, and DFT Investigations of $[\text{M}_2\text{Fe}_4(\text{CO})_{16}]^{3+}$ (<i>M</i> , Pt) ETQs	1.078	1
4761	Low-Valent, Multiply Bonded, Trigonal-Planar Sb Complex: Rational Syntheses, Dual Acidic/Basic Properties, and Unexpected Semiconducting Characteristics. <i>Inorganic Chemistry</i> , 2020, 59, 16073-16089.	1.9	5
4762	Removal of Berberine from Wastewater by MIL-101(Fe): Performance and Mechanism. <i>ACS Omega</i> , 2020, 5, 27962-27971.	1.6	31

#	ARTICLE	IF	CITATIONS
4763	A sandwich-type cluster containing Ge@Pd ₃ planar fragment flanked by aromatic nonagermanide caps. Nature Communications, 2020, 11, 5286.	5.8	19
4764	The bonding situation in heteromultimetallic carbonyl complexes. Dalton Transactions, 2020, 49, 16762-16771.	1.6	3
4765	van der Waals potential: an important complement to molecular electrostatic potential in studying intermolecular interactions. Journal of Molecular Modeling, 2020, 26, 315.	0.8	126
4766	The effect of metal alkali cations on the properties of hydrogen bonds in tautomeric forms of adenine and guanine mismatch. Journal of Molecular Graphics and Modelling, 2020, 100, 107705.	1.3	2
4767	Bulky electron donating side chain enhances the open-circuit voltage of benzodithiophene photovoltaic polymers. Materials Today Energy, 2020, 18, 100568.	2.5	2
4768	A study of glycine-based dithiocarbamates as effective corrosion inhibitors for cold rolled carbon steel in HCl solutions. Surfaces and Interfaces, 2020, 21, 100751.	1.5	9
4769	Investigation of Highly Efficient and Reversible Absorption of SO ₂ Using Ternary Functional Deep Eutectic Solvents. ACS Sustainable Chemistry and Engineering, 2020, 8, 16241-16251.	3.2	29
4770	The adsorption of chlorofluoromethane on pristine and Ge-doped silicon carbide nanotube: a PBC-DFT, NBO, and QTAIM study. Molecular Simulation, 2020, 46, 1405-1416.	0.9	33
4771	Molecular Origins of Heteroatom Engineering on the Emission Wavelength Tuning, Quantum Yield Variations and Fluorogenicity of NBD-like SCOTfluors. Chemistry - an Asian Journal, 2020, 15, 4082-4086.	1.7	8
4772	The adsorption of chlorofluoromethane on pristine, and Al- and Ga-doped boron nitride nanosheets: a DFT, NBO, and QTAIM study. Journal of Molecular Modeling, 2020, 26, 287.	0.8	35
4773	Unsaturated binuclear homoleptic nickel carbonyl anions Ni ₂ (CO) _n ⁺ (n = 4-6) featuring double three-center two-electron Ni-C-Ni bonds. Physical Chemistry Chemical Physics, 2020, 22, 23773-23784.	1.3	4
4774	Multiple d-d bonds between early transition metals in TM ₂ Lin (TM = Sc, Ti) superatomic molecule clusters. Nanoscale, 2020, 12, 20506-20512.	2.8	5
4775	Li center clusters MLi ₄ ⁺ (M = Al, Si, Ge) for dihydrogen storage. International Journal of Hydrogen Energy, 2020, 45, 24968-24979.	3.8	6
4776	Taking advantages of intramolecular hydrogen bonding to prepare mechanically robust and catalyst-free vitrimer. Polymer, 2020, 210, 123004.	1.8	44
4777	Experimental and computational evidence on gold-catalyzed regioselective hydration of phthalimido-protected propargylamines: an entry to β -amino ketones. Organic and Biomolecular Chemistry, 2020, 18, 9438-9447.	1.5	7
4778	Structure-directing sulfur...metal noncovalent semicoordination bonding. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 436-449.	0.5	12
4779	The X-ray constrained wavefunction of the [Mn(CO) ₄ {(C ₆ H ₅) ₂ P-S-C(Br) ₂ -(C ₆ H ₅) ₂ P(C ₆ H ₅) ₂ }] ⁺ complex: a theoretical and experimental study of dihalogen bonds and other noncovalent interactions. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 802-814.	0.5	3
4780	Discovery of Pyranoviolin A and Its Biosynthetic Gene Cluster in Aspergillus violaceofuscus. Frontiers in Microbiology, 2020, 11, 562063.	1.5	5

#	ARTICLE	IF	CITATIONS
4781	Visualization of Shallowâ€Groove Expansion of Au(111) Facet under Methane Pyrolysis. <i>Advanced Materials Interfaces</i> , 2020, 7, 2001245.	1.9	1
4782	Towards understanding metal aromaticity in different spin states: A density functional theory and information-theoretic approach analysis. <i>Chemical Physics Letters</i> , 2020, 761, 138065.	1.2	13
4783	Protein Matrix Control of Reaction Center Excitation in Photosystem II. <i>Journal of the American Chemical Society</i> , 2020, 142, 18174-18190.	6.6	46
4784	The simultaneous recognition mechanism of cations and anions using macrocyclicâ€iodine structures: insights from dispersion-corrected DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23795-23803.	1.3	2
4785	Acceptor plane expansion enhances horizontal orientation of thermally activated delayed fluorescence emitters. <i>Science Advances</i> , 2020, 6, .	4.7	80
4786	Versatility of the Cyano Group in Intermolecular Interactions. <i>Molecules</i> , 2020, 25, 4495.	1.7	8
4787	Equilibrium Geometries, Adiabatic Excitation Energies and Intrinsic C=C/Câ€H Bond Strengths of Ethylene in Lowest Singlet Excited States Described by TDDFT. <i>Symmetry</i> , 2020, 12, 1545.	1.1	5
4788	Decomposition mechanism of thiophene compounds in heavy oil under supercritical water. <i>Chemical Engineering Science</i> , 2020, 228, 115979.	1.9	6
4789	Elucidating the Key Role of the Cyano (â€Câ€N) Group to Construct Environmentally Friendly Fused-Ring Electron Acceptors. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23059-23068.	1.5	28
4790	Theoretical Prediction on a Novel Reduction-Responsive Nanoring Having a Disulfide Group for Facile Encapsulation and Release of Fullerenes C ₆₀ and C ₇₀ . <i>ACS Omega</i> , 2020, 5, 25400-25407.	1.6	2
4791	Solvent induced mononuclear and dinuclear mixed ligand Cu(<i>scp</i>) complex: structural diversity, supramolecular packing polymorphism and molecular docking studies. <i>New Journal of Chemistry</i> , 2020, 44, 18048-18068.	1.4	17
4792	N4Mg6M (M = Li, Na, K) superalkalis for CO ₂ activation. <i>Journal of Chemical Physics</i> , 2020, 153, 144301.	1.2	15
4793	Computational investigation of flavonol-based GLP-1R agonists using DFT calculations and molecular docking. <i>Computational and Theoretical Chemistry</i> , 2020, 1190, 113005.	1.1	4
4794	PES, molecular structure, spectroscopic (FT-IR, FT-Raman), electronic (UV-Vis, HOMO-LUMO), quantum chemical and biological (docking) studies on a potent membrane permeable inhibitor: dibenzoxepine derivative. <i>Heliyon</i> , 2020, 6, e04724.	1.4	52
4795	Impact of secondary donor units on the excited-state properties and thermally activated delayed fluorescence (TADF) efficiency of pentacarbazole-benzonitrile emitters. <i>Journal of Chemical Physics</i> , 2020, 153, 144708.	1.2	14
4796	Effects of different ester chains on the antioxidant activity of caffeic acid. <i>Bioorganic Chemistry</i> , 2020, 105, 104341.	2.0	15
4797	Alkylated benzimidazoles: Design, synthesis, docking, DFT analysis, ADMET property, molecular dynamics and activity against HIV and YFV. <i>Computational Biology and Chemistry</i> , 2020, 89, 107400.	1.1	22
4798	Insight into the Effect of Ligands on the Optical Properties of Germanium Quantum Dots and Their Applications in Persistent Cell Imaging. <i>Langmuir</i> , 2020, 36, 12375-12382.	1.6	4

#	ARTICLE	IF	CITATIONS
4799	Low-coordinate Sm(II) and Yb(II) complexes derived from sterically-hindered 1,2-bis(imino)acenaphthene (Ar-BIG-bian). Dalton Transactions, 2020, 49, 14445-14451.	1.6	12
4800	Room-temperature phosphorescence from a purely organic tetraphenylmethane derivative with formyl groups in both solution and crystalline states. Journal of Materials Chemistry C, 2020, 8, 14360-14364.	2.7	15
4801	Molecular Docking, Spectroscopic, and Computational Studies of 2-{3-(4-Chlorophenyl)-5-[4-(Propan-2-yl) Phenyl]-4, 5-Dihydro-1H-Pyrazol-1-yl}-1, 3-Thiazol-4(5H)-One. Polycyclic Aromatic Compounds, 2020, , 1-23.	1.4	2
4802	Structures and Properties of New Organic Conductors: BEDT-TTF, BEST and BETS Salts of the HOC ₂ H ₄ SO ₃ ⁻ Anion. Crystals, 2020, 10, 775.	1.0	7
4803	Ultralong and High-Efficiency Room Temperature Phosphorescence of Organic Phosphors-Doped Polymer Films Enhanced by 3D Network. Advanced Optical Materials, 2020, 8, 2001192.	3.6	47
4804	Agostic Hydrogens in η^5 -Norbornyl Metal Cyclopentadienyl Structures. European Journal of Inorganic Chemistry, 2020, 2020, 4180-4188.	1.0	0
4805	Therapeutic potential of graphitic carbon nitride as a drug delivery system for cisplatin (anticancer) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	1.5	72
4806	Highly sensitive determination of amanita toxins in biological samples using β -cyclodextrin collaborated molecularly imprinted polymers coupled with ultra-high performance liquid chromatography tandem mass spectrometry. Journal of Chromatography A, 2020, 1630, 461514.	1.8	8
4807	Doping atom to tune electronic characteristics and adsorption of cyclo[18] carbons: A theoretical study. Computational and Theoretical Chemistry, 2020, 1187, 112922.	1.1	16
4808	First-principles study for exploring the adsorption behavior of G-series nerve agents on graphdyine surface. Computational and Theoretical Chemistry, 2020, 1191, 113043.	1.1	43
4809	Theoretical design of new bridge-ring insensitive high energy compounds by selected normal Diels-Alder reactions between NH ₂ -substituted oxazoles and NO ₂ /NF ₂ /NHNO ₂ -substituted ethylenes/acetylenes. Defence Technology, 2021, 17, 1731-1739.	2.1	2
4810	Combined MD/QTAIM techniques to evaluate ligand-receptor interactions. Scope and limitations. European Journal of Medicinal Chemistry, 2020, 208, 112792.	2.6	19
4811	Alkaline earth metals serving as source of excess electron for alkaline earth metals to impart large second and third order nonlinear optical response; a DFT study. Journal of Molecular Graphics and Modelling, 2020, 101, 107759.	1.3	28
4812	The DFT study on neutral molecules with planar tetracoordinate oxygen surrounded by four carbon-based groups. Journal of Molecular Graphics and Modelling, 2020, 101, 107761.	1.3	0
4813	Adsorption properties study of boron nitride fullerene for the application as smart drug delivery agent of anti-cancer drug hydroxyurea by density functional theory. Journal of Molecular Liquids, 2020, 318, 114315.	2.3	53
4814	Accelerated discovery of high-efficient N-annulated perylene organic sensitizers for solar cells via machine learning and quantum chemistry. Materials Today Communications, 2020, 25, 101604.	0.9	9
4815	Antioxidant activity and mechanism of dihydrochalcone C-glycosides: Effects of C-glycosylation and hydroxyl groups. Phytochemistry, 2020, 179, 112393.	1.4	21
4816	Enhancing Stability and Formulation Capability of Fungicides by Cocrystallization through a Novel Multistep Slurry Conversion Process. Crystal Growth and Design, 2020, 20, 7356-7367.	1.4	14

#	ARTICLE	IF	CITATIONS
4817	Highly Efficient Conversion of Ketazines to Pyrazoline Derivatives Catalyzed by FeCl ₃ . Industrial & Engineering Chemistry Research, 2020, 59, 18748-18755.	1.8	6
4818	Triply Carbonyl-Bridged Ni ₂ (CO) ₅ Featuring Triple Three-Center Two-Electron Niâ€”Ni Bonds Instead of Niâ‰‰Ni Triple Bond. Inorganic Chemistry, 2020, 59, 15365-15374.	1.9	3
4819	Characterization of Pushâ€”Pull-Type Benzo[X]quinoline Derivatives (X = gorf): Environmentally Responsive Fluorescent Dyes with Multiple Functions. Journal of Organic Chemistry, 2020, 85, 13177-13190.	1.7	11
4820	All Boron Atoms in a ScB ₁₂ Monolayer Contribute to the Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2020, 124, 23221-23229.	1.5	14
4821	Can modified DNA base pairs with chalcogen bonding expand the genetic alphabet? A combined quantum chemical and molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2020, 22, 23754-23765.	1.3	6
4822	Borataalkene or boratabenzene? Understanding the aromaticity of 9-borataphenanthrene anions and its central ring. New Journal of Chemistry, 2020, 44, 18069-18073.	1.4	13
4823	Planar tetracoordinate carbon molecules with 14 valence electrons: examples of CB ₄ M _n ⁺² (M = Li, Au; <i>n</i> = 1â€”3) clusters. New Journal of Chemistry, 2020, 44, 18293-18302.	1.4	7
4824	The mechanism and diastereoselectivity in the formation of trifluoromethyl-containing spiro[pyrrolidin-3,2â€”oxindole] by a catalyst-free and mutually activated [3+2]-cycloaddition reaction: a theoretical study. New Journal of Chemistry, 2020, 44, 17465-17476.	1.4	6
4825	Comparative study of gold and silver interactions with amino acids and nucleobases. RSC Advances, 2020, 10, 34149-34160.	1.7	33
4826	Appearance of V-encapsulated tetragonal prism motifs in VSi ₁₀ ⁺ and VSi ₁₁ ⁺ clusters. Physical Chemistry Chemical Physics, 2020, 22, 22989-22996.	1.3	10
4827	Effect of charge transport channel and interaction of IDT type dyes on photoelectric characteristics. Journal of Molecular Liquids, 2020, 303, 112594.	2.3	12
4828	Synthesis, structure and ethylene polymerisation activity of Polyhedron, 2020, 188, 114704.	1.0	2
4829	Improving phase-transfer catalysis by enhancing non-covalent interactions. Physical Chemistry Chemical Physics, 2020, 22, 21015-21021.	1.3	10
4830	Electronic structure of triangular M ₃ (M = B, Al, Ga): nonclassical three-center two electron Î€ bond and Iÿ delocalization. Physical Chemistry Chemical Physics, 2020, 22, 18071-18077.	1.3	5
4831	Seeded-growth preparation of high-performance Ni/MgAl ₂ O ₄ catalysts for tar steam reforming. New Journal of Chemistry, 2020, 44, 13692-13700.	1.4	11
4832	Intermolecular Interactions in 1,6-Diaminohexane + Water Mixtures at 293.15 to 333.15 K. Russian Journal of Physical Chemistry A, 2020, 94, 1356-1362.	0.1	5
4833	Highâ€”Capacity and Stable Liâ€”O ₂ Batteries Enabled by a Trifunctional Soluble Redox Mediator. Angewandte Chemie - International Edition, 2020, 59, 19311-19319.	7.2	62
4834	Synthesis, crystal structure, Hirshfeld surface analysis, spectral characterization, reduced density gradient and nonlinear optical investigation on (E)-N'-(4-nitrobenzylidene)-2-(quinolin-8-yloxy) acetohydrazide monohydrate: A combined experimental and DFT approach. Journal of Molecular Structure, 2020, 1222, 128952.	1.8	25

#	ARTICLE	IF	CITATIONS
4835	Origin of core-to-core x-ray emission spectroscopy sensitivity to structural dynamics. Structural Dynamics, 2020, 7, 044102.	0.9	14
4836	Molecular Structural Properties of [n]-Annulene (n = 8, 10, 12, 14) and its Boron Nitride Derivatives: Analysis of NMR, NBO, ELF and PDI. Journal of Structural Chemistry, 2020, 61, 207-224.	0.3	0
4837	The effects of functional groups on the sorption of naphthalene on microplastics. Chemosphere, 2020, 261, 127592.	4.2	48
4838	Photo-physical properties of vinigrol revealed by two-photon absorption, electronic circular dichroism, Raman spectroscopy and Raman optical activity. Chemical Physics Letters, 2020, 755, 137798.	1.2	4
4839	Centrosymmetric and asymmetric dimers of 5-(quinolinium)-valeric acid bromide monohydrate in crystal field and in silico. Journal of Molecular Structure, 2020, 1222, 128912.	1.8	0
4840	A rare hetero-bimetallic Zn(II)/Ca(II) Schiff base complex: Synthesis, crystal structure, DFT, molecular docking and unveiling antimicrobial activity. Journal of Molecular Structure, 2020, 1222, 128951.	1.8	34
4841	Unveiling the structural and energetic properties of thiazole-water complex by microwave spectroscopy and theoretical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 242, 118720.	2.0	8
4842	Removal of Methyl Ethyl Ketone and Sec-Butanol from Hydrogen by Absorption with Ionic Liquids. Industrial & Engineering Chemistry Research, 2020, 59, 14476-14484.	1.8	5
4843	Structure and Stability of the Ionic Liquid Clusters [EMIM] _n [BF ₄] _{n+1} ⁺ (<i>n</i> = 1-9): Implications for Electrochemical Separations. Journal of Physical Chemistry Letters, 2020, 11, 6844-6851.	2.1	12
4844	Selectively Scissoring Hydrogen-Bonded Cytosine Dimer Structures Catalyzed by Water Molecules. ACS Nano, 2020, 14, 10680-10687.	7.3	10
4845	Macrocyclic Ligands with an Unprecedented Size-Selectivity Pattern for the Lanthanide Ions. Journal of the American Chemical Society, 2020, 142, 13500-13506.	6.6	37
4846	Ligand engineering to achieve enhanced ratiometric oxygen sensing in a silver cluster-based metal-organic framework. Nature Communications, 2020, 11, 3678.	5.8	122
4847	Multicomponent supramolecular assembly of <i>p</i> -hydroxybenzoic acid and malonic acid: a deep insight into the formation of selective cocrystals. CrystEngComm, 2020, 22, 5628-5637.	1.3	9
4848	Effect of charge-transfer states on the vibrationally resolved absorption spectra and exciton dynamics in ZnPc aggregates: Simulations from a non-Markovian stochastic Schrödinger equation. Journal of Chemical Physics, 2020, 153, 034116.	1.2	18
4849	Towards understanding physical origin of 2175Å... extinction bump in interstellar medium. Monthly Notices of the Royal Astronomical Society, 2020, 497, 2190-2200.	1.6	11
4850	The geometry, electronic and magnetic properties of VLi _n (<i>n</i> = 2-13) clusters using the first-principles and PSO method. Molecular Physics, 2020, 118, .	0.8	2
4851	A quantum chemical view of the interaction of RNA nucleobases and base pairs with the side chains of polar amino acids. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-16.	2.0	3
4852	Molecular Property Analysis of Vegetable Insulating Oil Based on Quantum Chemical Calculation. , 2020, , .		1

#	ARTICLE	IF	CITATIONS
4853	Antioxidant Activity of Selected Phenolic Acids—Ferric Reducing Antioxidant Power Assay and QSAR Analysis of the Structural Features. <i>Molecules</i> , 2020, 25, 3088.	1.7	101
4854	Boosting the Quantum Efficiency of Ultralong Organic Phosphorescence up to 52% via Intramolecular Halogen Bonding. <i>Angewandte Chemie</i> , 2020, 132, 17604-17608.	1.6	55
4855	Diels–Alder Reactivity of a Chiral Anthracene Template with Symmetrical and Unsymmetrical Dienophiles: A DFT Study. <i>ChemistryOpen</i> , 2020, 9, 748-761.	0.9	4
4856	Photoinduced Changes in Aromaticity Facilitate Electrocyclization of Dithienylbenzene Switches. <i>Journal of the American Chemical Society</i> , 2020, 142, 13941-13953.	6.6	38
4857	Influence of phenylpropanoid units of lignin and its oxidized derivatives on the stability and \hat{I}^2O_4 binding properties: DFT and QTAIM approach. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 5897-5905.	1.5	8
4858	Computational Rationalization of the Interaction of $Fe(CO)_4$ and Substituted Benzyne Ligands. <i>Journal of Structural Chemistry</i> , 2020, 61, 197-206.	0.3	1
4859	2-Aminobenzothiazole-Containing Copper(II) Complex as Catalyst in Click Chemistry: An Experimental and Theoretical Study. <i>Catalysts</i> , 2020, 10, 776.	1.6	8
4860	Structures and Chemical Bonding in Antimony(III) Bromide Complexes with Pyridine. <i>Chemistry - A European Journal</i> , 2020, 26, 16338-16348.	1.7	10
4861	Aromaticity of 1-Heterocyclopropenes Containing an Atom of Group 14 or 4. <i>Organometallics</i> , 2020, 39, 2749-2762.	1.1	17
4862	Electric field effects on organic photovoltaic heterojunction interfaces: The model case of pentacene/C60. <i>Computational and Theoretical Chemistry</i> , 2020, 1186, 112914.	1.1	14
4863	On new solvatomorphs of the metalloligand $[Ni(o-van-en)]$. <i>Inorganica Chimica Acta</i> , 2020, 512, 119874.	1.2	3
4864	Photodegradation of Hexafluoropropylene Oxide Trimer Acid under UV Irradiation. <i>Journal of Environmental Sciences</i> , 2020, 97, 132-140.	3.2	8
4865	Janus alkaline earthides with excellent NLO response from sodium and potassium as source of excess electrons; a first principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107668.	1.3	27
4866	Theoretical and experimental investigation on decomposition mechanism of eco-friendly insulation gas HFO1234zeE. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107671.	1.3	12
4867	The equilibrium molecular structure of 3-methyl-4-nitro- and 4-methyl-3-nitrofuraxans by gas-phase electron diffraction and coupled cluster calculations. <i>Journal of Molecular Structure</i> , 2020, 1222, 128856.	1.8	7
4868	Spectroscopic and molecular structure investigation of Propachlor herbicide: A combined experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2020, 1221, 128866.	1.8	6
4869	Theoretical study of closo-borate derivatives of general type $[B_nH_n-1COR]_2$ ($n=6, 10, 12$; $R=H, CH_3$). <i>Journal of Molecular Structure</i> , 2020, 1221, 128866.	1.0	15
4870	Substituent Effect on Triplet State Aromaticity of Benzene. <i>Journal of Organic Chemistry</i> , 2020, 85, 4289-4297.	1.7	35

#	ARTICLE	IF	CITATIONS
4871	Ab Initio Molecular Dynamics Simulations of Aqueous Glucosamine Solutions: Solvation Structure and Mechanism of Proton Transfer from Water to Amino Group. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6986-6997.	1.2	6
4872	Variation of Energy Transfer Rates across Protein-Water Contacts with Equilibrium Structural Fluctuations of a Homodimeric Hemoglobin. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1148-1159.	1.2	18
4873	Molecular Origins of Photoinduced Backward Intramolecular Charge Transfer. <i>Journal of Physical Chemistry C</i> , 2020, 124, 16820-16826.	1.5	19
4874	Effects of adding cyanovinyl moiety on the photovoltaic DSSCs phosphonic acid based cells. <i>Journal of Computational Electronics</i> , 2020, 19, 1629-1644.	1.3	8
4875	Unveiling the high reactivity of strained dibenzocyclooctyne in [3 + 2] cycloaddition reactions with diazoalkanes through the molecular electron density theory. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4100.	0.9	21
4876	An efficient Brønsted acidic polymer resin for the carbonylation of formaldehyde to glycolic acid. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2020, 130, 1027-1042.	0.8	4
4877	Computational simulation of fluorinated methane derivatives in type I clathrate hydrate. <i>Journal of Molecular Liquids</i> , 2020, 314, 113783.	2.3	6
4878	Theoretical and experimental study of choline chloride-carboxylic acid deep eutectic solvents and their hydrogen bonds. <i>Journal of Molecular Structure</i> , 2020, 1222, 128849.	1.8	69
4879	Synthesis and thermal properties of magnetite nano structures and DFT analysis of Fe ₃ O ₄ cluster as its smallest representative unit*. <i>Journal of Molecular Structure</i> , 2020, 1222, 128895.	1.8	4
4880	Promising architectures modifying the D-A architecture of 2,3-dipentylidithieno[3,2-f:2',3'-h]quinoxaline-based dye as efficient sensitizers in dye-sensitized solar cells: A DFT study. <i>Materials Science in Semiconductor Processing</i> , 2020, 120, 105260.	1.9	20
4881	First-principles screening and design of C275-based organic dyes for highly efficient dye-sensitized solar cells. <i>Solar Energy</i> , 2020, 207, 759-766.	2.9	3
4882	Gas-Phase Hydration of Perillaldehyde Investigated by Microwave Spectroscopy Assisted by Computational Chemistry. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6511-6520.	1.1	5
4883	Insights into the Assembly of the Pseudogemini Surfactant at the Oil/Water Interface: A Molecular Simulation Study. <i>Langmuir</i> , 2020, 36, 1839-1847.	1.6	20
4884	Photoinduced Charge Transfer in Push/Pull Systems of Two-Photon Absorption. <i>ACS Omega</i> , 2020, 5, 17275-17286.	1.6	5
4885	Selective aerobic oxidative cleavage of lignin C-C bonds over novel hierarchical Ce-Cu/MFI nanosheets. <i>Applied Catalysis B: Environmental</i> , 2020, 279, 119343.	10.8	49
4886	Theoretical study of selective hydrogenolysis of methyl vinyl carbinol over Au-Ni bimetallic catalyst: Toward constructing a working hypothesis for the role of dichloroethane solvent and perimeter sites. <i>Chemical Physics Letters</i> , 2020, 754, 137773.	1.2	1
4887	Insight into Intermolecular Charge Transfer Determined by Two Packing Mode Cocrystals. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17744-17751.	1.5	14
4888	Insights into C=O insertion in a carbene/alkyne metathesis cascade reaction catalyzed by Rh ₂ (OAc) ₄ : a DFT study. <i>Catalysis Science and Technology</i> , 2020, 10, 5513-5524.	2.1	2

#	ARTICLE	IF	CITATIONS
4889	Butadienyl Diiron Complexes: Nonplanar Metallacenes Aromatics Involving π - π Type Orbital Overlap. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 19048-19053.	7.2	17
4890	Probing Au π -O and Au π -P regium bonding interaction in AuX (X = F, Cl, Br) π -RPHOH (R = CH ₃ , F, CF ₃ , NH ₂ , CN) complexes. <i>Computational and Theoretical Chemistry</i> , 2020, 1179, 112800.	1.1	7
4891	Theoretical study on the desulfurization mechanisms of thiophene and benzothiophene under inert and oxidative atmospheres. <i>Fuel</i> , 2020, 280, 118683.	3.4	11
4892	Demystifying the mechanism of NMP ligands in promoting Cu-catalyzed acetylene hydrochlorination: insights from a density functional theory study. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 3204-3216.	3.0	23
4893	Theoretical investigation on transformation of Cr(II) to Cr(V) complexes bearing tetra π -N-heterocyclic carbene and group transfer reactivity. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26340.	1.0	6
4894	A multiscale study on photophysical properties of a novel fluorescent probe for imaging amyloid β in Alzheimer's disease. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26344.	1.0	4
4895	Rational design of an unusual 2D-MOF based on Cu(μ_2) and 4-hydroxypyrimidine-5-carbonitrile as linker with conductive capabilities: a theoretical approach based on high-pressure XRD. <i>Chemical Communications</i> , 2020, 56, 9473-9476.	2.2	6
4896	Computational insights into the coupling mechanism of benzoic acid, phenoxy acetylene and dihydroisoquinoline catalyzed by silver ion as polarizer and stabilizer. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5903.	1.7	4
4897	Adsorption of sarin and chlorosarin onto the Al ₁₂ N ₁₂ and Al ₁₂ P ₁₂ nanoclusters: DFT and TDDFT calculations. <i>Surface and Interface Analysis</i> , 2020, 52, 725-734.	0.8	4
4898	Adsorption of cytarabine and gemcitabine anticancer drugs on the BNNT surface: DFT and GD3-DFT approaches. <i>Adsorption</i> , 2020, 26, 1365-1384.	1.4	5
4899	Lithium isotope effect in extraction of lithium chloride by 4-Aminobenzo-15-crown-5 in water-anisole ionic liquid double solvent system. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2020, 325, 673-682.	0.7	5
4900	Cyclic Voltammetric and DFT Analysis of the Reduction of Manganese(III) Complexes with 2-Hydroxybenzophenones. <i>Electroanalysis</i> , 2020, 32, 2913-2925.	1.5	4
4901	Tuning Nonlinear Optical Behavior by Incorporation of the Chalcogenophene into Twistacenes. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10766-10775.	1.2	7
4902	Study on structural growth behavior and simulated photoelectron spectroscopy of Sc ₂ Si _n (O, ω = 1) ($n = 8$) clusters using G4(MP2) theory. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	0
4903	A MEDT computational study of the mechanism, reactivity and selectivity of non-polar [3+2] cycloaddition between quinazoline-3-oxide and methyl 3-methoxyacrylate. <i>Journal of Molecular Modeling</i> , 2020, 26, 328.	0.8	6
4904	Insight into the separation mechanism of acetate anion-based ionic liquids on CO ₂ and N ₂ : A multi-scale simulation study. <i>Journal of Molecular Liquids</i> , 2020, 320, 114408.	2.3	6
4905	Reversible Mechanochromic Luminescence of Tetranuclear Cuprous Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 17213-17223.	1.9	29
4906	Dipole Moment Variation Clears Up Electronic Excitations in the π -Stacked Complexes of Fluorescent Protein Chromophores. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 6288-6297.	2.5	5

#	ARTICLE	IF	CITATIONS
4907	General Method for Enantioselective Three-Component Carbonylation of Alkenes Enabled by Visible-Light Dual Photoredox/Nickel Catalysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 20390-20399.	6.6	136
4908	Theoretical study on reaction mechanism of phosphate-catalysed N ⁺ S acyl transfer of N-sulfanylethylamide (SEAlide). <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 9706-9711.	1.5	6
4909	Modelling the structural and reactivity landscapes of tucatinib with special reference to its wavefunction-dependent properties and screening for potential antiviral activity. <i>Journal of Molecular Modeling</i> , 2020, 26, 341.	0.8	35
4910	Bis(silanetellurone) with H ⁺ Te Interaction. <i>Inorganic Chemistry</i> , 2020, 59, 17811-17821.	1.9	9
4911	⁺ σ-Hole Interactions: A Comparative Investigation Based on Boron-Containing Molecules. <i>ChemistrySelect</i> , 2020, 5, 13223-13231.	0.7	12
4912	A topological study of the hexacoordinated carbon in the pentagonal-pyramidal benzene and hexamethylbenzene dications. <i>Chemical Physics Letters</i> , 2020, 758, 137912.	1.2	5
4913	Electride Characteristics of Some Binuclear Sandwich Complexes of Alkaline Earth Metals, M ₂ (L ⁺) ₂ (M = Be, Mg; L =) <i>TJ ETQq0 0 0 rgBT /Overlock 10 Tf 50 502 Td (C₅H₅)</i>	1.1	17
4914	Anchoring a bow-shaped boron single chain in binary BeB ₇ cluster: hybrid octagonal ring, multifold aromaticity, and dual electronic transmutation. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25574-25583.	1.3	6
4915	The Al-Al triple bond in Al ₂ X ₅ ⁺ and Al ₂ X ₆ ²⁺ (X = Li, Na) clusters with multiple alkali metal coordination. <i>New Journal of Chemistry</i> , 2020, 44, 21119-21124.	1.4	4
4916	From σ - to π - experimental and theoretical insights into the atmospheric degradation mechanism of dithiophosphinic acids. <i>RSC Advances</i> , 2020, 10, 40035-40042.	1.7	1
4917	Predicting the efficiency of polyethylene glycol-functionalised graphene in delivery of temozolomide anticancer drug and investigating the effect of pH on the drug release process: DFT and free energy calculations. <i>Molecular Simulation</i> , 2020, 46, 1474-1482.	0.9	7
4918	Experiment and simulation for CO ₂ capture using low transition temperature mixtures as solvents. <i>International Journal of Greenhouse Gas Control</i> , 2020, 103, 103178.	2.3	4
4919	Theoretical analysis of the spodium bonds in HgCl ₂ ·L (L = ClR, SR ₂ , and PR ₃) dimers. <i>Chemical Physics</i> , 2020, 539, 110978.	0.9	18
4920	Polynitro-acetone, dimethyl ether, and dimethylamine: a series of potential green and powerful oxidants for propellants. <i>Journal of Molecular Modeling</i> , 2020, 26, 347.	0.8	1
4921	Phosphorescent Tetradentate Platinum(II) Complexes Containing Fused 6/5/5 or 6/5/6 Metalloacycles. <i>Inorganic Chemistry</i> , 2020, 59, 18109-18121.	1.9	12
4922	Aqueous Systems with Tunable Fluorescence Including White-Light Emission for Anti-Counterfeiting Fluorescent Inks and Hydrogels. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 55269-55277.	4.0	39
4923	Tuning the photomechanical behavior and excellent elasticity of azobenzene <i>via</i> cocrystal engineering. <i>CrystEngComm</i> , 2020, 22, 8045-8053.	1.3	21
4924	Synthesis and properties of salts derived from C ₄ N ₁₈ ²⁺ , C ₄ N ₁₈ H ₃ ⁺ and C ₄ N ₁₈ H ₃ ⁺ anions. <i>Journal of Materials Chemistry A</i> , 2020, 8, 25035-25039.	5.2	29

#	ARTICLE	IF	CITATIONS
4925	Hydrogen generation from water splitting by catalysts of platinum-based clusters Pt ₃ X (X=Al, Si, Cu) and CO oxidation by their by-products. Chinese Journal of Chemical Physics, 2020, 33, 58-64.	0.6	4
4926	Theoretical studies on dihedral angle-bending isomers of M ₂ Pt ₂₀ /n clusters. Chinese Journal of Chemical Physics, 2020, 33, 450-458.	0.6	0
4927	Theoretical investigation on hydrogen bond interaction between adrenaline and hydrogen sulfide. Journal of Molecular Modeling, 2020, 26, 354.	0.8	18
4928	N-Heterocyclic carbene (NHC)-catalyzed oxidative [3+2] annulation of dioxindoles and enals: mechanism, role of NHC, role of a mixture of bases with different strength, and origin of stereoselectivity. Physical Chemistry Chemical Physics, 2020, 22, 28269-28276.	1.3	4
4929	Al ³⁺ regulated competition between TICT and ESIPT of a chemosensor. Journal of Luminescence, 2020, 228, 117657.	1.5	11
4930	Coassembly of C ₁₃ -Dipeptides: Gelations from Solutions and Precipitations. Biomacromolecules, 2020, 21, 5256-5268.	2.6	3
4931	Determinant Factor for Thermodynamic Stability of Sulfuric Acid-Amine Complexes. Journal of Physical Chemistry A, 2020, 124, 10246-10257.	1.1	8
4932	Computational Study on Metal-Ion-Decorated Prismane Molecules for Selective Adsorption of CO ₂ from Flue Gas Mixtures. ACS Omega, 2020, 5, 31146-31155.	1.6	4
4933	Efficient TiO ₂ /SubPc photocatalyst for degradation of organic dyes under visible light. New Journal of Chemistry, 2020, 44, 21192-21200.	1.4	12
4934	Microscopic insight into nanodiamond polymer composites: reinforcement, structural, and interaction properties. Nanoscale, 2020, 12, 24107-24118.	2.8	45
4935	Structure of Organic Compound (E)-3-((S)-1-Phenylethylamine)methylene R (+) Camphor. Crystallography Reports, 2020, 65, 1150-1155.	0.1	0
4936	Proton Transfer and Nitro Rotation Tuned Photoisomerization of Artificial Base Pair-ZP. Frontiers in Chemistry, 2020, 8, 605117.	1.8	15
4937	Comparison of the Reactivity and Structures for the Neutral and Cationic Bis(imino)pyridyl Iron and Cobalt Species by DFT Calculations. Catalysts, 2020, 10, 1396.	1.6	6
4938	Ground and excited state geometrical and optical properties of Au (n=13) nanoclusters: A first-principles study. Computational and Theoretical Chemistry, 2020, 1190, 113007.	1.1	4
4939	Theoretical Design of Dithienopicenocarbazole-Based Molecules by Molecular Engineering of Terminal Units Toward Promising Non-fullerene Acceptors. Frontiers in Chemistry, 2020, 8, 580252.	1.8	7
4940	Polyfuran-based chemical sensors: Identification of promising derivatives via DFT calculations and fully atomistic reactive molecular dynamics. European Polymer Journal, 2020, 141, 110085.	2.6	14
4941	N-(2-Aminoethyl)-2-(hexylthio) Acetamide-Functionalized Pillar[5]arene for the Selective Detection of Trp through Guest-Adaptive Multisupramolecular Interactions. Journal of Physical Chemistry A, 2020, 124, 9811-9817.	1.1	20
4942	The supramolecular self-assembly of 5-fluorouracil and caffeic acid through cocrystallization strategy opens up a new way for the development of synergistic antitumor pharmaceutical cocrystal. CrystEngComm, 2020, 22, 7992-8006.	1.3	19

#	ARTICLE	IF	CITATIONS
4943	Targeted Synthesis of NIR Luminescent Rhenium Diimine <i>cis,trans</i> -[Re(CO) ₂ (L) ₂] ⁿ⁺ Complexes Containing N-Donor Axial Ligands: Photophysical, Electrochemical, and Theoretical Studies. <i>ChemPlusChem</i> , 2020, 85, 2518-2527.	1.3	8
4944	Bicyclic Guanidine-Catalyzed Asymmetric Cycloaddition Reaction of Anthrones' Bifunctional Binding Modes and Origin of Stereoselectivity. <i>Journal of Organic Chemistry</i> , 2020, 85, 15139-15153.	1.7	7
4945	<i>In situ</i> textured carbon nitride photoanodes with enhanced photoelectrochemical activity by band-gap state modulation. <i>Journal of Materials Chemistry A</i> , 2020, 8, 24005-24012.	5.2	9
4946	Encapsulation of Highly Volatile Fragrances in Y Zeolites for Sustained Release: Experimental and Theoretical Studies. <i>ACS Omega</i> , 2020, 5, 31925-31935.	1.6	23
4947	Halogen bonding interactions in the XC ₅ H ₄ N·YCF ₃ (X = CH ₃ , H, Cl, CN, NO ₂ ; Y = Cl, Br, I) complexes. <i>Journal of Molecular Modeling</i> , 2020, 26, 344.	0.8	3
4948	Effect of the nature of lanthanide on intramolecular C-F†Ln dative interactions in hexafluoroisopropoxide complexes. <i>Russian Chemical Bulletin</i> , 2020, 69, 2082-2090.	0.4	2
4949	Isometric Thionated Naphthalene Diimides As Organic Cathodes for High Capacity Lithium Batteries. <i>Chemistry of Materials</i> , 2020, 32, 10575-10583.	3.2	26
4950	Controlling MÃ¶bius-Type Helicity and the Excited-State Properties of Cumulenes with Carbenes. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10100-10110.	1.1	16
4951	Intramolecular Energy Transfer in a Series of Star-Shaped Molecules with a Central Porphyrin Core and Four Oligocarbazole Arms. <i>Journal of Physical Chemistry C</i> , 2020, 124, 27356-27365.	1.5	2
4952	Codeposition of Levodopa and Polyethyleneimine: Reaction Mechanism and Coating Construction. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 54094-54103.	4.0	39
4953	Origin of the Enhanced Reusability and Electron Transfer of the Carbon-Coated Mn ₃ O ₄ Nanocube for Persulfate Activation. <i>ACS Catalysis</i> , 2020, 10, 14857-14870.	5.5	151
4954	Quantum Chemical Study of Interaction between Titanocene Dichloride Anticancer Drug and Al ₁₂ N ₁₂ Nano-Cluster. <i>Russian Journal of Inorganic Chemistry</i> , 2020, 65, 1726-1734.	0.3	12
4955	Isomerism and Biradical Character of Tetrapnictide Dianions: A Computational Study. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 3580-3586.	1.0	6
4956	F ₂ BMF (M = V, Nb, and Ta) and FBMF ₂ (M = Nb and Ta): A Combined Matrix Isolation Infrared Spectroscopic and Quantum Chemical Investigation. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8192-8200.	1.1	0
4957	Photoelectrochemical Performance Enhancement of ZnSe Nanorods versus Dots: Combined Experimental and Computational Insights. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10414-10420.	2.1	5
4958	Development of Immobilized SPINOL-Derived Chiral Phosphoric Acids for Catalytic Continuous Flow Processes. Use in the Catalytic Desymmetrization of 3,3-Disubstituted Oxetanes. <i>ACS Catalysis</i> , 2020, 10, 14971-14983.	5.5	19
4959	Theoretical study on the photochemistry of furoylazides: Curtius rearrangement and subsequent reactions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 28317-28324.	1.3	9
4960	The structure and hydrogen-bond properties of <i>N</i> -alkyl- <i>N</i> -methyl-pyrrolidinium bis(trifluoromethylsulfonyl)imide and DMSO mixtures. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 28021-28031.	1.3	11

#	ARTICLE	IF	CITATIONS
4961	The preferred conformation of the tetrafluoro-1,3-dithietane ⁻ isopropylamine complex as revealed by rotational spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 28339-28344.	1.3	2
4962	Quantum Chemical, Vibrational Spectroscopic and Molecular Docking Studies of 1-(Diphenylmethyl)Piperazine. <i>Polycyclic Aromatic Compounds</i> , 2020, , 1-21.	1.4	4
4963	Experimental and Molecular Dynamics Simulation Study on the Primary Nucleation of Penicillamine Racemate and Its Enantiomers in the Mixture Solvent of Water and Ethanol. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 21957-21968.	1.8	13
4964	Achieving Different Color Changes for Photochromic Compounds by Controlling Coordination Modes. <i>Journal of Physical Chemistry C</i> , 2020, 124, 27680-27686.	1.5	18
4965	Two conformational polymorphs of 4-methylhippuric acid. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 1077-1091.	0.5	3
4966	Intramolecular Hydrogen Bonds in Tip-Functionalized Single-Walled Carbon Nanotubes as pH-Sensitive Gates. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9542-9551.	1.1	6
4967	Achieving Ultrahigh Volumetric Energy Storage by Compressing Nitrogen and Sulfur Dual ⁺ Doped Carbon Nanocages via Capillarity. <i>Advanced Materials</i> , 2020, 32, e2004632.	11.1	56
4968	B36 bowl-like structure as nanocarrier for sulfonamides: a theoretical study. <i>Monatshefte für Chemie</i> , 2020, 151, 1785-1796.	0.9	2
4969	Heat-resistant and shape-memory metallo-supramolecules with simultaneously switchable fluorescence behavior supported by tridentate N3 group. <i>Polymer</i> , 2020, 208, 122886.	1.8	3
4970	Reply to "Comment on "Theoretical Insights into the Excited State Decays of a Donor ⁺ Acceptor Dyad: Is the Twisted and Rehybridized Intramolecular Charge-Transfer State Involved?" TM ". <i>Journal of Physical Chemistry B</i> , 2020, 124, 10582-10584.	1.2	1
4971	Conformation-Dependent Phosphorescence of Galactose-Decorated Phosphors and Assembling-Induced Phosphorescence Enhancement. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 52059-52069.	4.0	18
4972	Intermolecular Interactions Involving Heavy Alkenes H ₂ Si ⁺ H ₂ (T = C, Si, Ge, Sn,) Tj ETQq _{1.1} 0.784314 rgB	1.6	9
4973	Mössbauer isomer shifts and effective contact densities obtained by the exact two-component (X2C) relativistic method and its local variants. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26776-26786.	1.3	7
4974	Regulating the reactivity of black phosphorus via protective chemistry. <i>Science Advances</i> , 2020, 6, .	4.7	37
4975	Low-Dimensional Hybrid Indium/Antimony Halide Perovskites: Supramolecular Assembly and Electronic Properties. <i>Journal of Physical Chemistry C</i> , 2020, 124, 25686-25700.	1.5	23
4976	Revealing the role of nitrogen dopants in tuning the electronic and optical properties of graphene quantum dots <i>via</i> a TD-DFT study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 28230-28237.	1.3	17
4977	Improved Modeling of Thioamide FRET Quenching by Including Conformational Restriction and Coulomb Coupling. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10653-10662.	1.2	5
4978	A theoretical study on the alkali metal carboxylate ⁻ promoted <sc>L ⁻ Lactide</sc> polymerization. <i>Journal of Computational Chemistry</i> , 2020, 41, 2197-2202.	1.5	9

#	ARTICLE	IF	CITATIONS
4979	Mechanisms of Csp ² â€“H functionalization of aldehydes with triplet O ₂ catalyzed by NHPI: A density functional theory investigation. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4112.	0.9	7
4980	Understanding the Chemical Insights of Staple Motifs of Thiolateâ€“Protected Gold Nanoclusters. <i>Small</i> , 2021, 17, e2001836.	5.2	19
4981	A novel near-infrared fluorescent probe for intracellular detection of cysteine. <i>Analytical and Bioanalytical Chemistry</i> , 2020, 412, 7211-7217.	1.9	6
4982	The study on the interactions of two 1,2,3-triazoles with several biological macromolecules by multiple spectroscopic methodologies and molecular docking. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 243, 118795.	2.0	5
4983	Screening Borane Species for Dinitrogen Activation. <i>Inorganic Chemistry</i> , 2020, 59, 11770-11781.	1.9	34
4984	Comprehensive Photophysical Properties of Thiophene/Phenylene Co-oligomers Investigated by Theoretical and Experimental Studies. <i>Journal of Physical Chemistry C</i> , 2020, 124, 18946-18955.	1.5	4
4985	Density Functional Theoretical Study on the Electronic Structure of Rh ₂ O ₇ with Low Oxidation States. <i>ACS Omega</i> , 2020, 5, 19422-19428.	1.6	1
4986	A nature-inspired hydrogen-bonded supramolecular complex for selective copper ion removal from water. <i>Nature Communications</i> , 2020, 11, 3947.	5.8	86
4987	From the Linnettâ€“Gillespie model to the polarization of the spin valence shells of metals in complexes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 24201-24212.	1.3	4
4988	On the relations between backbone thiophene functionalization and charge carrier mobility of Aâ€“Dâ€“A type small molecules. <i>New Journal of Chemistry</i> , 2020, 44, 15177-15185.	1.4	6
4989	A Ti-MOF Decorated With a Pt Nanoparticle Cocatalyst for Efficient Photocatalytic H ₂ Evolution: A Theoretical Study. <i>Frontiers in Chemistry</i> , 2020, 8, 660.	1.8	8
4990	Crystal Structures and Fluorescence Spectroscopic Properties of a Series of Î±,Î±â€“Di(4â€“pyridyl)polyenes: Effect of Aggregationâ€“Induced Emission. <i>ChemPlusChem</i> , 2020, 85, 1968-1980.	1.3	3
4991	Tuning the optical properties of (TiO ₂) ₂ via the electric field. <i>Optik</i> , 2020, 221, 165395.	1.4	11
4992	Desymmetrized Vertex Design toward a Molecular Cage with Unusual Topology. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 20846-20851.	7.2	44
4993	A Sterically Hindered Derivative of 2,1,3â€“Benzotelluradiazole: Aâ€“Way to the First Structurally Characterised Monomeric Telluriumâ€“Nitrogen Radical Anion. <i>Chemistry - A European Journal</i> , 2020, 26, 14688-14699.	1.7	11
4994	Influence of alkali substituents on the strength, properties, and nature of tetrel bond between TH3F and pyridine. <i>Journal of Molecular Modeling</i> , 2020, 26, 224.	0.8	2
4995	Theoretical investigation on interactions between coinage-metal and IIIA-atom. <i>Journal of Molecular Modeling</i> , 2020, 26, 227.	0.8	1
4996	Hydroxynaphthalenecarboxamides and substituted piperazinylpropanediols, two new series of BRAF inhibitors. A theoretical and experimental study. <i>Bioorganic Chemistry</i> , 2020, 103, 104145.	2.0	8

#	ARTICLE	IF	CITATIONS
4997	Selective hydrogenation of acetylene catalyzed by nickel and nitrogen-doped C34: A density functional theory study. <i>Chemical Physics Letters</i> , 2020, 757, 137871.	1.2	4
4998	Asymmetric ITIC acceptor for asymmetric benzodithiophene polymer solar cells. <i>Dyes and Pigments</i> , 2020, 183, 108727.	2.0	3
4999	Theoretical insights on type I/II photoreactions of potential Zn(II) polypyridyl photosensitizers for two-photon photodynamic therapy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 242, 118771.	2.0	3
5000	Optical physics on chiral brominated azapirones: Bromophilone A and B. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 242, 118780.	2.0	5
5001	Lewis Amphiphilicity of 1,2,5-Chalcogenadiazoles for Crystal Engineering: Complexes with Crown Ethers. <i>Crystal Growth and Design</i> , 2020, 20, 5868-5879.	1.4	10
5002	Theoretical Prediction of the Potential Applications of Phenanthroline Derivatives in Separation of Transplutonium Elements. <i>Inorganic Chemistry</i> , 2020, 59, 11469-11480.	1.9	28
5003	Structures, Electronic, and Spectral Properties of Doped Boron Clusters $MB_{12}O_n$ (M = Li, Na, and K). <i>ACS Omega</i> , 2020, 5, 20525-20534.	1.6	16
5004	Revealing the Photophysical Mechanism of N,N' -Diphenyl-aniline Based Sensitizers with the DFT Framework: Theoretical Insights. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 13328-13341.	3.2	36
5005	Molecular engineering of dispersed nickel phthalocyanines on carbon nanotubes for selective CO ₂ reduction. <i>Nature Energy</i> , 2020, 5, 684-692.	19.8	365
5006	Globally stabilized bent carbon-carbon triple bond by hydrogen-free inorganic-metallic scaffolding Al ₄ F ₆ . <i>RSC Advances</i> , 2020, 10, 25275-25280.	1.7	0
5007	Molecular doping in few-molecule polymer-dopant complexes shows reduced Coulomb binding. <i>Journal of Materials Chemistry C</i> , 2020, 8, 11929-11935.	2.7	8
5008	Heteroligand Cu(II) Complexes with 2-Halogenopyridines: Crystal Structure and Features of Halogen-Halogen Contacts in the Solid State. <i>Journal of Structural Chemistry</i> , 2020, 61, 712-718.	0.3	8
5009	A CAM-B3LYP DFT Investigation of Atenolol Adsorption on the Surface of Boron Nitride and Carbon Nanotubes and Effect of Surface Carboxylic Groups. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 1678-1693.	0.1	1
5010	Reactivity of Aliphatic and Aromatic Nitrocompounds in the Triplet State with Respect to Amines. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 1603-1606.	0.1	1
5011	Theoretical Investigation on Structure-Property Relationship of Asymmetric Clusters (CH ₃ FBN ₃) _n (n = 1-6). <i>Journal of Chemistry</i> , 2020, 2020, 1-11.	0.9	0
5012	Detailed spectra, electronic properties, qualitative non-covalent interaction analysis, solvatochromism, docking and molecular dynamics simulations in different solvent atmosphere of cenobamate. <i>Structural Chemistry</i> , 2020, 31, 2475-2485.	1.0	45
5013	A thorough theoretical exploration of the effect mechanism of Fe on HCN heterogeneous formation from nitrogen-containing char. <i>Fuel</i> , 2020, 280, 118662.	3.4	29
5014	Theoretical Insight into Thermodynamically Optimal U@C ₈₄ : Three-Electron Transfer Rather Than Four-Electron Transfer. <i>Inorganic Chemistry</i> , 2020, 59, 12650-12658.	1.9	6

#	ARTICLE	IF	CITATIONS
5015	Synergy of activating substrate and introducing C-H...O interaction to achieve Rh ₂ (II)-catalyzed asymmetric cycloisomerization of 1, <i>n</i> -enynes. <i>Science China Chemistry</i> , 2020, 63, 1230-1239.	4.2	19
5016	An in-situ spectroscopy investigation of alkali metal interaction mechanism with the imide functional group. <i>Nano Research</i> , 2020, 13, 3224-3229.	5.8	11
5017	Optoelectronic properties of diathiafulvalene-functionalized diketopyrrolopyrrole...fullerene molecular dyad. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 242, 118767.	2.0	3
5018	Terminal Phosphinidene Complex Adducts with Neutral and Anionic O-Donors and Halides and the Search for a Differentiating Bonding Descriptor. <i>Inorganic Chemistry</i> , 2020, 59, 12829-12841.	1.9	22
5019	Directly linked metalloporphyrins: a quest for bio-inspired materials. <i>Materials Advances</i> , 2020, 1, 1895-1908.	2.6	4
5020	Dynamical properties of enzyme...substrate complexes disclose substrate specificity of the SARS-CoV-2 main protease as characterized by the electron density descriptors. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19069-19079.	1.3	29
5021	High...Capacity and Stable Li... ₂ Batteries Enabled by a Trifunctional Soluble Redox Mediator. <i>Angewandte Chemie</i> , 2020, 132, 19473-19481.	1.6	28
5022	Theoretical reinvestigation of the ozonolysis mechanism of allyl alcohol. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26387.	1.0	0
5023	The synergistic inhibitory effect and density functional theory study of 2,2...-[[[(Methyl-1H-benzotriazol-1-yl)methyl]imino]bisethanol and potassium oleate on copper in H ₂ O ₂ based alkaline slurries. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 603, 125275.	2.3	25
5024	Measurement, modelling and molecular dynamics analysis for isobaric vapour-liquid equilibria of binary or ternary system (diethylamine, ethyl acetate, triethylamine). <i>Journal of Chemical Thermodynamics</i> , 2020, 151, 106251.	1.0	4
5025	The interaction nature between hollow silica-based porous ionic liquids and CO ₂ : A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107694.	1.3	21
5026	Topological population analysis and pairing/unpairing electron distribution evolution: Atomic B ₃ ⁺ cluster bending mode, a case study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107696.	1.3	1
5027	Interpreting main features of the differential absorbance spectra of chlorinated natural organic matter: Comparison of the experimental and theoretical spectra of model compounds. <i>Water Research</i> , 2020, 185, 116206.	5.3	9
5028	Fluorescence Toggling Mechanism of Photochromic Phenylhydrazones: N...N Single Bond Rotation-Assisting... Photoisomerization Differs from Imine. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6411-6419.	1.1	5
5029	A microscopic and macroscopic investigation of the adsorption of N719 dye on ZnO nanopowders (ZNP) and ZnO nanorods (ZNR) for dye sensitized solar cells using statistical physics treatment and DFT simulation. <i>RSC Advances</i> , 2020, 10, 27615-27632.	1.7	12
5030	Modulating excited...state intramolecular proton transfer of 2...-(4...carboxyphenyl)...(2...hydroxyphenyl)benzothiazole depending on substituents: A DFT/TD...DFT study. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4109.	0.9	4
5031	Energetic Triazolo...Triazolo...Furazano...Pyrazines: A Promising Fused Tetracycle Building Block with Diversified Functionalities and Properties. <i>ChemistrySelect</i> , 2020, 5, 8557-8561.	0.7	8
5032	Microscopic mechanism for effect of sodium on NO heterogeneous reduction by char. <i>Journal of Fuel Chemistry and Technology</i> , 2020, 48, 663-673.	0.9	16

#	ARTICLE	IF	CITATIONS
5033	Sludge-derived biochar as efficient persulfate activators: Sulfurization-induced electronic structure modulation and disparate nonradical mechanisms. <i>Applied Catalysis B: Environmental</i> , 2020, 279, 119361.	10.8	240
5034	Unravelling phosphate adsorption on hydrous ferric oxide surfaces at the molecular level. <i>Chemosphere</i> , 2020, 261, 127776.	4.2	17
5035	Exploring two-dimensional graphene and boron-nitride as potential nanocarriers for cytarabine and clofarabine anti-cancer drugs. <i>Computational Biology and Chemistry</i> , 2020, 88, 107334.	1.1	10
5036	Optical properties of kalihinol derivatives in TPA, ECD and ROA. <i>Chemical Physics Letters</i> , 2020, 755, 137796.	1.2	3
5037	Structural characterization, electronic properties, and anxiolytic-like effect in adult zebrafish (<i>Danio rerio</i>) of cinnamaldehyde chalcone. <i>Journal of Molecular Structure</i> , 2020, 1222, 128954.	1.8	15
5038	Properties of gaseous $[B_{6X_6}]^{2-}$ dianions (X = Cl, Br, I). <i>Journal of Molecular Structure</i> , 2020, 1222, 128954.	1.3	12
5039	A DFT/TDDFT and QTAIM based investigation of the titanium-doped Boron-38 cluster. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	6
5040	Removal of sulfamethoxazole, sulfadiazine, and sulfamethazine by UV radiation and HO \cdot and SO $_4^{\cdot-}$ radicals using a response surface model and DFT calculations. <i>Environmental Science and Pollution Research</i> , 2020, 27, 41609-41622.	2.7	11
5041	Treatment of adsorption of dioxane by using SiCNT toward efficient remediation of refractory organic contaminants from wastewater: DFT and DFTB-MD simulations. <i>Journal of Molecular Liquids</i> , 2020, 316, 113869.	2.3	4
5042	Catalytic Effect of Alkali and Alkaline Earth Metals in Lignin Pyrolysis: A Density Functional Theory Study. <i>Energy & Fuels</i> , 2020, 34, 9734-9740.	2.5	32
5043	Changes in Structure and Reactivity of Ng $_2$ Encapsulated in Fullerenes: A Density Functional Theory Study. <i>Frontiers in Chemistry</i> , 2020, 8, 566.	1.8	7
5044	Structure and Stability of Aromatic Nitrogen Heterocycles Used in the Field of Energetic Materials. <i>Molecules</i> , 2020, 25, 3232.	1.7	16
5045	Arthrinins E, G, Three Botryane Sesquiterpenoids from the Plant Endophytic Fungus <i>Arthrinium</i> sp. HS66. <i>Natural Products and Bioprospecting</i> , 2020, 10, 201-207.	2.0	5
5046	Effects of π -bridge units on the properties of donor-acceptor type benzodithiophene-thienothiophene based polymers for organic solar cells. <i>Chemical Physics Letters</i> , 2020, 756, 137810.	1.2	7
5047	Investigation of polyvinylpyrrolidone as an inhibitor for trench super-filling of cobalt electrodeposition. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2020, 112, 232-239.	2.7	13
5048	Structural and electronic properties of graphene and its derivatives physisorbed by ionic liquids. <i>Diamond and Related Materials</i> , 2020, 109, 108005.	1.8	12
5049	Aerobically-initiated C(sp 3)-H bond amination through the use of activated azodicarboxylates. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 6258-6264.	1.5	11
5050	Noble Gas Binding Ability of an Au(I) Cation Stabilized by a Frustrated Lewis Pair: A DFT Study. <i>Frontiers in Chemistry</i> , 2020, 8, 616.	1.8	4

#	ARTICLE	IF	CITATIONS
5051	Theoretical Insights into the Effect of Cations, Anions, and Water on Fixation of CO ₂ Catalyzed by Different Ionic Liquids. <i>ChemSusChem</i> , 2020, 13, 6391-6400.	3.6	13
5052	Interatomic exchange-correlation interaction energy from a measure of quantum theory of atoms in molecules topological bonding: A diatomic case. <i>Journal of Computational Chemistry</i> , 2020, 41, 2213-2222.	1.5	16
5053	Achieving Good Molecular Stability in Nitrogen-rich Salts Based on Polyamino Substituted Furazan-triazole. <i>Crystal Growth and Design</i> , 2020, 20, 6084-6092.	1.4	18
5054	Classifying the chemical bonds involving the noble-gas atoms. <i>New Journal of Chemistry</i> , 2020, 44, 14536-14550.	1.4	17
5055	Metal-only Lewis Pairs of Rhodium with <i>s</i> , <i>p</i> and <i>d</i> -Block Metals. <i>Chemistry - A European Journal</i> , 2020, 26, 16833-16845.	1.7	22
5056	Design, molecular docking analysis of an anti-inflammatory drug, computational analysis and intermolecular interactions energy studies of 1-benzothiophene-2-carboxylic acid. <i>Computational Biology and Chemistry</i> , 2020, 88, 107348.	1.1	49
5057	Microscopic properties of two 1-(2-hydroxyethyl)-3-methylimidazolium-based ionic liquids and methanol mixtures. <i>Journal of Molecular Liquids</i> , 2020, 313, 113578.	2.3	5
5058	Interesting spin state properties of iron(II) polypyridine complex substituted by fluorine: A theoretical study. <i>Organic Electronics</i> , 2020, 85, 105884.	1.4	1
5059	Efficient strategies for improving the performance of EDOT derivatives and TPA derivatives-based hole transport materials for perovskite solar cells. <i>Solar Energy</i> , 2020, 208, 10-19.	2.9	14
5060	Step Forward to Stronger Neutral Organic Superbases: Fused Troponimines. <i>Journal of Organic Chemistry</i> , 2020, 85, 11375-11381.	1.7	10
5061	Photoinduced Charge Separation via the Double-Electron Transfer Mechanism in Nitrogen Vacancies g-C ₃ N ₅ /BiOBr for the Photoelectrochemical Nitrogen Reduction. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 38266-38274.	4.0	94
5062	Heterometallic metallacyclophanes constructed from side-off bicompartamental ligands. <i>Journal of Coordination Chemistry</i> , 2020, 73, 2773-2785.	0.8	0
5063	Revisiting (anti)aromaticity and chemical bond in planar B _x N _x clusters (x =) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.6	5
5064	Theoretical prediction of the impact sensitivities of energetic C-nitro compounds. <i>Journal of Molecular Modeling</i> , 2020, 26, 219.	0.8	4
5065	Self-association process of tetracycline antibiotic in different aqueous solutions: a joint experimental study and molecular dynamics simulation. <i>Journal of the Iranian Chemical Society</i> , 2020, 17, 2997-3007.	1.2	4
5066	Influence of P,S,O-Doping on g-C ₃ N ₄ for hydrogel formation and photocatalysis: An experimental and theoretical study. <i>Carbon</i> , 2020, 169, 338-348.	5.4	153
5067	Azomethine ylide addition impact on functionalized [60]Fullerene and [60]Boron-Nitride: Anticancer Doxorubicin and Boronic Chalcone drugs binding characteristics with mono- and bis-nanocarriers. <i>Colloids and Surfaces B: Biointerfaces</i> , 2020, 196, 111277.	2.5	7
5068	Mechanism study on the oxidation of ethylbenzene: A theoretical and computational approach. <i>Computational and Theoretical Chemistry</i> , 2020, 1188, 112974.	1.1	3

#	ARTICLE	IF	CITATIONS
5069	A comprehensive exploration of mercury adsorption sites on the carbonaceous surface: A DFT study. <i>Fuel</i> , 2020, 282, 118781.	3.4	34
5070	Ionic liquids simultaneously used as accelerants, stabilizers and extractants for improving the cannabidiol extraction from industrial hemp. <i>Industrial Crops and Products</i> , 2020, 155, 112796.	2.5	9
5071	Prediction of key photoelectric parameters at the interface of new subAPPC/C60 organic solar cell. <i>Materials Chemistry and Physics</i> , 2020, 255, 123616.	2.0	3
5072	Novel axial substituted subphthalocyanine and its TiO ₂ photocatalyst for degradation of organic water pollutant under visible light. <i>Optical Materials</i> , 2020, 109, 110202.	1.7	27
5073	Influence of geometry of mobile counteranions on conductivity, polarization and electrorheological effect of polymeric anionic liquids at ice point temperature. <i>Polymer</i> , 2020, 205, 122826.	1.8	15
5074	The origin of the high reactivity of triazolinediones (TADs) in Diels-Alder reactions from a theoretical perspective. <i>Tetrahedron</i> , 2020, 76, 131459.	1.0	4
5075	Mechanistic Insight into the Catalytic NO Oxidation by the MIL-100 MOF Platform: Toward the Prediction of More Efficient Catalysts. <i>ACS Catalysis</i> , 2020, 10, 9445-9450.	5.5	22
5076	Spiro-type host materials with rigidified skeletons for RGB phosphorescent OLEDs. <i>Journal of Materials Chemistry C</i> , 2020, 8, 12470-12477.	2.7	13
5077	The Lewis acidities of gold(I) and gold(III) derivatives: a theoretical study of complexes of AuCl and AuCl ₃ . <i>Structural Chemistry</i> , 2020, 31, 1909-1918.	1.0	11
5078	Mechanistic insight into the rhodium-catalyzed, P-directed selective C7 arylation of indoles: a DFT study. <i>Molecular Catalysis</i> , 2020, 495, 111147.	1.0	4
5079	An Excited State Intramolecular Proton Transfer-Based Fluorescent Probe with a Large Stokes Shift for the Turn-on Detection of Cysteine: A Detailed Theoretical Exploration. <i>ACS Omega</i> , 2020, 5, 19695-19701.	1.6	16
5080	An experimental and theoretical study of LuNC@C _{76,82} revealing a cage-cluster selection rule. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 4563-4571.	3.0	14
5081	Kinetic Investigation of the Pyrolysis of Isobutyric Anhydride and Isobutyric Acid. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 14747-14757.	1.8	3
5082	Accurate Ring Strain Energy Calculations on Saturated Three-Membered Heterocycles with One Group 13-16 Element. <i>Inorganic Chemistry</i> , 2020, 59, 11503-11513.	1.9	20
5083	Fast spin-flip enables efficient and stable organic electroluminescence from charge-transfer states. <i>Nature Photonics</i> , 2020, 14, 636-642.	15.6	331
5084	A key stacking factor for the effective formation of pyrene excimer in crystals: degree of π - π overlap. <i>Journal of Materials Chemistry C</i> , 2020, 8, 11830-11838.	2.7	67
5085	Adsorption behaviour of chronic blistering agents on graphdiyne; excellent correlation among SAPT, reduced density gradient (RDG) and QTAIM analyses. <i>Journal of Molecular Liquids</i> , 2020, 316, 113860.	2.3	79
5086	Steric effect in the formation of hydrogen bonded complexes of isopropylamine with alicyclic ethers by ultrasonic and DFT approach. <i>Journal of Molecular Liquids</i> , 2020, 317, 113910.	2.3	6

#	ARTICLE	IF	CITATIONS
5087	Cucurbit[7]uril as a possible nanocarrier for the antichagasic benzimidazole: a computational approach. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2020, 98, 93-103.	0.9	6
5088	Adsorption of H ₂ molecules on B/N-doped defected graphene sheets—a DFT study. <i>Structural Chemistry</i> , 2020, 31, 2413-2434.	1.0	6
5089	The electric fields enhance the non-covalent intermolecular interaction between H ₂ and (MgO). <i>Chemistry - an Asian Journal</i> , 2020, 15, 3096-3103.	0.9	5
5090	Theoretical investigation on anti-sandwich beryllium-boron clusters Be ₂ B (m=1-3): Fluxionality and multi-aromaticity. <i>Computational and Theoretical Chemistry</i> , 2020, 1188, 112949.	1.1	5
5091	Chemistry of bimetallic hexaborane(10) analogues: A combined experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2020, 512, 119898.	1.2	3
5092	A combined molecular dynamics and quantum mechanics study on the interaction of Fe ³⁺ and human serum albumin relevant to iron overload disease. <i>Journal of Molecular Liquids</i> , 2020, 317, 113933.	2.3	11
5093	Quantum chemical prediction of the spectroscopic properties and ionic composition of the molten NaF-AlF ₃ salts. <i>Journal of Molecular Liquids</i> , 2020, 317, 113937.	2.3	12
5094	Nature-Inspired Purpurin Polymer for Li-Ion Batteries: Mechanistic Insights into Energy Storage via Solid-State NMR and Computational Studies. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17939-17948.	1.5	6
5095	Unravelling the strain-promoted [3+2] cycloaddition reactions of phenyl azide with cycloalkynes from the molecular electron density theory perspective. <i>New Journal of Chemistry</i> , 2020, 44, 13633-13643.	1.4	30
5096	Role of Substituents at 3-position of Thienylethynyl Spacer on Electronic Properties in Diruthenium(II) Organometallic Wire-like Complexes. <i>Chemistry - an Asian Journal</i> , 2020, 15, 3304-3313.	1.7	4
5097	Molecular-Level Insight of Cu(I) Complexes with the 7,8-Bis(diphenylphosphino)-7,8-dicarba-nido-undecaborate Ligand as a Thermally Activated Delayed Fluorescence Emitter: Luminescent Mechanism and Design Strategy. <i>Inorganic Chemistry</i> , 2020, 59, 12039-12053.	1.9	18
5098	Longer and Stronger: Improving Persistent Luminescence in Size-Tuned Zinc Gallate Nanoparticles by Alcohol-Mediated Chromium Doping. <i>ACS Nano</i> , 2020, 14, 12113-12124.	7.3	50
5099	Tunable lifetimes and efficiencies of room temperature phosphorescent liquids by modulating the length and number of alkyl chains. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19746-19757.	1.3	8
5100	Influence of NiO decoration on adsorption capabilities of black phosphorus monolayer toward nitrogen dioxide: periodic DFT calculations. <i>Molecular Simulation</i> , 2020, 46, 1062-1072.	0.9	31
5101	Visible Light Electromagnetic Interaction of PM567 Chiral Dye for Asymmetric Photocatalysis, a First-Principles Investigation. <i>Catalysts</i> , 2020, 10, 882.	1.6	1
5102	Desymmetrized Vertex Design toward a Molecular Cage with Unusual Topology. <i>Angewandte Chemie</i> , 2020, 132, 21032-21037.	1.6	7
5103	Activation of the Unreactive Bond in C ₇₀ Fullerene toward Diels-Alder Reaction by Encapsulation of a Lithium Atom. <i>Chemistry - an Asian Journal</i> , 2020, 15, 3096-3103.	1.7	2
5104	Noncovalent Bonds between Tetrel Atoms. <i>ChemPhysChem</i> , 2020, 21, 1934-1944.	1.0	24

#	ARTICLE	IF	CITATIONS
5105	Insights into the mechanism and regiochemistry of the 1,3-dipolar cycloaddition reaction between benzaldehyde and diazomethane. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	18
5106	Defective phosphorene for highly efficient formaldehyde detection: Periodic density functional calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126792.	0.9	29
5107	Photocatalytic transformation fate and toxicity of ciprofloxacin related to dissociation species: Experimental and theoretical evidences. <i>Water Research</i> , 2020, 185, 116286.	5.3	99
5108	Dielectric Properties of CF ₃ SO ₂ F/N ₂ and CF ₃ SO ₂ F/CO ₂ Mixtures as a Substitute to SF ₆ . <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 15796-15804.	1.8	15
5109	Helic[1]tritycene[3]arene: Synthesis, Complexation, and Formation of [2]Rotaxane Shuttle. <i>Journal of Organic Chemistry</i> , 2020, 85, 11465-11474.	1.7	18
5110	Identification of a previously unreported co-crystal form of acetazolamide: a combination of multiple experimental and virtual screening methods. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20867-20879.	1.3	14
5111	Boosting the performance of A ⁻ D type hole-transporting materials for perovskite solar cells <i>via</i> tuning the acceptor group. <i>New Journal of Chemistry</i> , 2020, 44, 15244-15250.	1.4	21
5112	Confinement Effects of a Noble Gas Dimer Inside a Fullerene Cage: Can It Be Used as an Acceptor in a DSSC?. <i>Frontiers in Chemistry</i> , 2020, 8, 621.	1.8	13
5113	Theoretical study on the absorption of carbon dioxide by DBU-based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20050-20060.	1.3	9
5114	Panchromatic Organoboron Molecules with Tunable Absorption Spectra. <i>Chemistry - an Asian Journal</i> , 2020, 15, 3314-3320.	1.7	3
5115	Sensing mechanism elucidation of a chemosensor based on a <sc>metal-organic</sc> framework selective to explosive aromatic compounds. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26404.	1.0	14
5116	How do magnetic, structural, and electronic criteria of aromaticity relate to HOMO - LUMO gap? An evaluation for graphene quantum dot and its derivatives. <i>Chemical Physics</i> , 2020, 539, 110951.	0.9	16
5117	Insights into the intrinsic interaction between series of C1 molecules and surface of NiO oxygen carriers involved in chemical looping processes. <i>Chinese Journal of Chemical Engineering</i> , 2020, 28, 2771-2777.	1.7	6
5118	Effects of nitrilotriacetic acid and corrosion inhibitor on cobalt barrier chemical-mechanical polishing: Experimental and density functional theory analysis. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 605, 125392.	2.3	41
5119	Dinuclear uranyl coordination compound: Structural investigations and selective fluorescence sensing properties. <i>Polyhedron</i> , 2020, 189, 114745.	1.0	9
5120	Comparative Study of the Thermal Stabilities of the Experimentally Known High-Valent Fe(IV) Compounds Fe(1-norbornyl) ₄ and Fe(cyclohexyl) ₄ . <i>Journal of Physical Chemistry A</i> , 2020, 124, 6867-6876.	1.1	2
5121	New Insight on the Combined Effects of Hydrothermal Treatment and FeSO ₄ /Ca(ClO) ₂ Oxidation for Sludge Dewaterability Improvement: Moisture Distribution and Noncovalent Interaction Calculation. <i>ACS Omega</i> , 2020, 5, 15891-15900.	1.6	8
5122	Dominance of unique P-π phosphorus bonding with π donors: evidence using matrix isolation infrared spectroscopy and computational methodology. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20771-20791.	1.3	13

#	ARTICLE	IF	CITATIONS
5123	Oxygen migration and optical properties of coronene oxides and their persulfurated derivatives: insight into the electric field effect and the oxygen-site dependence. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20078-20086.	1.3	2
5124	DNA backbone interactions impact the sequence specificity of DNA sulfur-binding domains: revelations from structural analyses. <i>Nucleic Acids Research</i> , 2020, 48, 8755-8766.	6.5	16
5125	Dichotomous Siâ€“H Bond Activation by Alkoxide and Alcohol in Base-Catalyzed Dehydrocoupling of Silanes. <i>Inorganic Chemistry</i> , 2020, 59, 12240-12251.	1.9	16
5126	Synthesis, Spectroscopic, and Structural Characterization of Organyl Disulfanides and a Tetrasulfanide. <i>Inorganic Chemistry</i> , 2020, 59, 12322-12336.	1.9	10
5127	Electronic Structure and Nonadiabatic Dynamics of Atomic Silver Nanowireâ€“N₂ Systems. <i>Journal of Physical Chemistry C</i> , 2020, 124, 20834-20845.	1.5	15
5128	Enhanced metallicity boosts hydrogen evolution capability of dual-bimetallic Niâ€“Fe nitride nanoparticles. <i>Materials Today Physics</i> , 2020, 15, 100267.	2.9	67
5129	Spectroscopic evidence of n â†’ Î€* interactions involving carbonyl groups. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26669-26681.	1.3	22
5130	A theoretical study on dimerization and dissociation of acetic acid in ethanol solvent. <i>Computational and Theoretical Chemistry</i> , 2020, 1191, 113029.	1.1	1
5131	Substituent-regulated mechanism on reaction Cp ₂ NbH ₃ (Cp = Î· ⁵ -C ₅ H ₅) with RCi€CR (R = COOMe and Me). <i>Dalton Transactions</i> , 2020, 49, 15376-15384.	1.6	0
5132	Nile-Red-Based Fluorescence Probe for Selective Detection of Biothiols, Computational Study, and Application in Cell Imaging. <i>Molecules</i> , 2020, 25, 4718.	1.7	10
5133	A density functional theory and information-theoretic approach study of chiral molecules in external electric fields. <i>Chemical Physics Letters</i> , 2020, 757, 137858.	1.2	14
5134	Theoretical studies on oxadiazole-based layer stacking nitrogen-rich high-performance insensitive energetic materials. <i>Journal of Molecular Modeling</i> , 2020, 26, 298.	0.8	3
5135	High energy density materials based on fluorinated bridged trinitromethyl azo triazole derivatives: a quantum chemical study of thermodynamic and energetic properties. <i>SN Applied Sciences</i> , 2020, 2, 1.	1.5	0
5136	Impact of benzannulation on ESIPT in 2-(2â€“hydroxyphenyl)-oxazoles: a unified perspective in terms of excited-state aromaticity and intramolecular charge transfer. <i>RSC Advances</i> , 2020, 10, 39049-39059.	1.7	20
5137	Structural evolution in boron-based clusters B ₅ AlnO _l /+ (n=1â€“4): Al atoms transition from the periphery of the planar W-shaped B ₅ ring to the vertex of the bipyramid. <i>European Physical Journal D</i> , 2020, 74, 1.	0.6	4
5138	Room-Temperature Flexible Quasi-Solid-State Rechargeable Naâ€“O₂ Batteries. <i>ACS Central Science</i> , 2020, 6, 1955-1963.	5.3	25
5139	Nickel â€“ p-block metal mixed chalcogenides based on AuCu₃-type fragments: iodine-assisted synthesis as a way of obtaining new structures. <i>Dalton Transactions</i> , 2020, 49, 15081-15094.	1.6	5
5140	Halogen bonds on substituted dibromonitrobenzene derivatives. <i>Journal of Molecular Modeling</i> , 2020, 26, 319.	0.8	0

#	ARTICLE	IF	CITATIONS
5141	The disappearance of the stable slightly-bent isomer of germasilaallenes and the appearance of its cyclic isomer. <i>Polyhedron</i> , 2020, 192, 114821.	1.0	1
5142	DFT Study on the Mechanism of 4,4'-Bipyridine-Catalyzed Nitrobenzene Reduction by Diboron(4) Compounds. <i>Journal of Organic Chemistry</i> , 2020, 85, 13877-13885.	1.7	10
5143	Disubstituted Ferrocenyl Iodo- and Chalcogenoalkynes as Chiral Halogen and Chalcogen Bond Donors. <i>Organometallics</i> , 2020, 39, 3936-3950.	1.1	27
5144	Non-covalent sulfoxide π -(nitrosyl group) interactions involving coordinated nitrosyl in a Ru(η^5 -Cp*) π -nitrosyl complex with an η^2 -diimine ligand: structural and computational studies. <i>CrystEngComm</i> , 2020, 22, 7532-7537.	1.3	2
5145	Capturing unconventional metallofullerene M@C ₆₀ through activation of the unreactive [5,6] bond toward Diels-Alder reaction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 24249-24256.	1.3	5
5146	Theoretical investigation of perfect fullerene-like borospherene Ih-B20 protected by alkaline earth metal: multi-layered spherical electride molecules as electric field manipulated second-order nonlinear optical switches. <i>Dalton Transactions</i> , 2020, 49, 15267-15275.	1.6	5
5147	Tunable luminescent lead bromide complexes. <i>Journal of Materials Chemistry C</i> , 2020, 8, 15996-16000.	2.7	6
5148	An advanced and applicable heat-resistant explosive through controllable regiochemical modulation. <i>Journal of Materials Chemistry A</i> , 2020, 8, 23857-23865.	5.2	64
5149	Pauli energy and information-theoretic approach for evaluating dynamic and nondynamic electron correlation. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	2
5150	Molecular mechanism of CaCCinh-A01 inhibiting TMEM16A channel. <i>Archives of Biochemistry and Biophysics</i> , 2020, 695, 108650.	1.4	14
5151	Fluorinated vs Nonfluorinated PR ₂ (biaryl) Ligands and Their [AuCl(L)] Complexes: Synthesis, X-ray Structures, and Computational Study of Weak Interactions. <i>Bond, No Bond, and Beyond</i> . <i>Inorganic Chemistry</i> , 2020, 59, 16599-16610.	1.9	10
5152	Structure, stability, infrared spectra, and bonding of OHm(H ₂ O) ₇ (m = 0, \hat{A} \pm 1) clusters: ab initio study combining the particle swarm optimization algorithm. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26487-26501.	1.3	4
5153	Highly Efficient Thermally Activated Delayed Fluorescence via an Unconjugated Donor-Acceptor System Realizing EQE of Over 30%. <i>Advanced Materials</i> , 2020, 32, e2003885.	11.1	148
5154	Role of Fluorooxo-Functional Units in Symmetry Breaking and Second Harmonic Generation Response Contribution in Fluorooxoborate Nonlinear Optical Crystals. <i>Crystal Growth and Design</i> , 2020, 20, 7582-7587.	1.4	10
5155	Structural Effects of Amines in Enhancing Methanesulfonic Acid-Driven New Particle Formation. <i>Environmental Science & Technology</i> , 2020, 54, 13498-13508.	4.6	36
5156	π -Triple-Decker Sandwich-Containing Planar {B ₂ E ₂ Pd} Ring (E = S or Se). <i>Inorganic Chemistry</i> , 2020, 59, 16272-16280.	1.9	9
5157	High-Performance Anion Exchange Membranes with Para-Type Cations on Electron-Withdrawing CâO Links Free Backbone. <i>Macromolecules</i> , 2020, 53, 10988-10997.	2.2	36
5158	Are all planar and quasi-planar boron clusters aromatic? Counter examples of island or global π antiaromaticity from chemical bonding analysis. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25084-25094.	1.3	3

#	ARTICLE	IF	CITATIONS
5159	Synthesis, X-ray Structure, Hirshfeld Analysis of Biologically Active Mn(II) Pincer Complexes Based on s-Triazine Ligands. <i>Crystals</i> , 2020, 10, 931.	1.0	3
5160	Understanding the Influence of the Trifluoromethyl Group on the Selectivities of the [3+2] Cycloadditions of Thiocarbonyl <i>S</i> -methanides with α,β -Unsaturated Ketones. A MEDT study. <i>ChemistrySelect</i> , 2020, 5, 12791-12806.	0.7	4
5161	Theoretical prediction of F-doped hexagonal boron nitride: A promising strategy to enhance the capacity of adsorptive desulfurization. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 101, 107715.	1.3	11
5162	Assessment of PBE+U and HSE06 methods and determination of optimal parameter U for the structural and energetic properties of rare earth oxides. <i>Journal of Chemical Physics</i> , 2020, 153, 164710.	1.2	13
5163	A Digallane Gold Complex with a 12-Electron Auride Center: Synthesis and Computational Studies. <i>Organometallics</i> , 2020, 39, 4372-4379.	1.1	2
5164	ESP ^{ALIE} Analysis as a Theoretical Tool for Identifying the Coordination Atoms of Possible Multisite Extractants: Validation and Prediction. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 14353-14364.	3.2	7
5165	The KDEL trafficking receptor exploits pH to tune the strength of an unusual short hydrogen bond. <i>Scientific Reports</i> , 2020, 10, 16903.	1.6	11
5166	Theoretical investigation on QSAR of (2-Methyl-3-biphenyl) methanol analogs as PD-L1 inhibitor. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 459-467.	0.6	2
5167	Mechanistic Studies for Palladium Catalyzed Copolymerization of Ethylene with Vinyl Ethers. <i>Polymers</i> , 2020, 12, 2401.	2.0	14
5168	Isomeric Effect of Wide Bandgap Polymer Donors with High Crystallinity to Achieve Efficient Polymer Solar Cells. <i>Macromolecular Rapid Communications</i> , 2020, 41, e2000454.	2.0	10
5169	The conformational change of Plukenetia conophora oil derivatives and their acidic resistance, intra-fragment interactions, stability in different solvent media. <i>Journal of Molecular Modeling</i> , 2020, 26, 312.	0.8	0
5170	Rational designing an azo colorimetric sensor with high selectivity and sensitivity for uranium environmental monitoring. <i>Analytica Chimica Acta</i> , 2020, 1140, 153-167.	2.6	14
5171	Spectroscopic theoretical studies and wave function analysis on 1-Phenyl sulfonyl Pyrrole with quantum chemical computation techniques. <i>Materials Today: Proceedings</i> , 2020, 50, 2826-2826.	0.9	1
5172	Biodegradation mechanism of polycaprolactone by a novel esterase MGS0156: a QM/MM approach. <i>Environmental Sciences: Processes and Impacts</i> , 2020, 22, 2332-2344.	1.7	14
5173	Selective detection and removal of picric acid by C ₂ N surface from a mixture of nitro-explosives. <i>New Journal of Chemistry</i> , 2020, 44, 18646-18655.	1.4	11
5174	Probing on the Stable Structure of Silicon-Doped Charged Magnesium Nanomaterial Sensor: SiMgN \pm 1 (N = 2 \times 12) Clusters DFT Study. <i>Frontiers in Materials</i> , 2020, 7, .	1.2	9
5175	Tuning the Excited State of Tetradentate Pd(II) Complexes for Highly Efficient Deep-Blue Phosphorescent Materials. <i>Inorganic Chemistry</i> , 2020, 59, 13502-13516.	1.9	16
5176	Adsorption mechanism of toxic heavy metal ions on oxygen-passivated nanopores in graphene nanoflakes. <i>Journal of Materials Science</i> , 2020, 55, 15826-15844.	1.7	11

#	ARTICLE	IF	CITATIONS
5177	Highly Efficient Dehydration of Ethyl Acetate using Strong Hydrophilic Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 16751-16761.	1.8	6
5178	Cyclic Bis-alkylidene Complexes of Titanium and Zirconium: Synthesis, Characterization, and Reaction. <i>Chemistry - A European Journal</i> , 2020, 26, 16472-16479.	1.7	4
5179	Chiral discrimination in a mutated IDH enzymatic reaction in cancer: a computational perspective. <i>European Biophysics Journal</i> , 2020, 49, 549-559.	1.2	4
5180	Deciphering the Dynamics of Organic Nanoaggregates with AIEE Effect and Excited States: Lipophilic Benzothiadiazole Derivatives as Selective Cell Imaging Probes. <i>Journal of Organic Chemistry</i> , 2020, 85, 12614-12634.	1.7	31
5181	SERS Spectra of the Pesticide Chlorpyrifos Adsorbed on Silver Nanosurface: The Ag ₂₀ Cluster Model. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21702-21716.	1.5	31
5182	From inverse sandwich Ta ₂ B ₇ ⁺ and Ta ₂ B ₈ to spherical trihedral Ta ₃ B ₁₂ ⁺ : prediction of the smallest metallo-borospherene. <i>RSC Advances</i> , 2020, 10, 29320-29325.	1.7	20
5183	A novel anthracene derivative with an asymmetric structure as an electron transport material for stable Rec. 2020 blue organic light-emitting diodes. <i>Journal of Information Display</i> , 2020, 21, 197-201.	2.1	5
5184	Theoretical Analysis on Heteroleptic Cu(I)-Based Complexes for Dye-Sensitized Solar Cells: Effect of Anchors on Electronic Structure, Spectrum, Excitation, and Intramolecular and Interfacial Electron Transfer. <i>Molecules</i> , 2020, 25, 3681.	1.7	16
5185	Hg ⁺ ·Hg ⁺ ·Hg Interaction Stabilizes Unusual Trinuclear Double Sandwich Structure of Mercury(II) Porphyrins. <i>Inorganic Chemistry</i> , 2020, 59, 12988-12993.	1.9	4
5186	From Pyridine Adduct of Borabenzene to (In)finite Graphene Architectures Functionalized with N- ⁺ B Dative Bonds. Prototype Systems of Strong One- and Two-Photon Quantum Transitions Triggering Large Nonlinear Optical Responses. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21063-21074.	1.5	9
5187	Electric field induced intra-molecular self-redox: superalkali Li ₃ N ₃ Mg as a candidate for NLO molecular switches. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21928-21937.	1.3	7
5188	Molecular insight into the anion effect and free volume effect of CO ₂ solubility in multivalent ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20618-20633.	1.3	27
5189	<i>i>N</i>-Derivatives of Shannon entropy density as response functions. <i>Physical Chemistry Chemical Physics</i>, 2020, 22, 21535-21542.</i>	1.3	3
5190	Theoretical Insights for Materials Properties of Cyclic Organic Nanorings. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000110.	1.3	4
5191	A deep-red emission fluorescent probe with long wavelength absorption for viscosity detection and live cell imaging. <i>Analytical and Bioanalytical Chemistry</i> , 2020, 412, 7819-7826.	1.9	17
5192	Computational insight into the mechanism and origin of high regioselectivity in the ring-opening cyclization of spirocyclopropanes with stabilized sulfonium ylides by the DFT. <i>Journal of Molecular Modeling</i> , 2020, 26, 255.	0.8	0
5193	Polyene-Free Photoluminescent Polymers via Hydrothermal Hydrolysis of Polyacrylonitrile in Neutral Water. <i>ACS Macro Letters</i> , 2020, 9, 1403-1408.	2.3	8
5194	Methoxy-substituted bis-tridentate iridium(ⁱⁱⁱ) phosphors and fabrication of blue organic light emitting diodes. <i>Journal of Materials Chemistry C</i> , 2020, 8, 13590-13602.	2.7	14

#	ARTICLE	IF	CITATIONS
5195	Structural and electronic properties of exohedrally doped neutral silicon clusters LnSi _n (<i>n</i> = 5, 10; Ln = Sm, Eu, Yb). <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20545-20552.	1.3	20
5196	Separation of <i>m</i>-Cresol from Coal Tar Model Oil Using Propylamine-Based Ionic Liquids: Extraction and Interaction Mechanism Exploration. <i>ACS Omega</i> , 2020, 5, 23090-23098.	1.6	21
5197	Computational study of the substituent effect of halogenated fused-ring heteroaromatics on halogen bonding. <i>Journal of Molecular Modeling</i> , 2020, 26, 270.	0.8	5
5198	Bioinspired Nickel Complexes Supported by an Iron Metalloligand. <i>Inorganic Chemistry</i> , 2020, 59, 14251-14262.	1.9	20
5199	Mechanism for the reactivation of the peroxidase activity of human cyclooxygenases: investigation using phenol as a reducing cosubstrate. <i>Scientific Reports</i> , 2020, 10, 15187.	1.6	5
5200	Bonding Analysis of Compounds with Unusual Coordination of Carbon: Proposed Symmetric Systems with Six-Coordinate Carbon. <i>Molecules</i> , 2020, 25, 3937.	1.7	2
5201	Solid-State Effect Induced Thermally Activated Delayed Fluorescence with Tunable Emission: A Multiscale Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8540-8550.	1.1	18
5202	Virtual Screening of Marine Natural Compounds by Means of Chemoinformatics and CDFT-Based Computational Peptidology. <i>Marine Drugs</i> , 2020, 18, 478.	2.2	32
5203	Bimetallic Bis-NHC-Ir(III) Complex Bearing 2-Arylbenzo[<i>d</i>]oxazolyl Ligand: Synthesis, Catalysis, and Bimetallic Effects. <i>Organometallics</i> , 2020, 39, 3514-3523.	1.1	23
5204	Unveiling the mechanism and selectivity of [3+2] cycloaddition reactions of benzonitrile oxide to ethyl trans-cinnamate, ethyl crotonate and trans-2-penten-1-ol through DFT analysis. <i>Journal of Molecular Modeling</i> , 2020, 26, 279.	0.8	10
5205	Easily Constructed Imine-Bonded COFs for Iodine Capture at Ambient Temperature. <i>ACS Omega</i> , 2020, 5, 24262-24271.	1.6	32
5206	Synthesis and comparative studies of K-region functionalized pyrene derivatives. <i>New Journal of Chemistry</i> , 2020, 44, 16786-16794.	1.4	6
5207	Application of an inverse-design method for designing new branched thiophene oligomers for bulk-heterojunction solar cells. <i>Computational Condensed Matter</i> , 2020, 25, e00503.	0.9	0
5208	Why Can Cationic Halogen Bond Donors Activate the Ritter-Type Solvolysis of Benzhydryl Bromide but Cationic Hydrogen Bond Donors Can Not?. <i>ACS Omega</i> , 2020, 5, 21862-21872.	1.6	10
5209	On single-electron magnesium bonding formation and the effect of methyl substitution. <i>RSC Advances</i> , 2020, 10, 34413-34420.	1.7	1
5210	Excited-state absorption for zinc phthalocyanine from linear-response time-dependent density functional theory. <i>RSC Advances</i> , 2020, 10, 28066-28074.	1.7	6
5211	The noncoincidence phenomenon of acetylacetone C=O stretching in a binary mixture and the aggregation-induced split theory. <i>RSC Advances</i> , 2020, 10, 30982-30989.	1.7	7
5212	Theoretical investigation on the nature of 4-substituted Hantzsch esters as alkylation agents. <i>RSC Advances</i> , 2020, 10, 31425-31434.	1.7	12

#	ARTICLE	IF	CITATIONS
5213	Butadienyl Diiron Complexes: Nonplanar Metalla π -Aromatics Involving π - π Type Orbital Overlap. <i>Angewandte Chemie</i> , 2020, 132, 19210-19215.	1.6	3
5214	Synergistic and Diminutive Effects between Regium and Aerogen Bonds. <i>ChemPhysChem</i> , 2020, 21, 2426-2431.	1.0	17
5215	Metalated Ir π -CNP Complexes Containing Imidazolin π - π -ylidene and Imidazolidin π - π -ylidene Donors π Synthesis, Structure, Luminescence, and Metal π -Ligand Cooperative Reactivity. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 3944-3953.	1.0	6
5216	Theoretical predictions on pentaerythritol tetranitrate π -based high energy density compounds. <i>Journal of the Chinese Chemical Society</i> , 2020, 67, 1753-1762.	0.8	3
5217	Study of Aqueous Am(III)-Aliphatic Dicarboxylate Complexes: Coordination Mode-Dependent Optical Property and Stability Changes. <i>Inorganic Chemistry</i> , 2020, 59, 13912-13922.	1.9	9
5218	Tuning of Second-Order Nonlinear Optical Properties Based on [2.2]Paracyclophanes Isomer: the Relative Configuration and Polarizable Environment. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21692-21701.	1.5	12
5219	Influence of N-Base and O-Base Hybridization on Trier Bonds. <i>ACS Omega</i> , 2020, 5, 21300-21308.	1.6	4
5220	Photoinduced charge transfer in quasi-one-dimensional polymers in two-photon absorption. <i>RSC Advances</i> , 2020, 10, 33288-33298.	1.7	3
5221	Theoretical Investigation of the Circularly Polarized Luminescence of a Chiral Boron Dipyrromethene (BODIPY) Dye. <i>Frontiers in Chemistry</i> , 2020, 8, 801.	1.8	10
5222	One-Step Instantaneous Detection of Multiple Military and Improvised Explosives Facilitated by Colorimetric Reagent Design. <i>Analytical Chemistry</i> , 2020, 92, 13980-13988.	3.2	31
5223	Mechanistic Insights into the Oxidative Rearrangement Catalyzed by the Unprecedented Dioxygenase ChaP Involved in Chartreusin Biosynthesis. <i>Inorganic Chemistry</i> , 2020, 59, 13988-13999.	1.9	4
5224	π -Hole and Lone-Pair Hole Interactions in Chalcogen-Containing Complexes: A Comparative Study. <i>ACS Omega</i> , 2020, 5, 21631-21640.	1.6	23
5225	Spin Density Topology. <i>Molecules</i> , 2020, 25, 3537.	1.7	20
5226	Butterfly Methanes: Designing a Novel Class of anti π -van π Hoff Carbons. <i>ChemPhysChem</i> , 2020, 21, 2272-2278.	1.0	1
5227	Molecular electrostatic potential at nuclear position as a new concept in evaluation of the substitution effects of intramolecular B/N frustrated Lewis pairs in H ₂ splitting and CO ₂ reduction. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26416.	1.0	7
5228	B3LYP, M06 and B3PW91 DFT assignment of nd ₈ metal-bis-(N-heterocyclic carbene) complexes. <i>Journal of Molecular Modeling</i> , 2020, 26, 246.	0.8	6
5229	Multicenter-Emitting Carbon Dots: Color Tunable Fluorescence and Dynamics Monitoring Oxidative Stress In Vivo. <i>Chemistry of Materials</i> , 2020, 32, 8146-8157.	3.2	33
5230	Lighting Silver(I) Complexes for Solution-Processed Organic Light-Emitting Diodes and Biological Applications via Thermally Activated Delayed Fluorescence. <i>Inorganic Chemistry</i> , 2020, 59, 12122-12131.	1.9	23

#	ARTICLE	IF	CITATIONS
5231	Mechanistic Insights into the Oxidative Ring Expansion from Penicillin N to Deacetoxycephalosporin C Catalyzed by a Nonheme Iron(II) and \pm -KG-Dependent Oxygenase. <i>Inorganic Chemistry</i> , 2020, 59, 12218-12231.	1.9	8
5232	From π Bonds without σ Bonds to the Longest Metal–Metal Bond Ever: A Survey on Actinide–Actinide Bonding in Fullerenes. <i>Inorganic Chemistry</i> , 2020, 59, 12608-12615.	1.9	22
5233	F-Halogen Bond: Conditions for Its Existence. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7290-7299.	1.1	17
5234	Unconventional Type III Halogen–Halogen Interactions: A Quantum Mechanical Elucidation of π -Hole– π -Hole and Di- π -Hole Interactions. <i>ACS Omega</i> , 2020, 5, 21824-21835.	1.6	38
5235	Competition between the hydrogen bond and the halogen bond in a $[\text{CH}_3\text{OH}\cdots\text{CCl}_4]$ complex: a matrix isolation IR spectroscopy and computational study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22465-22476.	1.3	12
5236	Naphthalene Benzimidazole Based Neutral Ir(III) Emitters for Deep Red Organic Light-Emitting Diodes. <i>Inorganic Chemistry</i> , 2020, 59, 12461-12470.	1.9	16
5237	Electron-Precise Semiconducting ReGa_2Ge : Extending the IrIn_3 Structure Type to Group 7 of the Periodic Table. <i>Inorganic Chemistry</i> , 2020, 59, 12748-12757.	1.9	9
5238	Nonadiabatic Exciton and Charge Separation Dynamics at Interfaces of Zinc Phthalocyanine and Fullerene: Orientation Does Matter. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7388-7398.	1.1	18
5239	Adaptive π -Aromaticity in an Unsaturated Three-Membered Ring. <i>Chemistry - an Asian Journal</i> , 2020, 15, 3444-3450.	1.7	17
5240	Strategy Used to Control the Mechanism of Homogeneous Alkyne/Olefin Hydrogenation: AIMD Simulations and DFT Calculations. <i>Journal of Organic Chemistry</i> , 2020, 85, 11626-11634.	1.7	5
5241	Reactivity of Neutral Tantalum Sulfide Clusters Ta_3Sn ($n = 0-4$) with N_2 . <i>Journal of Physical Chemistry A</i> , 2020, 124, 7749-7755.	1.1	20
5242	Dyson-orbital concepts for description of electrons in molecules. <i>Journal of Chemical Physics</i> , 2020, 153, 070902.	1.2	66
5243	<p>Synergistic Combination of Sodium Aescinate-Stabilized, Polymer-Free, Twin-Like Nanoparticles to Reverse Paclitaxel Resistance</p>. <i>International Journal of Nanomedicine</i> , 2020, Volume 15, 5839-5853.	3.3	8
5244	Theoretical investigation on reverse intersystem crossing from upper triplet to lowest singlet: A π -hot exciton path for blue fluorescent OLEDs. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26399.	1.0	2
5245	Influence of Small Molecular Property on Antibody Response. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 10944-10950.	2.4	17
5246	Revealing the Mechanism and Origin of Reactivity of Au(I)-Catalyzed Functionalized Indenone Formation of Cyclic and Acyclic Acetals of Alkynylaldehydes. <i>Journal of Organic Chemistry</i> , 2020, 85, 12682-12691.	1.7	7
5247	The C_2N surface as a highly selective sensor for the detection of nitrogen iodide from a mixture of NX_3 ($\text{X} = \text{Cl}, \text{Br}, \text{I}$) explosives. <i>RSC Advances</i> , 2020, 10, 31997-32010.	1.7	35
5248	Theoretical study of the adsorption of amantadine on pristine, Al-, Ga-, P-, and As-doped boron nitride nanosheets: a PBC-DFT, NBO, and QTAIM study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	18

#	ARTICLE	IF	CITATIONS
5249	Random terpolymer based on thiophene-thiazolothiazole unit enabling efficient non-fullerene organic solar cells. <i>Nature Communications</i> , 2020, 11, 4612.	5.8	225
5250	Double aromaticity in a $BBe_6H_6^{+}$ cluster with a planar hexacoordinate boron structure. <i>Chemical Communications</i> , 2020, 56, 12597-12599.	2.2	26
5251	Theoretical studies on carbon dioxide adsorption in cation-exchanged molecular sieves. <i>RSC Advances</i> , 2020, 10, 32241-32248.	1.7	6
5252	Transition-Metal-Complex-Directed Synthesis of Hybrid Iodoargentates with Single-Crystal to Single-Crystal Structural Transformation and Photocatalytic Properties. <i>Inorganic Chemistry</i> , 2020, 59, 13962-13971.	1.9	16
5253	Guest-induced supramolecular chirality transfer in [2]pseudorotaxanes: experimental and computational study. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 7649-7655.	1.5	7
5254	Electronic structures of $NbGe_n$ ($n = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$) ($n = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$) Tj ETQq1 1 0.784314 rgBT group CASPT2 calculations. <i>Journal of Computational Chemistry</i> , 2020, 41, 2641-2652.	1.5	7
5255	Ultralong purely organic aqueous phosphorescence supramolecular polymer for targeted tumor cell imaging. <i>Nature Communications</i> , 2020, 11, 4655.	5.8	186
5256	Probing the structural evolution, electronic and spectral properties of beryllium doped magnesium and its ion clusters. <i>New Journal of Chemistry</i> , 2020, 44, 16929-16940.	1.4	16
5257	Novel homogeneous selective electrocatalysts for CO_2 reduction: an electrochemical and computational study of cyclopentadienyl-phenylendiamino-cobalt complexes. <i>Sustainable Energy and Fuels</i> , 2020, 4, 5609-5617.	2.5	5
5258	Density Functional Theory Calculation and Raman Scattering of the Antihistamine Ebastine. <i>Journal of Applied Spectroscopy</i> , 2020, 87, 608-614.	0.3	4
5259	Plasma-Assisted Chain Reactions of Rh_3^{+} Clusters with Dinitrogen: $N\equiv N$ Bond Dissociation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8222-8230.	2.1	15
5260	A Density Functional Theory Study toward Ring-Opening Reaction Mechanisms of 2,4,6-Trinitrotoluene's Meisenheimer Complex for the Biodegradation of Old Yellow Enzyme Flavoprotein Reductase. <i>ACS Omega</i> , 2020, 5, 23613-23620.	1.6	3
5261	An Insight into the Excitation States of Small Molecular Semiconductor Y6. <i>Molecules</i> , 2020, 25, 4118.	1.7	23
5262	Effect of Bulky Functional Groups on Donor and Acceptor Interactions and their Photoluminescence Properties. <i>ChemPhysChem</i> , 2020, 21, 2620-2626.	1.0	4
5263	Inverse sandwich complexes of $B_7M_2^{+}$, B_8M_2 , and $B_9M_2^{+}$ ($M = Zr, Hf$): the nonclassical $M\equiv M$ bonds embedded in monocyclic boron rings. <i>New Journal of Chemistry</i> , 2020, 44, 17705-17713.	1.4	6
5264	Study of weak interactions of boron nitride nanotubes with anticancer drug by quantum chemical calculations. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	4
5265	Designing Star-Shaped Subphthalocyanine-Based Acceptor Materials with Promising Photovoltaic Parameters for Non-fullerene Solar Cells. <i>ACS Omega</i> , 2020, 5, 23039-23052.	1.6	61
5266	Oxidation states of gallium (infrequent i and common iii) tunable i via medium-sized C_{60} and small-sized C_{28} fullerenes. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 4113-4117.	3.0	5

#	ARTICLE	IF	CITATIONS
5267	Ligand Effects of BrettPhos and RuPhos on Rate-Limiting Steps in Buchwald–Hartwig Amination Reaction Due to the Modulation of Steric Hindrance and Electronic Structure. <i>ACS Omega</i> , 2020, 5, 21385-21391.	1.6	11
5268	Regulating Photocatalysis by Spin-State Manipulation of Cobalt in Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2020, 142, 16723-16731.	6.6	333
5269	Distance-Selected Topochemical Dehydro-Diels–Alder Reaction of 1,4-Diphenylbutadiyne toward Crystalline Graphitic Nanoribbons. <i>Journal of the American Chemical Society</i> , 2020, 142, 17662-17669.	6.6	23
5270	<i>Ab initio</i> kinetics predictions for the role of pre-reaction complexes in hydrogen abstraction from 2-butanone by OH radicals. <i>RSC Advances</i> , 2020, 10, 33205-33212.	1.7	6
5271	All-metal Baird aromaticity. <i>Chemical Communications</i> , 2020, 56, 12522-12525.	2.2	25
5272	Nb ₂ BN ₂ ⁺ cluster anions reduce four carbon dioxide molecules: reactivity enhancement by ligands. <i>Dalton Transactions</i> , 2020, 49, 14081-14087.	1.6	7
5273	Reactions of Schiff Base-Substituted Diselenides and Tellurides with Ni(II), Pd(II) and Pt(II) Phosphine Complexes. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 4303-4312.	1.0	2
5274	Local and macrocyclic (anti)aromaticity of porphyrinoids revealed by the topology of the induced magnetic field. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21267-21274.	1.3	8
5275	Deciphering inhibitory activity of flavonoids against tau protein kinases: a coupled molecular docking and quantum chemical study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 411-424.	2.0	12
5276	Mutual Relations between Substituent Effect, Hydrogen Bonding, and Aromaticity in Adenine-Uracil and Adenine-Adenine Base Pairs. <i>Molecules</i> , 2020, 25, 3688.	1.7	5
5277	A density functional theory study on the electronic and adsorption characteristics of cyclo M ₉ N ₉ (M) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.8	12
5278	Comprehensive Analysis of Band Gap and Nanotwinning in Cd _{1-x} Mg _x S QDs. <i>Crystal Growth and Design</i> , 2020, 20, 6699-6706.	1.4	8
5279	Redox and structural properties of accessible actinide (Ac to Pu) metallocalixarenes (Ac to Pu): a relativistic DFT study. <i>RSC Advances</i> , 2020, 10, 26880-26887.	1.7	9
5280	A theoretical study of the reactivity of ethene and benzophenone with a hyper-coordinated alkene containing a so-called E=E (E = C, Si, Ge, Sn, and Pb) unit. <i>Dalton Transactions</i> , 2020, 49, 12842-12853.	1.6	6
5281	Phenothiazine versus Phenoxazine: Structural Effects on the Photophysical Properties of NIR-II AIE Fluorophores. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 43466-43473.	4.0	26
5282	Exploring the mechanism and counterion activity regulation in the Co ^{III} (salen)-catalyzed hydration of propylene oxide. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22417-22425.	1.3	5
5283	Optimization, Spectroscopic (Excited States, UV/Vis, Polarization) Studies, FMO, ELF, LOL, QTAIM, NBO Analysis and Electronic Properties of Two New Azomethine Derivatives: A Theoretical and Experimental Investigations. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 1848-1865.	0.1	7
5284	“ring” hole bond around difluoroethyne: stabilization of hydrogen bonding cyclohexamer and dicyclohexamer of ammonia molecules. <i>Journal of Molecular Modeling</i> , 2020, 26, 259.	0.8	1

#	ARTICLE	IF	CITATIONS
5285	Theoretical study of switching characteristics of molecular tweezers based on bis(Zn-salphen). <i>Journal of Molecular Modeling</i> , 2020, 26, 265.	0.8	0
5286	Breaking Kasha's Rule as a Mechanism for Solution-Phase Room-Temperature Phosphorescence from High-Lying Triplet Excited State. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8246-8251.	2.1	23
5287	N-{2-[(2-chlorothieno[3,2-d]pyrimidin-4-yl)amino]ethyl}-3-methoxybenzamide: design, synthesis, crystal structure, antiproliferative activity, DFT, Hirshfeld surface analysis and molecular docking study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 787-795.	2.0	4
5288	Anomalous Melting Point of Multicharge Ionic Liquids: Structural, Electrostatic, and Orbital Properties of [Ln(NO ₃) ₆] ³⁺ (Ln = Ce, Pr) Anions. <i>Inorganic Chemistry</i> , 2020, 59, 13700-13708.	1.9	7
5289	End-capped group manipulation of indacenodithienothiophene-based non-fullerene small molecule acceptors for efficient organic solar cells. <i>Nanoscale</i> , 2020, 12, 17795-17804.	2.8	18
5290	Effect on the aromaticity of heterocyclic ligands by coordination with ruthenium electron-withdrawing metal centers. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26412.	1.0	0
5291	Deep-Red Luminescence from Platinum(II) Complexes of N ² -Amido Ligands with Benzannulated N-Heterocyclic Donor Arms. <i>Inorganic Chemistry</i> , 2020, 59, 12504-12517.	1.9	22
5292	Negatively Curved Nanographene with Heptagonal and [5]Helicene Units. <i>Journal of the American Chemical Society</i> , 2020, 142, 14814-14819.	6.6	81
5293	A TDDFT investigation of the Photosystem II reaction center: Insights into the precursors to charge separation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 19705-19712.	3.3	9
5294	Insights into 2-Indolylmethanol-Involved Cycloadditions: Origins of Regioselectivity and Enantioselectivity. <i>Journal of Organic Chemistry</i> , 2020, 85, 11641-11653.	1.7	20
5295	Main-group metal cyclophane complexes with high coordination numbers. <i>RSC Advances</i> , 2020, 10, 30796-30805.	1.7	1
5296	Theoretical Insights into Y ₂ C ₂ @C ₈₂ : Vibrational Frequency Influencing the Thermodynamic Stability. <i>ChemistrySelect</i> , 2020, 5, 9806-9812.	0.7	0
5297	Theoretical Study on Thermally Activated Delayed Fluorescence Emitters in White Organic Light-Emitting Diodes: Emission Mechanism and Molecular Design. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7526-7537.	1.1	14
5298	Development and evaluation of a pH-responsive and water-soluble drug delivery system based on smart polymer coating of graphene nanosheets: an <i>in silico</i> study. <i>RSC Advances</i> , 2020, 10, 31106-31114.	1.7	8
5299	Behavior of Antibiotics in Natural Deep Eutectic Solvents. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 4669-4683.	1.0	9
5300	Maximizing Chiral Perturbation on Thermally Activated Delayed Fluorescence Emitters and Elaboration of the First Top-Emission Circularly Polarized OLED. <i>Advanced Functional Materials</i> , 2020, 30, 2004838.	7.8	94
5301	Effect of substitution on the bonding in He dimer confined within dodecahedrane: A computational study. <i>Journal of Computational Chemistry</i> , 2020, 41, 2398-2405.	1.5	5
5302	Stabilization of cyclic water tetramers and dimers in the crystal host of 2D coordination networks: electrical conductivity and dielectric studies. <i>New Journal of Chemistry</i> , 2020, 44, 15857-15870.	1.4	9

#	ARTICLE	IF	CITATIONS
5303	The Flow of the Redox Energy in Quercetin during Its Antioxidant Activity in Water. <i>International Journal of Molecular Sciences</i> , 2020, 21, 6015.	1.8	10
5304	Bioinspired succinyl- β -cyclodextrin membranes for enhanced uranium extraction and reclamation. <i>Environmental Science: Nano</i> , 2020, 7, 3124-3135.	2.2	16
5305	Exploring the Substituent Effect on the Structure and Electronic Properties of Si ₂ (para-C ₆ H ₄ X) ₂ Molecules. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 2760-2769.	0.1	2
5306	Enhanced Two-Photon Absorption of Cross-Conjugated Chalcone Derivatives: Modulation of the Effective π -Conjugated Structure. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10808-10816.	1.1	19
5307	Versatile Accumulated Surface Plasmon Resonance of Functionalized Nanosilver in Polymer Devices. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 21802-21810.	1.8	1
5308	Decisive Role of 5f-Orbital Covalence in the Structure and Stability of Pentavalent Transuranic Oxo [M ₆ O ₈] Clusters. <i>Inorganic Chemistry</i> , 2020, 59, 18068-18077.	1.9	5
5309	Molecular rotors with designed polar rotating groups possess mechanics-controllable wide-range rotational speed. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	6
5310	Multiscale modelling investigation of wood modification with acetic anhydride. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 28448-28458.	1.3	13
5311	Theoretical investigation on cis-trans isomerisation of azaphosphatriptycene- based molecular gear. <i>Supramolecular Chemistry</i> , 2020, 32, 569-577.	1.5	1
5312	Rapid Sequentially Palladium Catalyzed Four-Component Synthesis of Novel Fluorescent Biaryl-Substituted Isoxazoles. <i>Catalysts</i> , 2020, 10, 1412.	1.6	5
5313	Absorption of Toluene Using Deep Eutectic Solvents: Quantum Chemical Calculations and Experimental Investigation. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 22605-22618.	1.8	38
5314	Theoretical Investigations on the Excited-State Dynamics of an Al ³⁺ Fluorescence Sensor. <i>Journal of Physical Chemistry A</i> , 2020, 124, 11093-11101.	1.1	7
5315	How to Accomplish a Square C(N) ₄ Substructure of the Planar Tetracoordinate Carbon. <i>ACS Omega</i> , 2020, 5, 32583-32590.	1.6	0
5316	Manganese "gold" manganese complex with vinylidene and acetylide units. <i>Dalton Transactions</i> , 2020, 49, 17527-17531.	1.6	2
5317	Investigating the Complexation and Release Behaviors of Iodine in Poly(vinylpyrrolidone)-Iodine Systems through Experimental and Computational Approaches. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 22667-22676.	1.8	11
5318	Actinyl-Carboxylate Complexes [AnO ₂ (COOH) _n](H ₂ O) _m (An = U, Np, Pu, and Am; n = 1-3; m = 0, 2, 4; 2n + m = 6): Electronic Structures, Interaction Features, and the Potential to Adsorbents toward Cs Ion. <i>ACS Omega</i> , 2020, 5, 31974-31983.	1.6	2
5319	The Importance of Strain (Preorganization) in Beryllium Bonds. <i>Molecules</i> , 2020, 25, 5876.	1.7	2
5320	Efficient Decomposition of Perfluorinated Compounds In a High Photon Flux UV/sulfite system. <i>IOP Conference Series: Earth and Environmental Science</i> , 2020, 546, 042027.	0.2	1

#	ARTICLE	IF	CITATIONS
5321	Effect of Hydrogen Bond Donors and Acceptors on CO ₂ Absorption by Deep Eutectic Solvents. <i>Processes</i> , 2020, 8, 1533.	1.3	46
5322	Main-Group Metals Stabilized Polypyrrolic Uranyl(V) Complexes via Cation-Cation Interaction with the Uranyl <i>exo</i> -Oxo Atom: A Relativistic Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2020, 59, 18018-18026.	1.9	4
5323	Interrogating the Interplay between Hydrogen and Halogen Bonding in Graphitic Carbon Nitride Building Blocks. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10817-10825.	1.1	16
5324	Quantum Chemical Study of the Carbon Dioxide-Philicity of Surfactants: Effects of Tail Functionalization. <i>Langmuir</i> , 2020, 36, 15352-15361.	1.6	4
5325	Why Conventional Design Rules for C-H Activation Fail for Open-Shell Transition-Metal Catalysts. <i>ACS Catalysis</i> , 2020, 10, 15033-15047.	5.5	30
5326	On the Dynamic Mechanical Behavior and Importance of Weak Interactions in PS/PVME Blends. <i>ChemistrySelect</i> , 2020, 5, 14592-14595.	0.7	0
5327	Data of interaction of supported ionic liquids phases onto copper nanoparticles: A density functional theory study. <i>Data in Brief</i> , 2020, 33, 106562.	0.5	1
5328	Low-cost fabrication of highly dispersed atomically-thin MoS ₂ nanosheets with abundant active Mo-terminated edges. <i>Nano Materials Science</i> , 2021, 3, 205-212.	3.9	22
5329	Theoretical Investigation of the Mechanism, Performance and Kinetic Experimental Phenomena on Brønsted Acidic Ionic Liquids Catalyzed Dehydration of Sorbitol to Isosorbide. <i>ChemistrySelect</i> , 2020, 5, 14713-14720.	0.7	1
5330	Synthesis and characterization of aryltellurium compounds including mixed-valence derivatives. Evaluation of Te ²⁺ , Te ⁴⁺ and X ⁺ (X = Br, I) interactions. <i>Journal of Organometallic Chemistry</i> , 2020, 929, 121553.	0.8	0
5331	Tracing the driving forces responsible for the remarkable infectivity of 2019-nCoV: 1. Receptor binding domain in its bound and unbound states. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 28277-28285.	1.3	3
5332	Facile cyclization of sodium aminodiboranate to construct a boron-nitrogen-hydrogen ring. <i>Dalton Transactions</i> , 2020, 49, 16662-16666.	1.6	3
5333	Seven confluence principles: a case study of standardized statistical analysis for 26 methods that assign net atomic charges in molecules. <i>RSC Advances</i> , 2020, 10, 44121-44148.	1.7	14
5334	Solubility measurement, thermodynamic correlation and molecular simulations of uracil in (alcohol+water) binary solvents at (283.15-318.15) K. <i>Journal of Molecular Liquids</i> , 2020, 318, 114259.	2.3	26
5335	Stop Four Gaps with One Bush: Versatile Hierarchical Polybenzimidazole Nanoporous Membrane for Highly Durable Li-S Battery. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 55809-55819.	4.0	14
5336	High-Efficiency Thermal-Annealing-Free Organic Solar Cells Based on an Asymmetric Acceptor with Improved Thermal and Air Stability. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 57271-57280.	4.0	44
5337	Optical Properties of Artemisinin and Its Derivatives. <i>ACS Omega</i> , 2020, 5, 30849-30857.	1.6	2
5338	Mechanism of Gold Cyanidation in Bioleaching of Precious Metals from Waste Printed Circuit Boards. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 18975-18981.	3.2	9

#	ARTICLE	IF	CITATIONS
5339	Physicochemical Properties of Choline Chloride-Based Deep Eutectic Solvents with Polyols: An Experimental and Theoretical Investigation. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 18712-18728.	3.2	44
5340	Reactivity and Selectivity Controlling Factors in the Pd/Dialkylbiarylphosphine-Catalyzed C-C Cleavage/Cross-Coupling of an N-Fused Bicyclo[1.1.0]butane-2-Hydroxy-1,2-Lactam. <i>Journal of the American Chemical Society</i> , 2020, 142, 21140-21152.	6.6	20
5341	Simultaneous interlayer and intralayer space control in two-dimensional metal-organic frameworks for acetylene/ethylene separation. <i>Nature Communications</i> , 2020, 11, 6259.	5.8	85
5342	First-Principle Studies of Istradefylline with Emphasis on the Stability, Reactivity, Interactions and Wavefunction-Dependent Properties. <i>Polycyclic Aromatic Compounds</i> , 2020, , 1-15.	1.4	15
5343	Role of 3d transition metal doping in determining the electronic structure and properties of small magnesium clusters: a DFT-based comparison of neutral and cationic states. <i>Journal of Nanoparticle Research</i> , 2020, 22, 1.	0.8	6
5344	Reactive Molecular Dynamics Investigation of Toluene Oxidation under Electrostatic Fields: Effect of the Modeling of Local Charge Distribution. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10705-10716.	1.1	12
5345	Chemical Interactions at the Al/Poly-Epoxy Interface Rationalized by DFT Calculations and a Comparative XPS Analysis. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 57649-57665.	4.0	13
5346	Calculation of the UV Spectrum and Electrophilic Reactive Sites of Fentanyl Molecule Based on the Density Functional Theory. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 2586-2593.	0.1	3
5347	Bismuth Polycations Revisited: Alternative Synthesis and Electronic Structure of Bi ₆ Br ₇ , and Bonding in Main-Group Polyatomic Ions from a Direct Space Perspective. <i>Crystals</i> , 2020, 10, 940.	1.0	4
5348	Interaction between Trinuclear Radium Complexes of Pyrazolate and Anions, a Computational Study. <i>International Journal of Molecular Sciences</i> , 2020, 21, 8036.	1.8	7
5349	Search for optimal monomers for fabricating active layers in thin-film composite osmosis membranes by conceptual density functional theory. <i>Journal of Molecular Modeling</i> , 2020, 26, 334.	0.8	10
5350	Origin of diastereoselectivity and catalytic efficiency on Isothiourea-mediated cyclization of carboxylic acid with alkenyl ketone. <i>Computational and Theoretical Chemistry</i> , 2020, 1190, 113004.	1.1	1
5351	Separating Enthalpic, Configurational, and Solvation Entropic Components in Host-Guest Binding: Application to Cucurbit[7]uril Complexes through a Full <i>In Silico</i> Approach via Water Nanodroplets. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10486-10499.	1.2	5
5352	Volatile-char interactions during biomass pyrolysis: Contribution of amino group on graphitized carbon nanotube to xylose evolution based on experimental and theoretical studies. <i>Fuel</i> , 2020, 282, 118921.	3.4	23
5353	Ferrocene/anthraquinone based bi-redox molecule for symmetric nonaqueous redox flow battery. <i>Journal of Power Sources</i> , 2020, 480, 229132.	4.0	26
5354	Coupling-oxidation process promoted ring-opening degradation of 2-mecapto-5-methyl-1,3,4-thiadiazole in wastewater. <i>Water Research</i> , 2020, 186, 116362.	5.3	7
5355	Quantitative description of surface adsorption of surfactant in aqueous solution without the Gibbs equation. <i>Chemical Communications</i> , 2020, 56, 15076-15079.	2.2	5
5356	Ether functionalisation, ion conformation and the optimisation of macroscopic properties in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23038-23056.	1.3	34

#	ARTICLE	IF	CITATIONS
5357	Synthesis, Biological Evaluation and Stability Studies of Some Novel Aza-Acridine Aminoderivatives. <i>Molecules</i> , 2020, 25, 4584.	1.7	5
5358	Rotational Spectroscopy Meets Quantum Chemistry for Analyzing Substituent Effects on Non-Covalent Interactions: The Case of the Trifluoroacetophenone-Water Complex. <i>Molecules</i> , 2020, 25, 4899.	1.7	8
5359	Halogenated Diazabutadiene Dyes: Synthesis, Structures, Supramolecular Features, and Theoretical Studies. <i>Molecules</i> , 2020, 25, 5013.	1.7	28

5360

#	ARTICLE	IF	CITATIONS
5375	The nature of the chemical bonding in 5d transition-metal diatomic borides MB (M = Ir, Pt, Au). Journal of Chemical Physics, 2020, 152, 174301.	1.2	14
5376	Structural evolution and magnetic properties of ScLi _n (n = 2–13) clusters: A PSO and DFT investigation*. Chinese Physics B, 2020, 29, 077101.	0.7	5
5377	Effect of silanol on the thermal stability of poly[methyl(trifluoropropyl)siloxane]. Journal of Applied Polymer Science, 2020, 137, 49347.	1.3	9
5378	Regioselective Deuteration of a 3,4-Dialkoxypyrroline N-Oxide and Synthesis of 8-Indolizidines. European Journal of Organic Chemistry, 2020, 2020, 3423-3429.	1.2	0
5379	Computational studies on the conformational preference of N-(Thiazol-2-yl) benzamide. Journal of the Chinese Chemical Society, 2020, 67, 1800-1806.	0.8	2
5380	Synthesis, crystal structure, spectroscopic and hirshfeld surface analysis, NCI-RDG, DFT computations and antibacterial activity of new asymmetrical azines. Journal of Molecular Structure, 2020, 1217, 128376.	1.8	23
5381	Intermolecular interactions, vibrational spectra, and detonation performance of CL ₂ O/TNT cocrystal. Journal of the Chinese Chemical Society, 2020, 67, 1742-1752.	0.8	9
5382	Charge-Sensitive Cluster–Ligand Interactions Cause Altered Reactivity of Al _n [±] O ₂ Clusters with Benzene: Enhanced Stability of Al ₁₃ ⁺ Bz. Journal of Physical Chemistry A, 2020, 124, 4087-4094.	1.1	9
5383	Effect of the triptycene scaffold on the photophysical, electrochemical and electroluminescence properties of the iridium(III) complex. New Journal of Chemistry, 2020, 44, 8587-8594.	1.4	0
5384	A theoretical study of chemical bonding and topological and electrostatic properties of the anti-leprosy drug dapsone. Journal of Molecular Modeling, 2020, 26, 138.	0.8	7
5385	Alkali metal storage mechanism in organic semiconductor of perylene-3,4,9,10-tetracarboxylicdianhydride. Applied Surface Science, 2020, 524, 146396.	3.1	13
5386	Solvatochromism and intramolecular charge transfer in dialkylamino-substituted halogenated thienyl chalcone analogues. Chemical Physics, 2020, 537, 110854.	0.9	20
5387	Unusual spectroscopic and photophysical properties of solvatochromic BODIPY analogues of Prodan. Dyes and Pigments, 2020, 182, 108510.	2.0	9
5388	Synthesis and molecular dynamic simulation of a novel single ion conducting gel polymer electrolyte for lithium-ion batteries. Polymer, 2020, 201, 122568.	1.8	26
5389	General Density-Based Index to Analyze Charge Transfer Phenomena: From Models to Butterfly Molecules. Journal of Chemical Theory and Computation, 2020, 16, 4543-4553.	2.3	21
5390	Cycloaddition Reactions between H ₂ C = CHR (R = H, CN, CH ₃) and a Cyclic P/B Frustrated Lewis Pair: A DFT Study. Journal of Physical Chemistry A, 2020, 124, 4455-4462.	1.1	18
5391	Competition between tubular, planar and cage geometries: a complete picture of structural evolution of B _n (n = 31–50) clusters. Physical Chemistry Chemical Physics, 2020, 22, 12959-12966.	1.3	21
5392	From cyclic amines and acetonitrile to amidine zinc(II) complexes. RSC Advances, 2020, 10, 18200-18221.	1.7	9

#	ARTICLE	IF	CITATIONS
5393	Vibrational spectroscopic, NBO, AIM, and multiwfn study of tectorigenin: A DFT approach. <i>Journal of Molecular Structure</i> , 2020, 1217, 128443.	1.8	43
5394	Mechanism and Origins of Enantio- and Regioselectivities in Catalytic Asymmetric Minisci-Type Addition to Heteroarenes. <i>Journal of Organic Chemistry</i> , 2020, 85, 7207-7217.	1.7	10
5395	Suit[4]ane. <i>Journal of the American Chemical Society</i> , 2020, 142, 10273-10278.	6.6	18
5396	Macroscopic Polarization Change via Electron Transfer in a Valence Tautomeric Cobalt Complex. <i>Nature Communications</i> , 2020, 11, 1992.	5.8	41
5397	Can we utilize the higher Frenkel exciton state in biazulene diimides-based non-fullerene acceptors to promote charge separation at the donor/acceptor interface?. <i>New Journal of Chemistry</i> , 2020, 44, 9767-9774.	1.4	12
5398	Screening metal-dicorrole-based dyes with excellent photoelectronic properties for dye-sensitized solar cells by density functional calculations. <i>Journal of Porphyrins and Phthalocyanines</i> , 2020, 24, 1003-1012.	0.4	3
5399	New Crystal Forms for Biologically Active Compounds. Part 2: Anastrozole as N-Substituted 1,2,4-Triazole in Halogen Bonding and Lp- π Interactions with 1,4-Diodotetrafluorobenzene. <i>Crystals</i> , 2020, 10, 371.	1.0	14
5400	Partitioning a Molecule into the Atomic Basins and the Resultant Atomic Charges from Quantum Chemical Topology Analysis of the Kohn-Sham Potential. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5023-5032.	1.1	3
5401	Luminescent Zn(II) and Cd(II) complexes with chiral 2,2'-bipyridine ligands bearing natural monoterpene groups: synthesis, speciation in solution and photophysics. <i>Dalton Transactions</i> , 2020, 49, 7552-7563.	1.6	13
5402	A potential bio-antioxidant for mineral oil from cashew nutshell liquid: an experimental and theoretical approach. <i>Brazilian Journal of Chemical Engineering</i> , 2020, 37, 369-381.	0.7	10
5403	A NIR fluorescent probe based on phenazine with a large Stokes shift for the detection and imaging of endogenous H ₂ O ₂ in RAW 264.7 cells. <i>Analyst</i> , 2020, 145, 4196-4203.	1.7	12
5404	The Pd(0) and Pd(II) cocatalyzed isomerization of alkynyl epoxides to furans: a mechanistic investigation using DFT calculations. <i>Dalton Transactions</i> , 2020, 49, 9223-9230.	1.6	2
5405	Tetrachloroplatinate(II) anion as a square-planar tecton for crystal engineering involving halogen bonding. <i>CrystEngComm</i> , 2020, 22, 4180-4189.	1.3	18
5406	Highly improved carbon dioxide sensitivity and selectivity of black phosphorene sensor by vacancy doping: A quantum chemical perspective. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26265.	1.0	24
5407	Insights on Absolute and Relative Stereocontrol in Stereodivergent Cooperative Catalysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 9612-9624.	6.6	29
5408	Work function modification of PEDOT:PSS by mixing with barium acetylacetonate. <i>RSC Advances</i> , 2020, 10, 17673-17680.	1.7	13
5409	Cavity-trapped electrons: lithium doped tetracyano-2,6-naphthoquinodimethane (TNAP) systems. <i>Journal of Molecular Modeling</i> , 2020, 26, 118.	0.8	0
5410	Structural, electronic, and energetic investigations of acrolein adsorption on B36 borophene nanosheet: a dispersion-corrected DFT insight. <i>Journal of Molecular Modeling</i> , 2020, 26, 128.	0.8	21

#	ARTICLE	IF	CITATIONS
5411	Tuning Physicochemical Properties of Antipsychotic Drug Aripiprazole with Multicomponent Crystal Strategy Based on Structure and Property Relationship. <i>Crystal Growth and Design</i> , 2020, 20, 3747-3761.	1.4	34
5412	Chemosensing of Guanosine Triphosphate Based on a Fluorescent Dinuclear Zn(II)-Dipicolylamine Complex in Water. <i>Inorganic Chemistry</i> , 2020, 59, 7739-7751.	1.9	19
5413	Structure and bonding of molecular stirrers with formula $B_{7M_2}^{n+}$ and B_{8M_2} (M = Zn, Cd, Hg). <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12312-12320.	1.3	20
5414	Theoretical study of $D\alpha^2A^2\epsilon^2A$ triphenylamine and quinoline derivatives as sensitizers for dye-sensitized solar cells. <i>RSC Advances</i> , 2020, 10, 17255-17265.	1.7	14
5415	Organic Amines as Targeting Stabilizer at the Polymer/Fullerene Interface for Polymer:PC 61 BM Solar Cells. <i>Energy Technology</i> , 2020, 8, 2000266.	1.8	8
5416	Mechanism of antioxidant properties of quercetin and quercetin-DNA complex. <i>Journal of Molecular Modeling</i> , 2020, 26, 133.	0.8	53
5417	The reactivity enhancement in Diels-Alder cycloaddition of 1,3-diene by cation encapsulation to C60: a computational insight. <i>Structural Chemistry</i> , 2020, 31, 1821-1829.	1.0	3
5418	ZnO-chitosan/Rectorite Nanocomposite Exhibiting High Photocatalytic Activities under Visible-light Irradiation. <i>Journal Wuhan University of Technology, Materials Science Edition</i> , 2020, 35, 310-319.	0.4	6
5419	Analysis of the electronic delocalization in some isoelectronic analogues of B_{12} doped with beryllium and/or carbon. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12245-12259.	1.3	12
5420	Hydrogen vs. Halogen Bonds in 1-Halo-Closo-Carboranes. <i>Materials</i> , 2020, 13, 2163.	1.3	10
5421	Bio-Based Antimicrobial Ionic Materials Fully Composed of Natural Products for Elevated Air Purification. <i>Advanced Sustainable Systems</i> , 2020, 4, 2000046.	2.7	10
5422	Second Sphere Ligand Promoted Organoiridium Catalysts for Methanol Dehydrogenation under Mild Conditions. <i>ChemCatChem</i> , 2020, 12, 4024-4028.	1.8	8
5423	DFT Study of the Reaction Mechanism of N_2O Decomposition on Au_3^+ Clusters. <i>ChemistrySelect</i> , 2020, 5, 5391-5399.	0.7	2
5424	Size Dependence of $[C_n]$ Cycloparaphenylenes ($n = 9-20$): Relationship between Aromaticity and Third-Order Nonlinear Optical Properties. <i>Journal of Physical Chemistry C</i> , 2020, 124, 11081-11091.	1.5	16
5425	N-Terminal Derivatization-Assisted Identification of Individual Amino Acids Using a Biological Nanopore Sensor. <i>ACS Sensors</i> , 2020, 5, 1707-1716.	4.0	21
5426	Effect of Substituents in Hydrolyzed Cephalosporins on Intramolecular $O-H\cdots N$ Bond. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 925-932.	0.1	1
5427	Deciphering the role of acid additives in chiral diamine-catalyzed asymmetric aldol reactions of cyclohexanones with aldehydes. <i>Molecular Catalysis</i> , 2020, 486, 110881.	1.0	0
5428	Understand the Specific Regio- and Enantioselectivity of Fluostatin Conjugation in the Post-Biosynthesis. <i>Biomolecules</i> , 2020, 10, 815.	1.8	15

#	ARTICLE	IF	CITATIONS
5429	Cytotoxic Secondary Metabolites Isolated from the Marine Alga-Associated Fungus <i>Penicillium chrysogenum</i> LD-201810. <i>Marine Drugs</i> , 2020, 18, 276.	2.2	12
5430	The Mechanism of the Intramolecular Hydrocarbyl Metathesis within a Planar Triruthenium Cluster: Combining Core Flexibility with Hydride Mobility. <i>Chemistry - A European Journal</i> , 2020, 26, 13880-13889.	1.7	1
5431	Intermolecular hydrogen bond interactions in the thiourea/water complexes (Thio-(H ₂ O) _n) (n = 1, 5): X-ray, DFT, NBO, AIM, and RDG analyses. <i>Journal of Molecular Modeling</i> , 2020, 26, 161.	0.8	95
5432	Preorganization-enhanced halogen bonding via intramolecular hydrogen bonding: a theoretical study. <i>Structural Chemistry</i> , 2020, 31, 1999-2009.	1.0	0
5433	An innovative in vitro assay to study the effects of aromatic pollutants on porphyrin systems. <i>Environmental Pollution</i> , 2020, 264, 114606.	3.7	3
5434	(8-Amino)quinoline and (4-amino)phenanthridine complexes of Re(CO) ₃ halides. <i>Journal of Organometallic Chemistry</i> , 2020, 921, 121338.	0.8	6
5435	Insights on Betaine + Lactic Acid Deep Eutectic Solvent. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 11880-11892.	1.8	21
5436	Halogen Bonding in New Dichloride-Cobalt(II) Complex with Iodo Substituted Chalcone Ligands. <i>Crystals</i> , 2020, 10, 354.	1.0	7
5437	Cooperative interaction of sodium and chlorine ions with β -D-glucopyranose in aqueous solution from quantum mechanics and molecular dynamics. <i>Cellulose</i> , 2020, 27, 6793-6809.	2.4	3
5438	β -Functionalized ketene N,S-acetals as two-carbon synthons in the reaction with 1,2-naphthoquinone 1-methide. Synthesis of 3-amino-1H-benzo[f]chromenes. <i>Chemistry of Heterocyclic Compounds</i> , 2020, 56, 521-528.	0.6	4
5439	Keggin-type polyoxometalates as efficient catalysts for the synthesis of 4-methylcoumarins in solvent-free conditions, under conventional heating and microwave irradiations: Theoretical calculations and mechanism studies. <i>Chemical Data Collections</i> , 2020, 28, 100436.	1.1	5
5440	A pillar[5]arene-based fluorescent sensor for sensitive detection of L-Met through a dual-site collaborative mechanism. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 240, 118569.	2.0	14
5441	A study on the mechanism of oxidized quinoline removal from acid solutions based on persulfate-iron systems. <i>RSC Advances</i> , 2020, 10, 12504-12510.	1.7	7
5442	Modulation of the photoelectrochemical behavior of Au nanocluster@TiO ₂ electrode by doping. <i>Chemical Science</i> , 2020, 11, 6248-6255.	3.7	20
5443	Embellishing bis-1,2,4-triazole with four nitroamino groups: advanced high-energy-density materials with remarkable performance and good stability. <i>Journal of Materials Chemistry A</i> , 2020, 8, 11752-11760.	5.2	50
5444	Reaction Mechanism and Kinetics study on Addition of CCl ₄ to 1-hexene Catalyzed by Mo ₅ Q ₁₄ Quintuply-bond. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5726.	1.7	2
5445	Ab initio predictions for the reaction mechanism and orbital topological properties of the formation of Neptunimine, Plutonimine, and its side products. <i>Journal of Molecular Modeling</i> , 2020, 26, 163.	0.8	1
5446	Synthesis of a novel collector based on selective nitrogen coordination for improved separation of galena and sphalerite against pyrite. <i>Chemical Engineering Science</i> , 2020, 226, 115860.	1.9	39

#	ARTICLE	IF	CITATIONS
5447	Investigation of the deprotonation of tetracycline using differential absorbance spectra: A comparative experimental and DFT/TD-DFT study. <i>Science of the Total Environment</i> , 2020, 726, 138432.	3.9	14
5448	Unsymmetrical Functionalization of Bis-1,2,4-triazoles Skeleton: Exploring for Promising Energetic Materials. <i>ACS Applied Energy Materials</i> , 2020, 3, 6492-6500.	2.5	29
5449	Parameterization of Boronates Using VFFDT and Paramfit for Molecular Dynamics Simulation. <i>Molecules</i> , 2020, 25, 2196.	1.7	9
5450	Rational Design, Synthesis, Characterization and Evaluation of Iodinated 4,4'-Bipyridines as New Transthyretin Fibrillogenesis Inhibitors. <i>Molecules</i> , 2020, 25, 2213.	1.7	15
5451	Switching Xe/Kr adsorption selectivity in modified SBMOF-1: a theoretical study. <i>RSC Advances</i> , 2020, 10, 17195-17204.	1.7	18
5452	NWChem: Past, present, and future. <i>Journal of Chemical Physics</i> , 2020, 152, 184102.	1.2	425
5453	Biodegradation of Concentrated Benzoic Acid Using White-Rot Fungus <i>Hypocrea lixii</i> AH. <i>Environmental Engineering Science</i> , 2020, 37, 482-489.	0.8	2
5454	Symmetrical Noncovalent Interactions Br ^{δ+} ⋯Br ^{δ-} Observed in Crystal Structure of Exotic Primary Peroxide. <i>Symmetry</i> , 2020, 12, 637.	1.1	12
5455	Comparative investigation of σ-hole interactions of carbon-containing molecules with Lewis bases, acids and di-halogens. <i>Chemical Papers</i> , 2020, 74, 3569-3580.	1.0	18
5456	An sp ² -hybridized all-carboatomic ring, cyclo[18]carbon: Bonding character, electron delocalization, and aromaticity. <i>Carbon</i> , 2020, 165, 468-475.	5.4	188
5457	An sp ² -hybridized all-carboatomic ring, cyclo[18]carbon: Electronic structure, electronic spectrum, and optical nonlinearity. <i>Carbon</i> , 2020, 165, 461-467.	5.4	747
5458	Carboxymethyl cellulose improved adsorption capacity of polypyrrole/CMC composite nanoparticles for removal of reactive dyes: Experimental optimization and DFT calculation. <i>Chemosphere</i> , 2020, 255, 127052.	4.2	63
5459	Mechanisms of trehalose-mediated mitigation of Cd toxicity in rice seedlings. <i>Journal of Cleaner Production</i> , 2020, 267, 121982.	4.6	20
5460	Optoelectronic properties of cyclopentadithiophene-based donor-acceptor copolymers as donors in bulk heterojunction organic solar cells: A theoretical study. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 145, 109532.	1.9	17
5461	Theoretical investigation of the adsorption behaviors of fluorouracil as an anticancer drug on pristine and B-, Al-, Ga-doped C36 nanotube. <i>Journal of Molecular Liquids</i> , 2020, 309, 113209.	2.3	43
5462	Systematic study of synthesizing various heteroatom-substituted rhodamines from diaryl ether analogues. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 240, 118466.	2.0	17
5463	Tuning the Reactivity and Bonding Properties of Metal Square-Planar Complexes by the Substitution(s) on the Trans-Coordinated Pyridine Ring. <i>ACS Omega</i> , 2020, 5, 11768-11783.	1.6	9
5464	Monomolecular Dehydration of Ethanol into Ethylene over H-MOR Studied by Density Functional Theory. <i>ACS Omega</i> , 2020, 5, 9707-9713.	1.6	8

#	ARTICLE	IF	CITATIONS
5465	Mechanism of Palladium-Catalyzed Spiroannulation of Naphthols with Alkynes: A Density Functional Theory Study. <i>ChemCatChem</i> , 2020, 12, 3863-3869.	1.8	9
5466	DFT/TD-DFT Based Study to Decipher the Proton Transfer Process in Anion Sensing Mechanism of NTS Molecule. <i>ChemistrySelect</i> , 2020, 5, 5437-5450.	0.7	5
5467	Structural and electronic properties of the adsorption of nitric oxide molecule on copper clusters Cu _N (N=1-7): A DFT study. <i>Chemical Physics Letters</i> , 2020, 753, 137543.	1.2	6
5468	Syntheses, structure, Hirshfeld analysis and antimicrobial activity of four new Co(II) complexes with s-triazine-based pincer ligand. <i>Inorganica Chimica Acta</i> , 2020, 510, 119753.	1.2	17
5469	Selectivity of 18-crown-6 ether to alkali ions by density functional theory and molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , 2020, 311, 113305.	2.3	18
5470	Absorption and fluorescence properties of non-symmetric benzo-, furo-, and thieno-fused structures at the b bonds in the BODIPY frame. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 239, 118472.	2.0	3
5471	Amino and hydroxy substitution influences pyrene-DNA binding. <i>Science of the Total Environment</i> , 2020, 725, 138542.	3.9	14
5472	Influence of spin state and electron configuration on the active site and mechanism for catalytic hydrogenation on metal cation catalysts supported on NU-1000: insights from experiments and microkinetic modeling. <i>Catalysis Science and Technology</i> , 2020, 10, 3594-3602.	2.1	14
5473	Multipolar Porphyrin-Triazatruxene Arrays for Two-Photon Fluorescence Cell Imaging. <i>Chemistry - A European Journal</i> , 2020, 26, 13842-13848.	1.7	11
5474	Hydrogen sulphide H_2S and noble gases (Ng = He, Ne, Ar, Kr, Xe, Rn) complexes: A theoretical study of their dynamics, spectroscopy, and interactions. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26266.	1.0	4
5475	Volatile organic compounds enhancing sulfuric acid-based ternary homogeneous nucleation: The important role of synergistic effect. <i>Atmospheric Environment</i> , 2020, 233, 117609.	1.9	11
5476	Designing versatile sulfoximine as accepting unit to regulate the photophysical properties of TADF emitters towards high-performance OLEDs. <i>Chemical Engineering Journal</i> , 2020, 399, 125648.	6.6	20
5477	The bonds and aromaticities of $[NgB_xO_y]^+$ (Ng=Ar, Kr and Xe; $x=5$, $y=7$). <i>Computational and Theoretical Chemistry</i> , 2020, 1179, 112798.	1.1	1
5478	Theoretical research on nonlinear optical properties of sandwich compounds $M_3-NO_3-M_3$ (M, M'=Li, Tj). <i>ETQ</i> , 2020, 11, 10784314.	1.1	1
5479	Effect of O-containing functional groups produced by preoxidation on Zhundong coal gasification. <i>Fuel Processing Technology</i> , 2020, 206, 106480.	3.7	26
5480	Conceptual DFT and TDDFT study on electronic structure and reactivity of pure and sulfur doped (CrO ₃) (n=1-10) clusters. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 99, 107617.	1.3	7
5481	Pnicogen Bonds Pairing Anionic Lewis Acid with Neutral and Anionic Bases. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4998-5006.	1.1	24
5482	A Promising Phase Change Material with Record High Ionic Conductivity over a Wide Temperature Range of a Plastic Crystal Phase and Magnetic Thermal Memory Effect. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 28129-28138.	4.0	16

#	ARTICLE	IF	CITATIONS
5483	Remarkable second and third order nonlinear optical properties of organometallic $C_{60}Li_6$ - M_3O electrides. <i>New Journal of Chemistry</i> , 2020, 44, 9822-9829.	1.4	43
5484	C-F and C-H bond cleavage mechanisms of trifluoromethane ions in low-lying electronic states: threshold photoelectron-photoion coincidence imaging and theoretical investigations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13808-13817.	1.3	5
5485	Modification of geometrical and electronic structures of anionic and neutral silicon clusters by double-doped tantalum atoms. <i>Molecular Physics</i> , 2020, 118, e1770883.	0.8	3
5486	Defect engineering and zinc oxide doping of black phosphorene for nitrogen dioxide capture and detection: quantum-chemical calculations. <i>Applied Surface Science</i> , 2020, 523, 146527.	3.1	37
5487	A Thioxanthothioxanthene-based Hole Transporter with 2D Molecular Stacking for Efficient and Thermostable Perovskite Solar Cells. , 2020, 2, 691-698.		10
5488	A donor design strategy for triazine-carbazole blue thermally activated delayed fluorescence materials. <i>New Journal of Chemistry</i> , 2020, 44, 9743-9753.	1.4	15
5489	Unusual effects of the bulky 1-norbornyl group in cobalt carbonyl chemistry: low-energy structures with agostic hydrogen atoms. <i>New Journal of Chemistry</i> , 2020, 44, 8986-8995.	1.4	0
5490	Study of the influence of intermolecular interaction on classical and reverse substituent effects in <i>i</i> -substituted phenylboranes. <i>New Journal of Chemistry</i> , 2020, 44, 9656-9670.	1.4	13
5491	Red-emissive poly(phenylene vinylene)-derivated semiconductors with well-balanced ambipolar electrical transporting properties. <i>Journal of Materials Chemistry C</i> , 2020, 8, 10868-10879.	2.7	18
5492	Achieving Adaptive Aromaticity in Cyclo[10]carbon by Screening Cyclo[n]carbon ($n=8\sim 24$). <i>Chemistry - an Asian Journal</i> , 2020, 15, 2187-2191.	1.7	43
5493	A molecular-scale study on the role of methanesulfinic acid in marine new particle formation. <i>Atmospheric Environment</i> , 2020, 227, 117378.	1.9	21
5494	Structural and energetic investigation on the host/guest inclusion process of benzyl isothiocyanate into β -cyclodextrin using dispersion-corrected DFT calculations. <i>Carbohydrate Research</i> , 2020, 491, 107980.	1.1	18
5495	A novel in-situ chemical oxidation channel - Selective pH-dependence of refractory β -lactam antibiotics in the synergistic mechanism of persulfate and g-C ₃ N ₄ under visible light. <i>Chemical Engineering Journal</i> , 2020, 394, 124899.	6.6	28
5496	Nucleation mechanisms of iodic acid in clean and polluted coastal regions. <i>Chemosphere</i> , 2020, 253, 126743.	4.2	25
5497	Sorption of five organic compounds by polar and nonpolar microplastics. <i>Chemosphere</i> , 2020, 257, 127206.	4.2	79
5498	First-principles study on the structure and optical spectroscopy of the redox-active center of blue copper proteins. <i>Chemical Physics</i> , 2020, 537, 110859.	0.9	1
5499	Molecular simulation study on gas adsorption and separation performance of alkyl-functionalized HKUST materials. <i>Computational Materials Science</i> , 2020, 181, 109755.	1.4	7
5500	Efficiently luminescent cuprous iodide complexes supported by novel N ⁺ P-chelating ligands: Synthesis, structure and optoelectronic performances. <i>Dyes and Pigments</i> , 2020, 180, 108487.	2.0	12

#	ARTICLE	IF	CITATIONS
5501	NIR emitting platinum pincer complexes based on the N ^N C ligand containing {benz[4,5]imidazo[1,2-a]pyrazin} aromatic system; synthesis, characterization and photophysical study. <i>Inorganica Chimica Acta</i> , 2020, 511, 119776.	1.2	3
5502	Hydrogen detection on black phosphorene doped with Ni, Pd, and Pt: Periodic density functional calculations. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 16298-16309.	3.8	35
5503	Solvation of lithium ion in helium clusters: Structural properties and relative stabilities. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 98, 107582.	1.3	0
5504	Tannic acid modified single nanopore with multivalent metal ions recognition and ultra-trace level detection. <i>Nano Today</i> , 2020, 33, 100868.	6.2	96
5505	Conformation and bonding of 2-methoxy pyridine and its monohydrate from rotational spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 239, 118434.	2.0	5
5506	Density Functional Theory Studies of the Adsorption and Interactions between Selenium Species and Mercury on Activated Carbon. <i>Energy & Fuels</i> , 2020, 34, 9779-9786.	2.5	16
5507	Weakly Conjugated Phosphine Oxide Hosts for Efficient Blue Thermally Activated Delayed Fluorescence Organic Light-Emitting Diodes. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 30591-30599.	4.0	11
5508	Imidazolium-Based Ionic Liquids Introduced into π -Electron Donors: Highly Efficient Toluene Capture. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 9058-9069.	3.2	48
5509	Unveiling the Chemo- and Stereoselectivities of NHC-Catalyzed Reactions of an Aliphatic Ester with Aminochalcone. <i>Journal of Organic Chemistry</i> , 2020, 85, 8437-8446.	1.7	26
5510	Identifying the active sites of carbonaceous surface for the adsorption of gaseous arsenic trioxide: A theoretical study. <i>Chemical Engineering Journal</i> , 2020, 402, 125800.	6.6	34
5511	Aminated C20 fullerene as a promising nanosensor for detection of A-234 nerve agent. <i>Computational and Theoretical Chemistry</i> , 2020, 1186, 112907.	1.1	19
5512	Theoretical insights into the performance of graphene derivatives, h-BN and BNC heterostructures in the adsorption and elimination of atrazine: An all-electron DFT study. <i>Diamond and Related Materials</i> , 2020, 108, 107967.	1.8	10
5513	Uptake of formaldehyde onto doped phosphorene nanosheets: A cluster DFT study of single and co-adsorption states. <i>Journal of Alloys and Compounds</i> , 2020, 831, 154885.	2.8	26
5514	A comparison of ether- and alkyl-imidazolium-based ionic liquids diluted with CH ₃ CN: A combined FTIR and DFT study. <i>Journal of Molecular Liquids</i> , 2020, 313, 113542.	2.3	18
5515	Exploring non-covalent interactions for metformin-thyroid hormones stabilization: Structure, Hirshfeld atomic charges and solvent effect. <i>Journal of Molecular Liquids</i> , 2020, 313, 113590.	2.3	10
5516	π -Stacking Driven Aggregation and Folding of Squaramides. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5832-5839.	1.1	6
5517	Probing Solute-Solvent Interactions of Transition Metal Complexes Using L-Edge Absorption Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5636-5645.	1.2	8
5518	The tetrotum cluster Li ₂ FeB ₁₄ and its possible use for constructing boron nanowires. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15013-15021.	1.3	3

#	ARTICLE	IF	CITATIONS
5519	Charge transfer characteristics of fullerene-free polymer solar cells <i>via</i> multi-state electronic coupling treatment. <i>Sustainable Energy and Fuels</i> , 2020, 4, 4137-4157.	2.5	2
5520	Unexpected Electronic Behavior of Organic Azide and <i>Metal-Carbyne</i> in Their 1,3-Dipolar Cycloaddition Reaction. <i>Chinese Journal of Chemistry</i> , 2020, 38, 1565-1570.	2.6	10
5521	Nonlinear optical response of sodium based superalkalis decorated graphdiyne surface: A DFT study. <i>Optik</i> , 2020, 218, 165033.	1.4	22
5522	Re ₆ C ₃₂ : A Magnetic Pentagonal Icositetrahedron Molecule. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4440-4444.	1.1	0
5523	Theoretical Framework of 1,3-Thiazolium-5-Thiolates Mesoionic Compounds: Exploring the Nature of Photophysical Property and Molecular Nonlinearity. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5563-5569.	1.1	16
5524	New Discovery of Metal-Organic Framework UTSA-280: Ultrahigh Adsorption Selectivity of Krypton over Xenon. <i>Journal of Physical Chemistry C</i> , 2020, 124, 14603-14612.	1.5	19
5525	Theoretical Investigation on Copper(I) Complexes Featuring a Phosphonic Acid Anchor with Asymmetric Ligands for DSSC. <i>ACS Applied Electronic Materials</i> , 2020, 2, 2141-2150.	2.0	8
5526	Density Functional Theory Study on the Mechanism of Iridium-Catalyzed Benzylamine <i>ortho</i> -C-H Alkenylation with Ethyl Acrylate. <i>ACS Omega</i> , 2020, 5, 15446-15453.	1.6	4
5527	Insights into the Anchoring of Polysulfides and Catalytic Performance by Metal Phthalocyanine Covalent Organic Frameworks as the Cathode in Lithium-Sulfur Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 10185-10192.	3.2	37
5528	Highly efficient luminescence from space-confined charge-transfer emitters. <i>Nature Materials</i> , 2020, 19, 1332-1338.	13.3	413
5529	A transition metal-gallium cluster formed <i>via</i> insertion of α -Ga. <i>Chemical Communications</i> , 2020, 56, 8139-8142.	2.2	3
5530	Theoretical elucidation of the multi-functional synthetic methodology for switchable Ni(0)-catalyzed C-H allylations, alkenylations and dienylations with allenes. <i>Catalysis Science and Technology</i> , 2020, 10, 4219-4228.	2.1	8
5531	Charge density of 4-methyl-3-[(tetrahydro-2H-pyran-2-yl)oxy]thiazole-2(3H)-thione. A comprehensive multipole refinement, maximum entropy method and density functional theory study. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 450-468.	0.5	3
5532	Theoretical Insight into the Interaction between Chloramphenicol and Functional Monomer (Methacrylic Acid) in Molecularly Imprinted Polymers. <i>International Journal of Molecular Sciences</i> , 2020, 21, 4139.	1.8	36
5533	A density functional theory study on the atmospheric reaction of CH ₃ O ₂ with HS: Mechanism and kinetics. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26330.	1.0	0
5534	Axially Chiral Biphenyl Compound-Based Thermally Activated Delayed Fluorescent Materials for High-Performance Circularly Polarized Organic Light-Emitting Diodes. <i>Advanced Science</i> , 2020, 7, 2000804.	5.6	71
5535	Density functional theory studies of effects of boron replacement on the structure and property of RDX and HMX. <i>Journal of the Chinese Chemical Society</i> , 2020, 67, 1977-1985.	0.8	2
5536	Tautomers of homophthalic anhydride in the ground and excited electronic states: analysis through energy, hardness and vibrational signatures. <i>Journal of Molecular Modeling</i> , 2020, 26, 173.	0.8	7

#	ARTICLE	IF	CITATIONS
5537	Thermodynamic inhibition effects of an ionic liquid (choline chloride), a naturally derived substance (urea), and their mixture (deep eutectic solvent) on CH ₄ hydrates. <i>Chemical Engineering Journal</i> , 2020, 399, 125830.	6.6	27
5538	Long-lasting direct capture of xylene from air using covalent-triazine frameworks through multiple C-H⋯N weak interactions. <i>Chemical Engineering Journal</i> , 2020, 400, 125888.	6.6	8
5539	Hydrogen adsorption on BN-embedded tetrabenzopentacene as a promising nanoflake for energy storage: Theoretical insights. <i>Diamond and Related Materials</i> , 2020, 108, 107968.	1.8	11
5540	Size dependent hydrogen-bonded methanol wires regulating the fluorescence On-Off of 1-H-pyrrolo[3,2-h]quinoline⋅(MeOH) _{n=1,2} complexes with ESMP. <i>Journal of Molecular Liquids</i> , 2020, 306, 112894.	2.3	14
5541	Vibrational spectrum of 1-ethyl-3-methylimidazolium tetrafluoroborate on graphene surface. <i>Journal of Molecular Liquids</i> , 2020, 311, 113340.	2.3	5
5542	New oxyalkyl derivatives of trifluoromethanesulfonamide: Dynamic rivalry between different types of chain and cyclic associates in different phase states. <i>Journal of Molecular Structure</i> , 2020, 1219, 128534.	1.8	3
5543	Two new C ₁₉ -diterpenoid alkaloids from <i>Aconitum smirnovii</i> . <i>Phytochemistry Letters</i> , 2020, 38, 96-100.	0.6	4
5544	Synthesis, structure and in vitro anticancer activity of Pd(II) complexes of mono- and bis-pyrazolyl-s-triazine ligands. <i>Polyhedron</i> , 2020, 187, 114665.	1.0	5
5545	SBA-15-Supported Imidazolium Ionic Liquid through Different Linkers as a Sustainable Catalyst for the Synthesis of Cyclic Carbonates: A Kinetic Study and Theoretical DFT Calculations. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 12632-12644.	1.8	42
5546	Design, synthesis and investigations of a series of energetic salts through the variation of amines and concentration of picrate anions. <i>CrystEngComm</i> , 2020, 22, 4842-4852.	1.3	6
5547	Spectroscopic evidence for intact carbonic acid stabilized by halide anions in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19459-19467.	1.3	10
5548	Components of the interaction energy of the odd-electron halogen bond: an <i>ab initio</i> study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15389-15400.	1.3	6
5549	Electronic structure and stability of Al ₆ CMn (M=Li, Na, K; n=2, 4, 6) clusters. <i>Computational and Theoretical Chemistry</i> , 2020, 1178, 112780.	1.1	3
5550	Second-order NLO properties of bis-cyclometalated iridium(III) complexes with ^β -diketiminato ancillary ligand: Substituent and redox effect. <i>Inorganica Chimica Acta</i> , 2020, 511, 119835.	1.2	4
5551	Solid-state effect on luminescent properties of thermally activated delayed fluorescence molecule with aggregation induced emission: A theoretical perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 241, 118634.	2.0	11
5552	Complexes of HArF and AuX (X = F, Cl, Br, I). Comparison of H⋯F bonds, halogen bonds, F⋯shared bonds and covalent bonds. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5891.	1.7	6
5553	The aromatic fullerene-like silicon cage with 12 Si ₅ pentagons stabilized by a V ₃ unit. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	6
5554	A DFT study of the mechanism of H transfer during steam gasification. <i>Combustion and Flame</i> , 2020, 219, 327-338.	2.8	22

#	ARTICLE	IF	CITATIONS
5555	Assessing the ecotoxicity of ionic liquids on <i>Vibrio fischeri</i> using electrostatic potential descriptors. <i>Journal of Hazardous Materials</i> , 2020, 397, 122761.	6.5	16
5556	A divergent mode of activation of a nitrosyl iron complex with unusual antiangiogenic activity. <i>Journal of Inorganic Biochemistry</i> , 2020, 210, 111133.	1.5	7
5557	On the Interaction between Superatom Al ₁₂ Be and DNA Nucleobases/Base Pairs: Bonding Nature and Potential Applications in O ₂ Activation and CO Oxidation. <i>ACS Omega</i> , 2020, 5, 15325-15334.	1.6	5
5558	Covalent vs Charge-Shift Nature of the Metal–Metal Bond in Transition Metal Complexes: A Unified Understanding. <i>Journal of the American Chemical Society</i> , 2020, 142, 12277-12287.	6.6	37
5559	Cobalt/Lewis Acid Catalysis for Hydrocarbofunctionalization of Alkynes via Cooperative C–H Activation. <i>Journal of the American Chemical Society</i> , 2020, 142, 12878-12889.	6.6	51
5560	Iridium-Catalyzed Enantioselective Transfer Hydrogenation of Ketones Controlled by Alcohol Hydrogen-Bonding and sp ³ C–H Noncovalent Interactions. <i>Advanced Synthesis and Catalysis</i> , 2020, 362, 4655-4661.	2.1	15
5561	The strategy for improving the stability of nitroform derivatives—high-energetic oxidant based on hexanitroethane. <i>Journal of Molecular Modeling</i> , 2020, 26, 181.	0.8	3
5562	Theoretical study on structures of Am(III) carbonate complexes. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2020, 325, 527-535.	0.7	3
5563	Azafluorene derivatives as inhibitors of SARS CoV-2 RdRp: Synthesis, physicochemical, quantum chemical, modeling and molecular docking analysis. <i>Journal of Molecular Structure</i> , 2020, 1220, 128741.	1.8	28
5564	New donor-acceptor-donor type of organic semiconductors based on the regioisomers of diketopyrrolopyrroles: A DFT study. <i>Materials Today Communications</i> , 2020, 25, 101364.	0.9	11
5565	Wavelength-Dependent Ultraviolet Photodissociation of Protonated Tryptamine. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5280-5287.	1.1	5
5566	Halogen Bonding Between Anions: Association of Anion Radicals of Tetraiodo- <i>p</i> -benzoquinone with Iodide Anions. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 17197-17201.	7.2	13
5567	Hydrogen bond interactions of hydrated aluminum nitrate with <sc>PVDF</sc>, <sc>PVDF@TrFE</sc> and <sc>PVDF@HFP</sc>: A density functional theory-based illustration. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26328.	1.0	13
5568	Spectroscopic (FTIR and UV-Vis) Analysis, Supramolecular Studies, XRD Structural Characterization and Theoretical Studies of Two Flavone-Oxime Derivatives. <i>ChemistrySelect</i> , 2020, 5, 6365-6372.	0.7	0
5569	Molecular and dissociative adsorption of tetrachlorodibenzodioxin on M-doped graphenes (M = B, Al). <i>Tj ETQq0 0 0 ggBT /Overl</i>	0.8	0
5570	Novel axial substituted subphthalocyanines and their TiO ₂ nanocomposites: Synthesis, structure, theoretical calculation and their photocatalytic properties. <i>Materials Today Communications</i> , 2020, 25, 101264.	0.9	6
5571	A novel D-A-D-typed rod-like fluorescent material for efficient Fe(III) and Cr(VI) detection: Synthesis, structure and properties. <i>Sensors and Actuators B: Chemical</i> , 2020, 320, 128377.	4.0	12
5572	Asymmetric Induction with a Chiral Amine Catalyzed by a Ru-PNP Pincer Complex: Insight from Theoretical Investigation. <i>Inorganic Chemistry</i> , 2020, 59, 8404-8411.	1.9	13

#	ARTICLE	IF	CITATIONS
5573	Coordination of a Central Atom by Multiple Intramolecular Pnictogen Bonds. <i>Inorganic Chemistry</i> , 2020, 59, 9315-9324.	1.9	19
5574	Chemoselective Cross-Coupling of <i>gem</i> -Borazirconocene Alkanes with Aryl Halides. <i>Journal of the American Chemical Society</i> , 2020, 142, 11506-11513.	6.6	27
5575	Metallophilic interactions: observations of the shortest metallophilic interactions between closed shell (d^{10} , d^{10} , d^{10} , d^8 , d^8) metal ions [$M = Hg$ and Pd and $M = Cu$, Ag , Au , and Pd]. <i>Dalton Transactions</i> , 2020, 49, 9099-9117.	1.6	30
5576	Distinctly Diverse PLQY and Inverse Solid-State Luminescent Properties in Structure-Similar Diphenyl Sulfone TADF Molecules: A Role of Ca^{2+} . <i>Advanced Theory and Simulations</i> , 2020, 3, 2000037.	1.3	3
5577	Halogen Bonding Between Anions: Association of Anion Radicals of Tetraiodo- <i>p</i> -benzoquinone with Iodide Anions. <i>Angewandte Chemie</i> , 2020, 132, 17350-17354.	1.6	4
5578	Self-assembly of multifunctional hydrogels with polyoxometalates helical arrays using nematic peptide liquid crystal template. <i>Journal of Colloid and Interface Science</i> , 2020, 578, 218-228.	5.0	16
5579	Molecular and supramolecular structures of self-assembled Cu(II) and Co(II) complexes with 4,4'-[6-(3,5-dimethyl-1H-pyrazol-1-yl)-1,3,5-triazine-2,4-diyl]dimorpholine ligand. <i>Journal of Molecular Structure</i> , 2020, 1219, 128584.	1.8	3
5580	Computational study of catalyst-controlled regiodivergent pathways in hydroboration of 1,3-dienes: mechanism and origin of regioselectivity. <i>Organic Chemistry Frontiers</i> , 2020, 7, 2157-2167.	2.3	11
5581	A semipinacol rearrangement of vinylogous β -ketol cocatalyzed by a cinchona-based primary amine and N-Boc-phenylglycines: mechanisms, roles of catalysts and the origin of enantioselectivity. <i>Organic Chemistry Frontiers</i> , 2020, 7, 1845-1861.	2.3	6
5582	Efficient and chromaticity stable green and white organic light-emitting devices with organic-inorganic hybrid materials. <i>RSC Advances</i> , 2020, 10, 21206-21221.	1.7	4
5583	Photodegradation of seven bisphenol analogues by Bi ₅ O ₇ /UiO-67 heterojunction: Relationship between the chemical structures and removal efficiency. <i>Applied Catalysis B: Environmental</i> , 2020, 277, 119222.	10.8	66
5584	Comparative enantioseparation of chiral 4,4'-bipyridine derivatives on coated and immobilized amylose-based chiral stationary phases. <i>Journal of Chromatography A</i> , 2020, 1625, 461303.	1.8	20
5585	Molecular mechanism for the encapsulation of the doxorubicin in the cucurbit[<i>n</i>]urils cavity and the effects of diameter, protonation on loading and releasing of the anticancer drug: Mixed quantum mechanical/ molecular dynamics simulations. <i>Computer Methods and Programs in Biomedicine</i> , 2020, 196, 105563.	2.6	9
5586	2-((9H-fluoren-9-ylidene)methyl)pyridine as a new functional block for aggregation induced emissive and stimuli-responsive materials. <i>Dyes and Pigments</i> , 2020, 181, 108595.	2.0	3
5587	Theoretical insights into hydrogen sensing capabilities of black phosphorene modified through ZnO doping and decoration. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 16918-16928.	3.8	35
5588	1,2,4-triazole-3-thione Schiff bases compounds: Crystal structure, hirshfeld surface analysis, DFT studies and biological evaluation. <i>Journal of Molecular Structure</i> , 2020, 1219, 128591.	1.8	16
5589	Fluorenone-based molecules for resistive memory devices: Tuning memory behavior by adjusting end groups. <i>Synthetic Metals</i> , 2020, 266, 116431.	2.1	3
5590	How Stable and Powerful Can Metal <i>cyclo</i> -Pentazolate Salts Be? An Answer through Theoretical Crystal Design. <i>Crystal Growth and Design</i> , 2020, 20, 4794-4801.	1.4	6

#	ARTICLE	IF	CITATIONS
5591	How to Stabilize a Heptagon-Containing C ₈₀ Cage by Endohedral Derivation. <i>Inorganic Chemistry</i> , 2020, 59, 8099-8107.	1.9	2
5592	Anionic behavior and single-molecule crystal in fullerene confinements: A contribution from $\langle \text{scp} \rangle \text{DFT} \langle \text{scp} \rangle$ energy decomposition and cooperativity analyses. <i>Journal of Computational Chemistry</i> , 2020, 41, 1912-1920.	1.5	8
5593	Mechanism of hydrogen generation on stable Mo-edge of 2H-MoS ₂ in water from density functional theory. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	6
5594	Structure, stability and bonding features of Al _n Si _m clusters. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	4
5595	Solvent effect on excited-state intramolecular proton transfer process based on "naked" diazaborepins. <i>Computational and Theoretical Chemistry</i> , 2020, 1185, 112898.	1.1	7
5596	Theoretical insights into the spectral properties of a salicylideneaniline-based fluorescence chemosensor (SB1) and its sensing mechanism for cyanide anion. <i>Journal of Molecular Liquids</i> , 2020, 312, 113295.	2.3	17
5597	Understanding the Interaction Mechanism of Char and CaSO ₄ Oxygen Carrier in Chemical Looping Combustion: Semi-empirical Tight-Binding Method Calculation and Grand Canonical Monte Carlo Simulation. <i>Energy & Fuels</i> , 2020, 34, 8600-8607.	2.5	6
5598	Effective Separation and Purification of Nitrogen-Containing Aromatics from the Light Portion of a High-Temperature Coal Tar Using Choline Chloride and Malonic Acid: Experimental and Molecular Dynamics Simulation. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 9464-9471.	3.2	21
5599	Reaction mechanism of synthetic thorium sulfides: theoretical calculation study. <i>Journal of Molecular Modeling</i> , 2020, 26, 123.	0.8	0
5600	Density functional theory studies on cytosine analogues for inducing double-proton transfer with guanine. <i>Scientific Reports</i> , 2020, 10, 9671.	1.6	8
5601	Insight into structural properties of polyethylene glycol monolaurate in water and alcohols from molecular dynamics studies. <i>RSC Advances</i> , 2020, 10, 21760-21771.	1.7	8
5602	Synthesis, spectroscopic characterization and computational study of Ru(II)/DMSO complexes with monocoordinated carbazate ligands. <i>Journal of Coordination Chemistry</i> , 2020, 73, 1605-1618.	0.8	1
5603	A Detailed DFT Study on Electronic Structures and Nonlinear Optical Properties of Doped C ₃₀ . <i>ChemistrySelect</i> , 2020, 5, 6987-6999.	0.7	22
5604	Mechanism of a catalytic silver(I)-complex: assisted electroless deposition of inductance coil on poly(ethylene terephthalate) film. <i>Journal of Materials Science: Materials in Electronics</i> , 2020, 31, 8165-8173.	1.1	1
5605	High sensitivity of graphdiyne nanoflake toward detection of phosgene, thiophosgene and phosgenoxime; a first-principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107658.	1.3	45
5606	Mechanism of sonication time on structure and adsorption properties of 3D peanut shell/graphene oxide aerogel. <i>Science of the Total Environment</i> , 2020, 739, 139983.	3.9	24
5607	Lasing Properties Activation by Constitutional Isomerism of an Electron-Accepting Group. <i>Journal of Physical Chemistry C</i> , 2020, 124, 13845-13857.	1.5	0
5608	Carbon monoxide formation from trimethylamine-boranecarboxylate: DFT studies of S _N i and chelotropic mechanisms. <i>RSC Advances</i> , 2020, 10, 16038-16044.	1.7	2

#	ARTICLE	IF	CITATIONS
5609	Diversity and uniformity in anion- π complexes of thiocyanate with aromatic, olefinic and quinoidal π -acceptors. <i>Dalton Transactions</i> , 2020, 49, 8734-8743.	1.6	19
5610	Molecular docking studies, structural and spectroscopic properties of monomeric and dimeric species of benzofuran-carboxylic acids derivatives: DFT calculations and biological activities. <i>Computational Biology and Chemistry</i> , 2020, 87, 107311.	1.1	61
5611	Single Si-Doped Graphene as a Catalyst in Oxygen Reduction Reactions: An In Silico Study. <i>ACS Omega</i> , 2020, 5, 15268-15279.	1.6	21
5612	The effect of introducing an ether group into an imidazolium-based ionic liquid in binary mixtures with DMSO. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15734-15742.	1.3	29
5613	Manganon ⁰ - and rhenia-copper carboranes based on the medium-size non-icosahedral 5,6-dicarba-nido-decaborane. <i>Journal of Organometallic Chemistry</i> , 2020, 911, 121141.	0.8	1
5614	Studies of the stability, nucleophilic substitution reactions, DNA/BSA interactions, cytotoxic activity, DFT and molecular docking of some tetra- and penta-coordinated gold(Au^{I}) complexes. <i>New Journal of Chemistry</i> , 2020, 44, 11172-11187.	1.4	17
5615	Conformational and electronic study of dopamine interacting with the D_2 dopamine receptor. <i>Journal of Computational Chemistry</i> , 2020, 41, 1898-1911.	1.5	9
5616	New boron-capped cage manganese(II) complex with terminal thiophene-2-carboxaldehyde groups: Crystal structure and density functional theory investigation for electron transfer. <i>Journal of Molecular Structure</i> , 2020, 1219, 128481.	1.8	2
5617	Towards low-impact-sensitivity through crystal engineering: New energetic co-crystals formed between Picric acid, Trinitrotoluene and 9-Vinylanthracene. <i>Journal of Molecular Structure</i> , 2020, 1219, 128614.	1.8	8
5618	Theoretical analysis of the absorption spectrum, electronic structure, excitation, and intramolecular electron transfer of Zn^{II} porphyrin dyes for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14846-14856.	1.3	8
5619	All-nitrogen ion-based compounds as energetic oxidizers: a theoretical study on $[\text{N}_5^+][\text{NO}_3^-]$, $[\text{N}_5^+][\text{N}(\text{NO}_2)_2^-]$, $[\text{NO}_2^+][\text{N}_5^-]$ and NO_2N_3 . <i>New Journal of Chemistry</i> , 2020, 44, 11188-11195.	1.4	3
5620	Changes in Electron Structure of the Triple Bond in Substituted Acetylene and Diacetylene Derivatives. <i>ChemPhysChem</i> , 2020, 21, 1847-1857.	1.0	6
5621	Computational Insight into the Mechanism of Mannich Reaction between Glycinate and Aryl N -diphenylphosphinyl Imine Catalyzed by N -Quaternized Pyridoxal. <i>ChemistrySelect</i> , 2020, 5, 6504-6513.	0.7	3
5622	Investigation on spectra (UV-Vis, vibrational, NMR, HRMS), electronic structure (DFT calculations), molecular docking and antidiabetic activity of N -((benzo[d]thiazol-2-ylthio)methyl)- N -cyclohexylcyclohexanamine - A Mannich base. <i>Journal of Molecular Structure</i> , 2020, 1219, 128604.	1.8	7
5623	Triggered singlet fission via tuning current density vectors (CDV) in the ground-state and excited-state. <i>Organic Electronics</i> , 2020, 84, 105795.	1.4	1
5624	Hydrogen Migration-Triggered Diradicaloid Singlet-Fission Switch. <i>Journal of the American Chemical Society</i> , 2020, 142, 11791-11803.	6.6	11
5625	The halogen bond with isocyano carbon reduces isocyanide odor. <i>Nature Communications</i> , 2020, 11, 2921.	5.8	46
5626	Probing the Origin of Adaptive Aromaticity in 16-Valence-Electron Metallapentalenes. <i>Chemistry - A European Journal</i> , 2020, 26, 12964-12971.	1.7	28

#	ARTICLE	IF	CITATIONS
5627	Structures and properties of $[Ag(Ag_2S)_n]^+$ clusters with $n = 1-9$: a density functional theory study. <i>Journal of Nanoparticle Research</i> , 2020, 22, 1.	0.8	8
5628	A theoretical investigation of different point charges combined with GAFF and OPLS-AA for acetic anhydride. <i>Chemical Physics Letters</i> , 2020, 754, 137707.	1.2	5
5629	Electronic structures and bonding of graphdiyne and its BN analogs: Transition from quasi-planar to planar sheets. <i>Journal of Alloys and Compounds</i> , 2020, 846, 155987.	2.8	5
5630	Intramolecular bonding properties in actinide embedded nearly planar superatoms. <i>Chemical Physics Letters</i> , 2020, 752, 137574.	1.2	4
5631	Perylene derivative films: Emission from higher singlet excited state. <i>Journal of Luminescence</i> , 2020, 226, 117478.	1.5	1
5632	Halogen bond and internal dynamics in the π -complex of pyridine-chlorotrifluoromethane: A rotational study. <i>Journal of Molecular Spectroscopy</i> , 2020, 371, 111323.	0.4	8
5633	Theoretical study on the ESIPT of fluorescent probe molecules N-(2-(4-(dimethylamino)phenyl)-3-hydroxy-4-oxo-4h-chromen-6-yl) butyramide in different solvents. <i>Journal of Molecular Liquids</i> , 2020, 314, 113614.	2.3	14
5634	Structures, stabilities and electronic properties of the bimetal V2-doped Sin ($n = 1-10$) clusters: a density functional investigation. <i>European Physical Journal D</i> , 2020, 74, 1.	0.6	0
5635	The electrochemical properties and PIM1 kinase enzyme inhibition of some 2-(hydroxy phenyl amino) naphthalene-1,4-dione derivatives. <i>Journal of Molecular Liquids</i> , 2020, 307, 112874.	2.3	1
5636	Trace amounts of $Cu(OAc)_2$ boost the efficiency of cumene oxidation catalyzed by carbon nanotubes washed with HCl. <i>Catalysis Science and Technology</i> , 2020, 10, 2523-2530.	2.1	22
5637	Theoretical studies on full-color thermally activated delayed fluorescence molecules. <i>Journal of Materials Chemistry C</i> , 2020, 8, 5839-5846.	2.7	13
5638	Trishomoaromatic ($B_3N_3Ph_6$) Dianion: Characterization and Two-Electron Reduction. <i>Angewandte Chemie</i> , 2020, 132, 8953-8957.	1.6	4
5639	Anion-Anion Complexes Established between Aspartate Dimers. <i>ChemPhysChem</i> , 2020, 21, 1052-1059.	1.0	17
5640	The oxo exchange reaction mechanism of americium(VI): a density functional theory study. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2020, 324, 857-868.	0.7	1
5641	Theoretical Insight into Palladium(II)-Counterion-Ligand Cooperative Regiodivergent Syntheses of Indolo[3,2- <i>c</i>]coumarins and Benzofuro[3,2- <i>c</i>]quinolinones from Diphenylethyne Derivatives. <i>Inorganic Chemistry</i> , 2020, 59, 4741-4752.	1.9	6
5642	Monoalkylation of aniline with trichloroacetimidate catalyzed by (Δ)-camphorsulfonic acid through an S_N1 reaction based on dual hydrogen-bonding activation modes. <i>New Journal of Chemistry</i> , 2020, 44, 5526-5534.	1.4	1
5643	Delocalization of the Unpaired Electron in the Quercetin Radical: Comparison of Experimental ESR Data with DFT Calculations. <i>International Journal of Molecular Sciences</i> , 2020, 21, 2033.	1.8	11
5644	Which Stereoinductor Is Better for Asymmetric Functionalization of α -Amino Acids in a Nickel(II) Coordination Environment? Experimental and DFT Considerations. <i>Chemistry - A European Journal</i> , 2020, 26, 7074-7082.	1.7	9

#	ARTICLE	IF	CITATIONS
5645	Sâˆ™Hâ€¦ O and Oâˆ™Hâ€¦ O Hydrogen Bondsâ€¦Comparison of Dimers of Thiocarboxylic and Carboxylic Acids. <i>ChemPhysChem</i> , 2020, 21, 1653-1664.	1.0	10
5646	Synthesis, characterization and thermal properties of 1,10-phenanthroline mixed-ligand complexes of cobalt(II) and copper(II): metal-mediated transformations of the dicyanamide ion. <i>Chemical Papers</i> , 2020, 74, 3003-3016.	1.0	10
5647	Carvedilol serves as a novel CYP1B1 inhibitor, a systematic drug repurposing approach through structure-based virtual screening and experimental verification. <i>European Journal of Medicinal Chemistry</i> , 2020, 193, 112235.	2.6	31
5648	Thermal hazard analysis and initial decomposition mechanism of 5-(4-pyridyl)tetrazolate-methylene tetrazole. <i>Fuel</i> , 2020, 269, 117434.	3.4	14
5649	Molecular structure, spectroscopic (FT-IR, FT-Raman, NMR, UV-VIS), chemical reactivity and biological examinations of Ketorolac. <i>Journal of Molecular Structure</i> , 2020, 1210, 128040.	1.8	18
5650	Antioxidant Properties of Camphene-Based Thiosemicarbazones: Experimental and Theoretical Evaluation. <i>Molecules</i> , 2020, 25, 1192.	1.7	23
5651	Biomimetic micro cell cathode for high performance lithiumâ€¦sulfur batteries. <i>Nano Energy</i> , 2020, 72, 104680.	8.2	42
5652	Effects of carboxylic acid auxiliary ligands on the magnetic properties of azido-Cu(II) complexes: A density functional theory study. <i>Polyhedron</i> , 2020, 182, 114506.	1.0	14
5653	A new FRET probe for ratiometric fluorescence detecting mitochondria-localized drug activation and imaging endogenous hydroxyl radicals in zebrafish. <i>Chemical Communications</i> , 2020, 56, 4432-4435.	2.2	36
5654	A novel energetic framework combining the advantages of furazan and triazole: a design for high-performance insensitive explosives. <i>Dalton Transactions</i> , 2020, 49, 4675-4679.	1.6	15
5655	A Nonâ€¦Fullerene Acceptor with Chlorinated Thienyl Conjugated Side Chains for Highâ€¦Performance Polymer Solar Cells via Toluene Processing. <i>Chinese Journal of Chemistry</i> , 2020, 38, 697-702.	2.6	20
5656	Investigation of the hydrogen, halogen and pnicoen dimers by means of molecular face calculated by ab initio method. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	2
5657	Computational Analysis of the Selective Formation of the C4Î±â€¦C8â€² Bond in the Intermolecular Coupling of Catechin Derivatives. <i>Journal of Organic Chemistry</i> , 2020, 85, 5010-5018.	1.7	2
5658	Intramolecular Charge Transfer in 5-Halogen Cytidines Revealed by Femtosecond Time-Resolved Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2020, 124, 2560-2567.	1.2	6
5659	Bioâ€¦Inspired Isoalloxazine Redox Moieties for Rechargeable Aqueous Zincâ€¦Ion Batteries. <i>Chemistry - an Asian Journal</i> , 2020, 15, 1290-1295.	1.7	31
5660	Theoretical investigation on the structure and stability of some neutral noble gas compounds containing Xeâ€¦Xe bond. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26185.	1.0	4
5661	Sorption of aromatic organophosphate flame retardants on thermally and hydrothermally produced biochars. <i>Frontiers of Environmental Science and Engineering</i> , 2020, 14, 1.	3.3	14
5662	Stretching the Pâ€¦C Bond. Variations on Carbenes and Phosphanes. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2660-2671.	1.1	5

#	ARTICLE	IF	CITATIONS
5663	Antiadiabatic View of Fast Environmental Effects on Optical Spectra. <i>Physical Review Letters</i> , 2020, 124, 107401.	2.9	17
5664	The differences and cooperativity between Ge (Sn)-O tetrel bonds and X (X=F, Cl, Br, and I) -O halogen bonds. <i>Chemical Physics</i> , 2020, 534, 110748.	0.9	2
5665	ESIPT triggered TICT of an Al ³⁺ fluorescence sensor and its sensing mechanism. <i>Journal of Luminescence</i> , 2020, 223, 117203.	1.5	8
5666	Synthesis, crystal structure, spectroscopic and nonlinear optical properties of organic salt: A combined experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2020, 1210, 128039.	1.8	9
5667	An analysis of spectroscopic, computational and biological activity studies of L-shaped sulfamoylbenzoic acid derivatives: A third order nonlinear optical material. <i>Journal of Molecular Structure</i> , 2020, 1210, 128070.	1.8	17
5668	A rational design of excellent light-absorbing dyes with different N-substituents at the phenothiazine for high efficiency solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 234, 118241.	2.0	17
5669	Discovery of a Superatom inside the Fullerene Cage. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2694-2699.	1.1	5
5670	Halogen-bonded building block for 2D self-assembly: Triggered by hydrogen-bonding motifs relative to the terminal functions of the side chains. <i>Applied Surface Science</i> , 2020, 515, 145983.	3.1	17
5671	Amino Acid Residues Vary the Self-Assembly and Photophysical Properties of Diphenylamine-Cyanostilbene-Capped Amphiphiles. <i>ChemPhotoChem</i> , 2020, 4, 481-486.	1.5	8
5672	Assessing the Recyclability of Supramolecularly Assembled Organocatalytic Species: A Theoretical Insight. <i>Israel Journal of Chemistry</i> , 2020, 60, 475-484.	1.0	2
5673	Models for predicting impact sensitivity of energetic materials based on the trigger linkage hypothesis and Arrhenius kinetics. <i>Journal of Molecular Modeling</i> , 2020, 26, 65.	0.8	33
5674	H-bond interactions between arsenite and deoxynucleotides at different pH values: A combined computational and experimental study. <i>Chemosphere</i> , 2020, 251, 126395.	4.2	5
5675	Chiral thermally activated delayed fluorescence emitters with dual conformations based on a pair of enantiomeric donors containing asymmetric carbons. <i>Dyes and Pigments</i> , 2020, 178, 108336.	2.0	10
5676	A porous g-C ₃ N ₄ nanosheets containing nitrogen defects for enhanced photocatalytic removal meropenem: Mechanism, degradation pathway and DFT calculation. <i>Environmental Research</i> , 2020, 184, 109339.	3.7	67
5677	Jet fuel range hydrocarbons production through competitive pathways of hydrocracking and isomerization over HPW-Ni/MCM-41 catalyst. <i>Fuel</i> , 2020, 269, 117465.	3.4	22
5678	Expanding the horizons of covalent organic frameworks to electrochemical sensors; A case study of CTF-FUM. <i>Microporous and Mesoporous Materials</i> , 2020, 300, 110146.	2.2	30
5679	Designing alkoxy-induced based high performance near infrared sensitive small molecule acceptors for organic solar cells. <i>Journal of Molecular Liquids</i> , 2020, 305, 112829.	2.3	76
5680	Excitation wavelength dependent ICT character and ISC efficiency in a photocleavage agent of 1-aminoanthraquinone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 234, 118200.	2.0	7

#	ARTICLE	IF	CITATIONS
5681	Theoretical study of T shaped phenothiazine/carbazole based organic dyes with naphthalimide as π -spacer for DSSCs. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 233, 118201.	2.0	22
5682	The Role of the Hydrogen Bond between Piperazine and Fullerene Molecules in Stabilizing Polymer:Fullerene Solar Cell Performance. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 15472-15481.	4.0	15
5683	Relative Position and Relative Rotation in Supramolecular Systems through the Analysis of the Principal Axes of Inertia: Ferrocene/Cucurbit[7]uril and Ferrocenyl Azide/ β -Cyclodextrin Case Studies. <i>ACS Omega</i> , 2020, 5, 5013-5025.	1.6	6
5684	Analysis of the structures, stabilities and electronic properties of MB ₁₆ (M) Tj ETQq1 1.0.784314. <i>rgBT / Q</i>	1.4	29
5685	Supramolecular lead (<sc>ii</sc>) architectures engineered by tetrel bonds. <i>CrystEngComm</i> , 2020, 22, 2389-2396.	1.3	29
5686	Experimental and DFT study of the effect of mercaptosuccinic acid on cyanide-free immersion gold deposition. <i>RSC Advances</i> , 2020, 10, 9768-9776.	1.7	5
5687	Synthesis of anionic ionic liquids@TpBd-(SO ₃) ₂ for the selective adsorption of cationic dyes with superior capacity. <i>RSC Advances</i> , 2020, 10, 5443-5453.	1.7	10
5688	TDDFT study on the photophysical properties of coumarinyl chalcones and sensing mechanism of a derived fluorescent probe for hydrogen sulfide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 234, 118263.	2.0	18
5689	Visible-light-induced photocatalyst-free C-3 functionalization of indoles with diethyl bromomalonate. <i>Green Chemistry</i> , 2020, 22, 2543-2548.	4.6	24
5690	Designing a new class of excess electron compounds with unique electronic structures and extremely large non-linear optical responses. <i>New Journal of Chemistry</i> , 2020, 44, 6411-6419.	1.4	22
5691	Insights into N-heterocyclic carbene and Lewis acid cooperatively catalyzed oxidative [3 + 3] annulation reactions of α,β -unsaturated aldehyde with 1,3-dicarbonyl compounds. <i>Organic Chemistry Frontiers</i> , 2020, 7, 1113-1121.	2.3	25
5692	Crystal Structure of the Heteroligand Complex [(2-Br-5-MePy) ₂ CoCl ₂] \cdot (2-Br-5-MePy): Formation of Supramolecular Associates due to the Halogen Bond. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2020, 46, 37-41.	0.3	7
5693	Heteroleptic Binuclear Iodoacetate Copper(II) Complexes with 3-Bromopyridine and 4-Ethylpyridine: Crystal Structures and Peculiarities of Contacts Halogen \cdots Halogen. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2020, 46, 119-124.	0.3	6
5694	Turn-on fluorescence in a stable Cd(II) metal-organic framework for highly sensitive detection of Cr ³⁺ in water. <i>Dyes and Pigments</i> , 2020, 178, 108359.	2.0	23
5695	Ultra-high capacity hydrogen storage of B ₆ Be ₂ and B ₈ Be ₂ clusters. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 12932-12939.	3.8	31
5696	Selectivity in the flotation of copper with xanthate over other ions present in wastewater: An experimental and computational study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 98, 107587.	1.3	7
5697	A smart reaction-based fluorescence probe for ratio detection of hydrazine and its application in living cells. <i>Microchemical Journal</i> , 2020, 156, 104809.	2.3	23
5698	Activatable Formation of Emissive Excimers for Highly Selective Detection of β -Galactosidase. <i>Analytical Chemistry</i> , 2020, 92, 5733-5740.	3.2	27

#	ARTICLE	IF	CITATIONS
5699	Coinage metalides: a new class of excess electron compounds with high stability and large nonlinear optical responses. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8476-8484.	1.3	26
5700	Gold-catalyzed domino cyclization enabling construction of diverse fused azaspiro tetracyclic scaffolds: a cascade catalysis mechanism due to a substrate and counterion. <i>Catalysis Science and Technology</i> , 2020, 10, 2415-2426.	2.1	8
5701	Câ€“Hâ€“Au interactions and optical properties of [(P,P) ₄ Au ₆] ²⁺ molecular gold nanoclusters. <i>Dalton Transactions</i> , 2020, 49, 4797-4804.	1.6	13
5702	Investigation on the Interaction Mechanism of the Solvent Extraction for Mercaptan Removal from Liquefied Petroleum Gas. <i>Energy & Fuels</i> , 2020, 34, 4788-4798.	2.5	16
5703	Perfluoroolefin complexes <i>versus</i> perfluorometallacycles and perfluorocarbene complexes in cyclopentadienylcobalt chemistry. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7616-7624.	1.3	2
5704	A novel hot exciton blue fluorophores and white organic light-emitting diodes with simplified configuration. <i>Scientific Reports</i> , 2020, 10, 5114.	1.6	11
5705	Introducing Trifluoromethyl to Strengthen Hydrogen Bond for High Efficiency Organic Solar Cells. <i>Frontiers in Chemistry</i> , 2020, 8, 190.	1.8	9
5706	A promising insensitive energetic material based on a fluorodinitromethyl explosophore group and 1,2,3,4-tetrahydro-1,3,5-triazine: synthesis, crystal structure and performance. <i>RSC Advances</i> , 2020, 10, 11816-11822.	1.7	10
5707	Halogen Bonding Provides Heterooctameric Supramolecular Aggregation of Diaryliodonium Thiocyanate. <i>Crystals</i> , 2020, 10, 230.	1.0	25
5708	Sensing Performance Investigations on Two-Photon Fluorescent Probes for Detecting Î²-Amyloid in Alzheimerâ€™s Disease. <i>Sensors</i> , 2020, 20, 1760.	2.1	5
5709	Widely Electronically Tunable 2,6-Disubstituted Dithieno[1,4]thiazinesâ€™ Electron-Rich Fluorophores Up to Intense NIR Emission. <i>Chemistry - A European Journal</i> , 2020, 26, 12978-12986.	1.7	5
5710	The origin of regioselectivity in Cu-catalyzed hydrocarbonylative coupling of alkynes with alkyl halides. <i>Organic Chemistry Frontiers</i> , 2020, 7, 1137-1148.	2.3	12
5711	Sulfur vs. Selenium as Bridging Ligand in Diâ€“ron Complexes: A Theoretical Analysis. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1525-1538.	1.0	10
5712	Carbonyl Bridge-Based pâ€“r Conjugated Polymers as High-Performance Electrodes of Organic Lithium-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 18457-18464.	4.0	39
5713	The role of dipole moment in two fused-ring electron acceptor and one polymer donor based ternary organic solar cells. <i>Materials Chemistry Frontiers</i> , 2020, 4, 1507-1518.	3.2	22
5714	Functionalizing triptycene to create 3D high-performance non-fullerene acceptors. <i>RSC Advances</i> , 2020, 10, 12004-12012.	1.7	3
5715	Phosphine Oxides as Spectroscopic Halogen Bond Descriptors: IR and NMR Correlations with Interatomic Distances and Complexation Energy. <i>Molecules</i> , 2020, 25, 1406.	1.7	21
5716	Scavenging of Hydrogen Peroxide by Allyl Methyl Sulfide and Diallyl Sulfide, Two Garlic Active Compounds: A Theoretical Study. <i>ChemistrySelect</i> , 2020, 5, 3234-3242.	0.7	4

#	ARTICLE	IF	CITATIONS
5717	Sulfur Dioxide Complexes of Main-Group Elements: from SO ₂ ⁰ to SO ₂ ⁺ and SO ₂ ²⁺ upon Coordination to Aluminum and Silicon Difluorides. <i>Inorganic Chemistry</i> , 2020, 59, 4703-4710.	1.9	9
5718	Adsorption of Phosgene Gas on Pristine and Copper-Decorated B ₁₂ N ₁₂ Nanocages: A Comparative DFT Study. <i>ACS Omega</i> , 2020, 5, 7641-7650.	1.6	114
5719	Design of new pincer fullerene ligands thorough [2+3] cycloaddition of the azomethine ylides to fullerene cage: a DFT study. <i>Molecular Simulation</i> , 2020, 46, 565-572.	0.9	4
5720	Synthesis and micro-mechanistic studies of histidine modified montmorillonite for lead(II) and copper(II) adsorption from wastewater. <i>Chemical Engineering Research and Design</i> , 2020, 157, 142-152.	2.7	38
5721	Unique magnetic shielding and bonding in Pnictogen nortricyclane Zintl clusters. <i>Chemical Physics Letters</i> , 2020, 749, 137414.	1.2	9
5722	Inhibitive and adsorption behavior of thiazazole derivatives on carbon steel corrosion in CO ₂ -saturated oilfield produced water: Effect of substituent group on efficiency. <i>Journal of Colloid and Interface Science</i> , 2020, 572, 91-106.	5.0	114
5723	Computational Study of Photocatalytic CO ₂ Reduction by a Ni(II) Complex Bearing an S ₂ N ₂ -Type Ligand. <i>Organometallics</i> , 2020, 39, 1176-1186.	1.1	4
5724	Linear and Star-Shaped Extended Di- and Tristyrylbenzenes: Synthesis, Characterization and Optical Response to Acid and Metal Ions. <i>Chemistry - A European Journal</i> , 2020, 26, 8137-8143.	1.7	4
5725	Theoretical study on carbonaceous materials as high efficient carriers for crizotinib drug in liquid water by density functional theory approach. <i>Structural Chemistry</i> , 2020, 31, 1553-1561.	1.0	4
5726	Glyoxylic Sulfuric Anhydride from the Gas-Phase Reaction between Glyoxylic Acid and SO ₃ : A Potential Nucleation Precursor. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3261-3268.	1.1	10
5727	Structure and C-N tetrel-bonding of the isopropylamine-CO ₂ complex studied by microwave spectroscopy and theoretical calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8467-8475.	1.3	22
5728	Using dialkyl amide <i>via</i> forming hydrophobic deep eutectic solvents to separate citric acid from fermentation broth. <i>Green Chemistry</i> , 2020, 22, 2526-2533.	4.6	22
5729	Boosting the hole transport of conductive polymers by regulating the ion ratio in ionic liquid additives. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9796-9807.	1.3	9
5730	Theoretical design of bis-azole derivatives for energetic compounds. <i>RSC Advances</i> , 2020, 10, 13185-13195.	1.7	7
5731	Acceptor-donor-acceptor type molecules for high performance organic photovoltaics chemistry and mechanism. <i>Chemical Society Reviews</i> , 2020, 49, 2828-2842.	18.7	326
5732	Charge density modulation on asymmetric fused-ring acceptors for high-efficiency photovoltaic solar cells. <i>Materials Chemistry Frontiers</i> , 2020, 4, 1747-1755.	3.2	15
5733	Beryllium bonding: insights from the σ - and π -hole analysis. <i>Journal of Molecular Modeling</i> , 2020, 26, 94.	0.8	7
5734	Enforced Planar FOX-7-like Molecules: A Strategy for Thermally Stable and Insensitive π -Conjugated Energetic Materials. <i>Journal of the American Chemical Society</i> , 2020, 142, 7153-7160.	6.6	95

#	ARTICLE	IF	CITATIONS
5735	Isolation of an elusive phosphatetrahedrane. <i>Science Advances</i> , 2020, 6, eaaz3168.	4.7	31
5736	Functionalized Pt(II) and Ir(III) NIR Emitters and Their Covalent Conjugates with Polymer-Based Nanocarriers. <i>Bioconjugate Chemistry</i> , 2020, 31, 1327-1343.	1.8	22
5737	Remarkable improvement in phosgene detection with a defect-engineered phosphorene sensor: first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9677-9684.	1.3	36
5738	A metal-free blue chromophore derived from plant pigments. <i>Science Advances</i> , 2020, 6, eaaz0421.	4.7	24
5739	Judicious Choice of N-Heterocycles for the Realization of Sky-Blue-to Green-Emitting Carbazolygold(III) C ⁺ C ⁻ N Complexes and Their Applications for Organic Light-Emitting Devices. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 9684-9692.	7.2	23
5740	Both Configuration and QM Region Size Matter: Zinc Stability in QM/MM Models of DNA Methyltransferase. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3121-3134.	2.3	28
5741	Exploring the Nature of the Energy Barriers on the Mechanism of the Zirconocene-Catalyzed Ethylene Polymerization: A Quantitative Study from Reaction Force Analysis. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8198-8209.	1.5	3
5742	Charge transfer co-crystals based on donor-acceptor interactions for near-infrared photothermal conversion. <i>Chemical Communications</i> , 2020, 56, 5223-5226.	2.2	62
5743	Superior thermally robust energetic materials featuring <i>Z</i> - <i>E</i> isomeric bis(3,4-diamino-1,2,4-triazol-5-yl)-1 <i>H</i> -pyrazole: self-assembly nitrogen-rich tubes and templates with Hofmeister anion capture architecture. <i>CrystEngComm</i> , 2020, 22, 3144-3154.	1.3	12
5744	Over 15% Efficiency Polymer Solar Cells Enabled by Conformation Tuning of Newly Designed Asymmetric Small-Molecule Acceptors. <i>Advanced Functional Materials</i> , 2020, 30, 2000383.	7.8	55
5745	High selective hydroxylation of phenol catalyzed by PNP ligand-containing [FeFe]-hydrogenase model complexes. <i>Journal of Chemical Technology and Biotechnology</i> , 2020, 95, 2180-2186.	1.6	2
5746	Theoretical design and rotational conformation analysis of molecular bevel gear with triptycene as rotator. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	2
5747	Molecular Mechanisms and Structural Basis of Retigabine Analogues in Regulating KCNQ2 Channel. <i>Journal of Membrane Biology</i> , 2020, 253, 167-181.	1.0	15
5748	Computational insight into polynitromethyl- and polydifluoroaminomethyl-substituted energetic derivatives of 2,3-dihydro pyrazino [2,3- <i>e</i>] [1, 2, 3, 4] tetrazine. <i>Journal of Molecular Modeling</i> , 2020, 26, 78.	0.8	2
5749	Optical Properties of Novel Conjugated Nanohoops: Revealing the Effects of Topology and Size. <i>Journal of Physical Chemistry C</i> , 2020, 124, 7353-7360.	1.5	51
5750	Multistimuli-Responsive Fluorescent Organogelator Based on Triphenylamine-Substituted Acylhydrazone Derivative. <i>ACS Omega</i> , 2020, 5, 5675-5683.	1.6	21
5751	Structures, stabilities and aromatic properties of endohedrally transition metal doped boron clusters M@B ₂₂ , M = Sc and Ti: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8077-8087.	1.3	8
5752	Photoelectron spectroscopy and computational investigations of the electronic structures and noncovalent interactions of cyclodextrin-closedodecaborate anion complexes $\beta\text{-CD}\cdot\text{B}_{12}\text{X}_{12}^{2-}$ ($\beta = \hat{1}, \hat{2}, \hat{3}$; X = H, F). <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7193-7200.	1.3	14

#	ARTICLE	IF	CITATIONS
5753	Does Chlorine in CH ₃ Cl Behave as a Genuine Halogen Bond Donor?. Crystals, 2020, 10, 146.	1.0	18
5754	Toward an Understanding of the Formation and Desolvation of Methanol Solvate, and Structure of Methanolysis Product: A Case Study of Nicosulfuron. Crystals, 2020, 10, 157.	1.0	4
5755	Anion Recognition by Neutral and Cationic Iodotriazole Halogen Bonding Scaffolds. Molecules, 2020, 25, 798.	1.7	3
5756	Trishomoaromatic (B ₃ N ₃ Ph ₆) Dianion: Characterization and Two-Electron Reduction. Angewandte Chemie - International Edition, 2020, 59, 8868-8872.	7.2	10
5757	Interaction and selectivity of 14-crown-4 derivatives with Li ⁺ , Na ⁺ , and Mg ²⁺ metal ions. Journal of Molecular Modeling, 2020, 26, 67.	0.8	22
5758	Deep blue electro-fluorescence and highly efficient chemical warfare agent sensor: Functional versatility of weak coupling hybridized locally excited and charge-transfer excited state. Dyes and Pigments, 2020, 177, 108317.	2.0	15
5759	Electrochemical Deposition of Copper on Epitaxial Graphene. Applied Sciences (Switzerland), 2020, 10, 1405.	1.3	14
5760	Exploring the effects of solvents on an organic explosive: Insights from the electron structure, electrostatic potential, and conformational transformations of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane. International Journal of Quantum Chemistry, 2020, 120, e26202.	1.0	1
5761	An Overall Comprehension of Anti-Aromatic Porphyrinoids Using 3D Graphical Chemical Shielding Description. Advanced Theory and Simulations, 2020, 3, 2000007.	1.3	1
5762	Revisiting van der Waals Radii: From Comprehensive Structural Analysis to Knowledge-Based Classification of Interatomic Contacts. ChemPhysChem, 2020, 21, 359-359.	1.0	4
5763	Intermolecular Interactions between Halogen-Substituted <i>p</i> -Benzoquinones and Halide Anions: Anion-Complexes versus Halogen Bonding. ChemPlusChem, 2020, 85, 441-449.	1.3	8
5764	Periodic trends and complexation chemistry of tetravalent actinide ions with a potential actinide decorporation agent 5-LiO(Me ₃ ,2-HOPO): A relativistic density functional theory exploration. Journal of Computational Chemistry, 2020, 41, 1427-1435.	1.5	13
5765	The oxidation of cyclo-olefin by the S=O ₂ ground-state complex [FeIV(O)(TQA)(NCMe)] ²⁺ . Journal of Biological Inorganic Chemistry, 2020, 25, 371-382.	1.1	2
5766	The study of bicyclic amidine-based ionic liquids as promising carbon dioxide capture agents. Journal of Molecular Liquids, 2020, 304, 112805.	2.3	22
5767	Reaction of chloroauric acid with histidine in microdroplets yields a catalytic Au ⁺ (His) ₂ complex. Chemical Science, 2020, 11, 2558-2565.	3.7	25
5768	Azaphenanthrene derivatives as inhibitor of SARS CoV-2 Mpro: Synthesis, physicochemical, quantum chemical and molecular docking analysis. Chemical Data Collections, 2020, 28, 100470.	1.1	2
5769	Graphene-BN-organic nanoflake complexes: DFT, IGM and SAPTO insights. Diamond and Related Materials, 2020, 107, 107905.	1.8	19
5770	The effects of amino acid sequence and solvent polarity on the self-assembling of cyclic peptide nanotubes and molecular channel formation inside the lipid bilayer. Journal of Molecular Liquids, 2020, 314, 113660.	2.3	10

#	ARTICLE	IF	CITATIONS
5771	Expanding the hole delocalization range in excited molecules for stable organic light-emitting diodes employing thermally activated delayed fluorescence. <i>Journal of Materials Chemistry C</i> , 2020, 8, 10021-10030.	2.7	14
5772	A LSER-based model to predict the solubilizing effect of drugs by inclusion with cucurbit[7]uril. <i>RSC Advances</i> , 2020, 10, 24542-24548.	1.7	2
5773	Synthesis, crystal structure, antiproliferative activity, DNA binding and density functional theory calculations of 3-(pyridin-2-yl)-8-tert-butylcoumarin and its copper(II) complex. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5875.	1.7	5
5774	Modified Lennard-Jones potentials for nanoscale atoms. <i>Journal of Computational Chemistry</i> , 2020, 41, 1985-2000.	1.5	5
5775	Spectroscopy driven DFT computation for a structure of the monomeric Cu ²⁺ -Curcumin complex and thermodynamics driven evaluation of its binding to DNA: Pseudo-binding of Curcumin to DNA. <i>Journal of Molecular Structure</i> , 2020, 1221, 128732.	1.8	6
5776	Structural, spectroscopic and computational investigations on (4,6-dimethyl-benzofuran-3-yl)-acetic acid hydrazide. <i>Journal of Molecular Structure</i> , 2020, 1220, 128748.	1.8	17
5777	Computational Insight into 1,2-Diamine, -Diether, and -Amino Ether Chiral Ligand-Mediated Carbolithiation: A Case of Enantioinduction Reversal. <i>Journal of Organic Chemistry</i> , 2020, 85, 8933-8943.	1.7	4
5778	π-Aromaticity-Induced Stabilization of Heterometallic Supertetrahedral Clusters [Zn ₆ Ge ₁₆] ⁴⁺ and [Cd ₆ Ge ₁₆] ⁴⁺ . <i>Angewandte Chemie - International Edition</i> , 2020, 59, 17286-17290.	7.2	31
5779	N-Heterocyclic Carbene Organocatalysis: With or Without Carbenes?. <i>Chemistry - A European Journal</i> , 2020, 26, 10140-10151.	1.7	17
5780	Electronic structure and second-order nonlinear optical properties of linear [3]spirobifluorenylene compounds. <i>New Journal of Chemistry</i> , 2020, 44, 10484-10491.	1.4	5
5781	Designing Hole Transport Materials with High Hole Mobility and Outstanding Interface Properties for Perovskite Solar Cells. <i>ChemPhysChem</i> , 2020, 21, 1866-1872.	1.0	3
5782	Thiourea-based polyimide/RGO composite cathode: A comprehensive study of storage mechanism with alkali metal ions. <i>Science China Materials</i> , 2020, 63, 1929-1938.	3.5	13
5783	Mn-Doped black phosphorene for ultrasensitive hydrogen sulfide detection: periodic DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15549-15558.	1.3	26
5784	In-plane polarization induced by the hydrogen bonding and π-π stacking of functionalized PDI supramolecules for the efficient photocatalytic degradation of organic pollutants. <i>Materials Chemistry Frontiers</i> , 2020, 4, 2673-2687.	3.2	24
5785	Forcing dimethylacridine crooking to improve the efficiency of orange-red thermally activated delayed fluorescent emitters. <i>Journal of Materials Chemistry C</i> , 2020, 8, 10416-10421.	2.7	4
5786	Fluoroacetate dehalogenase catalyzed dehalogenation of halogenated carboxylic acids: A QM/MM approach. <i>Chemosphere</i> , 2020, 254, 126803.	4.2	9
5787	Charge Recombination in Polaron Pairs: A Key Factor for Operational Stability of Blue-Phosphorescent Light-Emitting Devices. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000028.	1.3	6
5788	Rational Control of Charge Transfer Excitons Toward High-Contrast Reversible Mechanoresponsive Luminescent Switching. <i>Angewandte Chemie</i> , 2020, 132, 17733-17739.	1.6	17

#	ARTICLE	IF	CITATIONS
5789	Effects of heterocyclic ring and amino-ethyl-amino group on the electronic and photophysical properties of a triphenylamine-pyrimidine dye. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26355.	1.0	6
5790	Hydration and swelling: a theoretical investigation on the cooperativity effect of H-bonding interactions between p-hydroxy hydroxymethyl calix[4]/[5]arene and H ₂ O by many-body interaction and density functional reactivity theory. <i>Journal of Molecular Modeling</i> , 2020, 26, 190.	0.8	2
5791	Platinum(II), palladium(II) and gold(I) benzimidazolin-2-ylidene as potential probes for determination of N-heterocyclic carbene donor strengths and steric bulks by DFT calculations. <i>Journal of Chemical Sciences</i> , 2020, 132, 1.	0.7	3
5792	Synthesis of O-doped coal-based carbon electrode materials by ultrasound-assisted bimetallic activation for application in supercapacitors. <i>Applied Surface Science</i> , 2020, 529, 147074.	3.1	36
5793	Insight into the degradation of ammonium dibutyl dithiophosphate by natural pyrrhotite-activated peroxydisulfate: Activation mechanisms, DFT studies. <i>Chemical Engineering Journal</i> , 2020, 401, 126105.	6.6	20
5794	Probing the structural and electronic properties of anionic europium-doped silicon clusters by density functional theory and comparison of experimental photoelectron spectroscopy. <i>Chemical Physics</i> , 2020, 538, 110918.	0.9	10
5795	Adsorptive removal of diclofenac sodium from aqueous solution by magnetic COF: Role of hydroxyl group on COF. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 603, 125238.	2.3	53
5796	Ca ²⁺ mediated mechanism of octa-brominated dioxin/furan formation via BDE-209 thermolysis: Introducing the Mayer bond order difference. <i>Journal of Hazardous Materials</i> , 2020, 400, 123229.	6.5	12
5797	Gold decorated B12N12 nanocluster as an effective sulfasalazine drug carrier: A theoretical investigation. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 124, 114296.	1.3	37
5798	One step synthesis of red-emitting fluorescence turn-on probe for nitroreductase and its application to bacterial detection and oral cancer cell imaging. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 241, 118637.	2.0	17
5799	Single-atom silver induced amorphization of hollow tubular g-C ₃ N ₄ for enhanced visible light-driven photocatalytic degradation of naproxen. <i>Science of the Total Environment</i> , 2020, 742, 140642.	3.9	34
5800	Origins of Salt Formation and Cocrystallization: A Combined Experimental and Theoretical Study. <i>Crystal Growth and Design</i> , 2020, 20, 5834-5842.	1.4	18
5801	Adaptive π Aromaticity and Triplet Ground State in Tetraatomic Boron Species. <i>Organometallics</i> , 2020, 39, 2602-2608.	1.1	16
5802	Tailoring of the core structure towards promising small molecule hole-transporting materials for perovskite solar cells: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16359-16367.	1.3	15
5803	Density functional study of the optoelectronic and photovoltaic properties of cyclopentadithiophene-benzothiadiazole donor-acceptor copolymer: Effect of structural modification. <i>AIP Conference Proceedings</i> , 2020, , .	0.3	0
5804	Synthesis, characterization and SAR studies of bis(imino)pyridines as antioxidants, acetylcholinesterase inhibitors and antimicrobial agents. <i>Bioorganic Chemistry</i> , 2020, 102, 104073.	2.0	19
5805	The second-order NLO property of a photoswitchable heteroditopic ion-pair receptor based on 2-pyridyl acylhydrazone linking with 2,6-pyridine bisamide: The impacts of metal cations and anions. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107652.	1.3	2
5806	Why could the CrO _x /SiO ₂ and VO _x /SiO ₂ catalysts show so different behaviors in ethylene polymerization? A theoretical approach. <i>Molecular Catalysis</i> , 2020, 493, 111090.	1.0	4

#	ARTICLE	IF	CITATIONS
5807	The obvious advantage of amino-functionalized metal-organic frameworks: As a persulfate activator for bisphenol F degradation. <i>Science of the Total Environment</i> , 2020, 741, 140464.	3.9	43
5808	Regulating the NLO response of anthraquinone-supported thiourea-linked crown ether macrocycle by introducing metal cations: A DFT study. <i>Journal of Theoretical and Computational Chemistry</i> , 2020, 19, 2050017.	1.8	2
5809	Designing a novel material with considerable nonlinear optical responses based on the bicorannulenyl molecule. <i>Journal of Molecular Modeling</i> , 2020, 26, 201.	0.8	4
5810	Study of Electronic and Vibrational Structures of Reduced, Neutral, and Oxidized Ni ₃ (dpa) ₄ X ₂ Using Density Functional Theory and Raman Spectroscopy. <i>ACS Omega</i> , 2020, 5, 15620-15630.	1.6	5
5811	Efficient Deep Blue Platinum Acetylide Phosphors with Acyclic Diaminocarbene Ligands. <i>Chemistry - A European Journal</i> , 2020, 26, 16028-16035.	1.7	20
5812	Spectroscopic elucidation (FT-IR, FT-Raman and UV-visible) with NBO, NLO, ELF, LOL, drug likeness and molecular docking analysis on 1-(2-ethylsulfonyl-ethyl)-2-methyl-5-nitro-imidazole: An antiprotozoal agent. <i>Computational Biology and Chemistry</i> , 2020, 88, 107330.	1.1	77
5813	Water dissociation and H migration on metal decorated B40: A density functional theory (DFT) study. <i>Journal of Molecular Liquids</i> , 2020, 315, 113759.	2.3	8
5814	Fe-decorated all-boron B40 fullerene serving as a potential promising active catalyst for CO oxidation: A DFT mechanistic approach. <i>Polyhedron</i> , 2020, 188, 114699.	1.0	16
5815	The role of chlorine oxide radical (ClO•) in the degradation of polychloro-1,3-butadienes in UV/chlorine treatment: kinetics and mechanisms. <i>Water Research</i> , 2020, 183, 116056.	5.3	25
5816	Reactivity of Cobalt Clusters Co _n ^{±0} with Ammonia: Co ₃ ⁺ Cluster Catalysis for NH ₃ Dehydrogenation. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5879-5886.	1.1	13
5817	Perspective on theoretical methods and modeling relating to electro-catalysis processes. <i>Chemical Communications</i> , 2020, 56, 9937-9949.	2.2	52
5818	Computational Insights on the Mechanism of the Chemiluminescence Reaction of New Group of Chemiluminogens 10-Methyl-9-thiophenoxycarbonylacridinium Cations. <i>International Journal of Molecular Sciences</i> , 2020, 21, 4417.	1.8	3
5819	Self-Assembled Biomimetic Capsules for Self-Preservation. <i>Small</i> , 2020, 16, e2000930.	5.2	9
5820	Characterization of charge transfer excited states in [2Fe ²⁺ S] iron-sulfur clusters using conventional configuration interaction techniques. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	10
5821	Unravelling the regio- and stereoselective synthesis of bicyclic N,O-nucleoside analogues within the molecular electron density theory perspective. <i>Structural Chemistry</i> , 2020, 31, 2147-2160.	1.0	13
5822	Theoretical Characterization of Catalytically Active Species in Reductive Hydroxymethylation of Styrene with CO ₂ over a Bisphosphine-Ligated Copper Complex. <i>Inorganic Chemistry</i> , 2020, 59, 9667-9682.	1.9	8
5823	Influence of Different Molecular Design Strategies on Photovoltaic Properties of a Series of Triphenylamine-Based Organic Dyes for Dye-Sensitized Solar Cells: Insights from Theoretical Investigations. <i>Journal of Physical Chemistry C</i> , 2020, 124, 15036-15044.	1.5	17
5824	Nature of fluorine interactions in wheel and axle topology based hexa-coordinated Sn(IV)-porphyrins: an experimental and theoretical analysis. <i>CrystEngComm</i> , 2020, 22, 5049-5059.	1.3	2

#	ARTICLE	IF	CITATIONS
5825	Cooperativity effects between regium-bonding and pnictogen-bonding interactions in ternary MFA·Â·PH ₃ O·Â·MF (M = Cu, Ag, Au): an ab initio study. <i>Molecular Physics</i> , 2020, 118, .	0.8	7
5826	Influence of Tethered Ions on Electric Polarization and Electrorheological Property of Polymerized Ionic Liquids. <i>Molecules</i> , 2020, 25, 2896.	1.7	13
5827	Detection of hydrolyzed plutonium chloride compounds generated by moisture intrusion of pyroprocessing hot cell using density functional theory. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2020, 325, 101-110.	0.7	2
5828	Direct oxidation of methane to methanol on Co embedded N-doped graphene: Comparing the role of N ₂ O and O ₂ as oxidants. <i>Applied Catalysis A: General</i> , 2020, 602, 117716.	2.2	11
5829	Investigation of excited state proton transfer mechanism for 2-(benzo[d]thiazol-2-yl)naphthalene-1,3-diol in different solvents. <i>Chemical Physics</i> , 2020, 538, 110914.	0.9	6
5830	Density functional theory study of non-metal catalysts with different CN ratios for acetylene hydrochlorination. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 603, 125230.	2.3	2
5831	Highly Efficient, Reversible, and Selective Absorption of SO ₂ in 1-Ethyl-3-methylimidazolium Chloride Plus Imidazole Deep Eutectic Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 13696-13705.	1.8	51
5832	Force Fields for Macromolecular Assemblies Containing Diketopyrrolopyrrole and Thiophene. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5150-5162.	2.3	9
5833	Efficient and Environmentally Friendly Adsorbent Based on Î²-Ketoenol-Pyrazole-Thiophene for Heavy-Metal Ion Removal from Aquatic Medium: A Combined Experimental and Theoretical Study. <i>ACS Omega</i> , 2020, 5, 17324-17336.	1.6	17
5834	Impact of alkyl chain length and water on the structure and properties of 1-alkyl-3-methylimidazolium chloride ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 17687-17704.	1.3	38
5835	Determinants for proton location and electron coupled proton transfer in hydrogen bonded pentafluorophenol anion clusters. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16712-16720.	1.3	0
5836	The ditetrel bond: noncovalent bond between neutral tetrel atoms. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16606-16614.	1.3	29
5837	N-Borylated Hydroxylamines [B ₁₂ H ₁₁ NH ₂ OH] as a Novel Type of Substituted Derivative of the closo-Dodecaborate Anion. <i>Russian Journal of Inorganic Chemistry</i> , 2020, 65, 795-799.	0.3	15
5838	Gaining Insight into the Effect of Organic Interface Layer on Suppressing Ion Migration Induced Interfacial Degradation in Perovskite Solar Cells. <i>Advanced Functional Materials</i> , 2020, 30, 2000837.	7.8	29
5839	Fe-quaterpyridine complex: a comprehensive DFT study on the mechanism of CO ₂ -to-CO conversion. <i>Journal of Materials Science</i> , 2020, 55, 14301-14314.	1.7	3
5840	Density functional studies of hydrogen passivated nanoclusters of carbon, silicon, germanium and their respective ionic analogues. <i>Chemical Physics Letters</i> , 2020, 755, 137759.	1.2	0
5841	Optimizing small conjugated molecules for solar-cell applications using an inverse-design method. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107654.	1.3	2
5842	The molecular structure, spectroscopic features and electronic properties of tioxolone under the external electric field. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 231, 118108.	2.0	25

#	ARTICLE	IF	CITATIONS
5843	Degradation of levofloxacin in aqueous solution by non-thermal plasma combined with Ag ₃ PO ₄ /activated carbon fibers: Mechanism and degradation pathways. Separation and Purification Technology, 2020, 250, 117264.	3.9	42
5844	π-Aromaticity-Induced Stabilization of Heterometallic Supertetrahedral Clusters [Zn ₆ Ge ₁₆] ⁴⁺ and [Cd ₆ Ge ₁₆] ⁴⁺ . Angewandte Chemie, 2020, 132, 17439-17443.	1.6	9
5845	Rational Control of Charge Transfer Excitons Toward High-Contrast Reversible Mechanoresponsive Luminescent Switching. Angewandte Chemie - International Edition, 2020, 59, 17580-17586.	7.2	83
5846	Insights into the adsorption of Pb(II) over trimercapto-s-triazine trisodium salt-modified lignin in a wide pH range. Chemical Engineering Journal Advances, 2020, 1, 100002.	2.4	8
5847	Structure and interaction properties of MBIL [Bmim][FeCl ₄] and methanol: A combined FTIR and simulation study. Journal of Molecular Liquids, 2020, 309, 113061.	2.3	26
5848	Nickel-catalyzed hydroalkenylation of styrene with phenylpropanal: theoretical studies on the mechanism, regioselectivity, and role of phenylboronic acid. Organic Chemistry Frontiers, 2020, 7, 2207-2215.	2.3	5
5849	Efficient blue electroluminescence with an external quantum efficiency of 9.20% and CIE _y ≤ 0.08 without excimer emission. RSC Advances, 2020, 10, 25059-25072.	1.7	5
5850	Integrated solvent-process design methodology based on COSMO-SAC and quantum mechanics for TMQ (2,2,4-trimethyl-1,2-H-dihydroquinoline) production. Chemical Engineering Science, 2020, 226, 115894.	1.9	14
5851	Weak hydrogen bonds between alkyl halides and amides: The microwave spectroscopic and theoretical study of the difluoromethane-formamide complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 241, 118681.	2.0	5
5852	Catalytic Mechanism of K and Ca on the Volatile-Biochar Interaction for Rapid Pyrolysis of Biomass: Experimental and Simulation Studies. Energy & Fuels, 2020, 34, 9741-9753.	2.5	34
5853	(2-Pyridyloxy)arsines as ligands in transition metal chemistry: a stepwise As(III) → As(II) → As(I) reduction. Dalton Transactions, 2020, 49, 10042-10051.	1.6	3
5854	Analytic intermolecular potential energy surface and first-principles prediction of the rotational profiles for a symmetric top ion-atom complex: A case study of H ₃ O ⁺ Ar. Journal of Chemical Physics, 2020, 152, 214302.	1.2	2
5855	Homogeneous photocatalytic degradation of sulfamethazine induced by Fe(III)-carboxylate complexes: Kinetics, mechanism and products. Chemical Engineering Journal, 2020, 402, 126122.	6.6	35
5856	Unveiling the relationship between the phosphorescent quantum yield and structural modification to construct high-performance Pt(II) complex. Inorganica Chimica Acta, 2020, 512, 119861.	1.2	2
5857	A new alendronate doped HAP nanomaterial for Pb ²⁺ , Cu ²⁺ and Cd ²⁺ effect absorption. Journal of Hazardous Materials, 2020, 400, 123143.	6.5	65
5858	Morphology of alumina in NaF-AlF ₃ systems determined by Raman spectroscopy and quantum mechanical calculations. Journal of Molecular Liquids, 2020, 315, 113747.	2.3	8
5859	Theoretical Investigations of Lu ₂ C ₈₄ : Unexpected Impact of Metal Electronic Configuration toward the Metal-Metal π -Bond in Fullerene. Inorganic Chemistry, 2020, 59, 10113-10122.	1.9	8
5860	Unveiling the Role of Hydrogen Bonding and g-Tensor in the Interaction of Ru-Bis-DMSO with Amino Acid Residue and Human Serum Albumin. Journal of Physical Chemistry B, 2020, 124, 6459-6474.	1.2	2

#	ARTICLE	IF	CITATIONS
5861	Metal-Organic Framework Based on β -Cyclodextrin Gives High Ethylene Gas Adsorption Capacity and Storage Stability. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 34095-34104.	4.0	75
5862	Phosphine ligand-coated Cu nanoparticle-catalyzed selective semihydrogenation of alkynes: electronic or hindrance effects of the ligand?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16905-16913.	1.3	0
5863	N-t-Butyl- β -aryl Nitrones as Potent Spin Traps: DFT Analysis of Electron Localization Function Topology, Local Selectivity, Reactivity and Solvent Effects. <i>Asian Journal of Chemistry</i> , 2020, 32, 1191-1196.	0.1	1
5864	Boosting the Quantum Efficiency of Ultralong Organic Phosphorescence up to 52% via Intramolecular Halogen Bonding. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 17451-17455.	7.2	253
5865	The (Dioximate)Ni ^{II} System: Ligand Oxidation and Binding Modes of Triiodide Species. <i>Inorganic Chemistry</i> , 2020, 59, 2316-2327.	1.9	13
5866	Photoinduced Charge Transfer in Donor-Bridge-Acceptor in One- and Two-photon Absorption: Sequential and Superexchange Mechanisms. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4968-4981.	1.5	39
5867	Switching of Self-Assembly to Solvent-Assisted Assembly of Molecular Motor: Unveiling the Mechanisms of Dynamic Control on Solvent Exchange. <i>Langmuir</i> , 2020, 36, 1773-1792.	1.6	10
5868	LiB13: A New Member of Tetrahedral-Typed B13 Ligand Half-Surround Cluster. <i>Scientific Reports</i> , 2020, 10, 1642.	1.6	14
5869	Is the origin of green fluorescence in unsymmetrical four-ring bent-core liquid crystals single or double proton transfer?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4731-4740.	1.3	11
5870	Color tuning of an active pharmaceutical ingredient through cocrystallization: a case study of a metronidazole-pyrogallol cocrystal. <i>CrystEngComm</i> , 2020, 22, 1404-1413.	1.3	19
5871	Potential molecular semiconductor devices: cyclo-C _n (<i>n</i> = 10 and 14) with higher stabilities and aromaticities than acknowledged cyclo-C ₁₈ . <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4823-4831.	1.3	31
5872	Hydrogen storage capability of cage-like Li ₃ B ₁₂ clusters. <i>Journal of Applied Physics</i> , 2020, 127, .	1.1	9
5873	Shellmycin A-D, Novel Bioactive Tetrahydroanthra- β -Pyrone Antibiotics from Marine <i>Streptomyces</i> sp. Shell-016. <i>Marine Drugs</i> , 2020, 18, 58.	2.2	13
5874	A High-Power Aqueous Zinc-Organic Radical Battery with Tunable Operating Voltage Triggered by Selected Anions. <i>ChemSusChem</i> , 2020, 13, 2239-2244.	3.6	59
5875	Switching between H ₄ ckel and M ₄ bius aromaticity: a density functional theory and information-theoretic approach study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4715-4730.	1.3	25
5876	A molecular electron density theory study of the Grignard reagent-mediated regioselective direct synthesis of 1,5-disubstituted-1,2,3-triazoles. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4062.	0.9	20
5877	High first-order hyperpolarizabilities of thiobarbituric acid derivative-based donor-acceptor nonlinear optical-phores: Multiple theoretical investigations of substituents and conjugated bridges effect. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26176.	1.0	7
5878	Comparative cation sensing properties of a newly designed urea linked ferrocene-benzimidazole dyad: a DFT study. <i>Journal of Molecular Modeling</i> , 2020, 26, 50.	0.8	3

#	ARTICLE	IF	CITATIONS
5879	Stabilizing Pd on magnetic phosphine-functionalized cellulose: DFT study and catalytic performance under deep eutectic solvent assisted conditions. <i>Carbohydrate Polymers</i> , 2020, 235, 115947.	5.1	23
5880	The effect of sodium chloride concentration on the mutarotation and structure of d-xylose in water: Experimental and theoretical investigation. <i>Carbohydrate Research</i> , 2020, 489, 107941.	1.1	5
5881	Thermodynamic behavior of [OMIM]-based ionic liquid and H ₂ O systems: Experimental, model prediction and mechanism insights. <i>Journal of Molecular Liquids</i> , 2020, 301, 112493.	2.3	5
5882	Physical mechanism of the photoinduced charge transfer in multibranched compounds during one- and two-photon absorption. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 231, 118144.	2.0	3
5883	Soft interactions with hard Lewis acids: generation of mono- and dicationic alkaline-earth metal arene-complexes by direct oxidation. <i>Chemical Science</i> , 2020, 11, 2068-2076.	3.7	29
5884	H-Bonding on spin centres enhances spin-spin coupling for organic diradicals. <i>Journal of Materials Chemistry C</i> , 2020, 8, 3402-3408.	2.7	8
5885	High triplet energy materials for efficient exciplex-based and full-TADF-based white OLEDs. <i>Dyes and Pigments</i> , 2020, 177, 108259.	2.0	5
5886	Structural analysis of intramolecular 1,5-type O ⁻ O and S ⁻ O interactions in diethyl 2-oxo and diethyl 2-thioxo-1H benzo[d]imidazole-1,3(2H)-dicarboxylate: Experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2020, 1209, 127929.	1.8	2
5887	Theoretical study on the intermolecular interactions between energetic oxidizer and pyrazine - 1, 4 - dioxide. <i>Materials Today Communications</i> , 2020, 24, 101020.	0.9	5
5888	A water-soluble fluorescence sensor with high specificity for detecting hydrazine in river water detection and A549 cell imaging. <i>Sensors and Actuators B: Chemical</i> , 2020, 311, 127914.	4.0	34
5889	A quasi-plane IrB ₁₈ cluster with high stability. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5942-5948.	1.3	11
5890	On the existence of a local dipolar plasmon mode in doped small gold atomic arrays. <i>Physical Review B</i> , 2020, 101, .	1.1	2
5891	Zinc-Doped Boron Phosphide Nanocluster as Efficient Sensor for SO ₂ . <i>Journal of Chemistry</i> , 2020, 2020, 1-12.	0.9	45
5892	Regium Bonds between Silver(I) Pyrazolates Dinuclear Complexes and Lewis Bases (N ₂ , OH ₂ , NCH, SH ₂), Tj ETQq1 1.0.784314 rgBT /Dv	1.0	17
5893	How Different Substitution Positions of F, Cl Atoms in Benzene Ring of 5-Methylpyrimidine Pyridine Derivatives Affect the Inhibition Ability of EGFR L858R/T790M/C797S Inhibitors: A Molecular Dynamics Simulation Study. <i>Molecules</i> , 2020, 25, 895.	1.7	9
5894	Boron-Based Chiral Helix Be ₆ B ₁₀ ²⁺ and Be ₆ B ₁₁ ⁺ Clusters: Structures, Chemical Bonding, and Formation Mechanism. <i>Chemistry - an Asian Journal</i> , 2020, 15, 1094-1104.	1.7	14
5895	Mechanism study of TADF and phosphorescence in dinuclear copper (I) molecular crystal using QM/MM combined with an optimally tuned range-separated hybrid functional. <i>Organic Electronics</i> , 2020, 81, 105667.	1.4	13
5896	Extension of π -conjugation and enhancement of electron-withdrawing ability at terminal indenedione for A-D-A small molecules for application in organic solar cells. <i>Organic Electronics</i> , 2020, 81, 105679.	1.4	10

#	ARTICLE	IF	CITATIONS
5897	How Many Pnictogen Bonds can be Formed to a Central Atom Simultaneously?. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2046-2056.	1.1	29
5898	Iodization Threshold in Size-Dependent Reactions of Lead Clusters Pb _n ⁺ with Iodomethane. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2505-2512.	1.1	5
5899	Effect of SDBS solution on the surface potential properties of the Zhaozhuang coal. <i>Surface and Interface Analysis</i> , 2020, 52, 442-453.	0.8	3
5900	Theoretical study on novel superalkali doped graphdiyne complexes: Unique approach for the enhancement of electronic and nonlinear optical response. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107573.	1.3	68
5901	DFT study on the "Silver effect" in gold-catalyzed hydroamination of terminal alkynyl sulfamides. <i>Molecular Catalysis</i> , 2020, 486, 110847.	1.0	2
5902	Hydrogen bond capability tunable different "relay-race" mechanisms of the excited-state proton transfer process for 4-methoxy-3-hydroxyflavone. <i>Organic Electronics</i> , 2020, 81, 105678.	1.4	7
5903	Theoretical Evaluation of the Molecular Inclusion Process between Chlordecone and Cyclodextrins: A New Method for Mitigating the Basis Set Superposition Error in the Case of an Implicit Solvation Model. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2115-2125.	2.5	12
5904	Novel inorganic aromatic mixed-valent superalkali electride CaN ₃ Ca: an alkaline-earth-based high-sensitivity multi-state nonlinear optical molecular switch. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5985-5994.	1.3	5
5905	Energetic azide-based coordination polymers: Sensitivity tuning through diverse structural motifs. <i>Chemical Engineering Journal</i> , 2020, 390, 124587.	6.6	36
5906	Metalloids as halogen bond acceptors: A combined crystallographic data and theoretical investigation. <i>Chemical Physics Letters</i> , 2020, 745, 137270.	1.2	7
5907	Effects of pH and electrolytes on the sheet-to-sheet aggregation mode of graphene oxide in aqueous solutions. <i>Environmental Science: Nano</i> , 2020, 7, 984-995.	2.2	13
5908	An intramolecular 1,5-chalcogen bond on the conformational preference of carbonyl thiocarbamate species. <i>New Journal of Chemistry</i> , 2020, 44, 5243-5253.	1.4	9
5909	Fusion of thienyl into the backbone of electron acceptor in organic photovoltaic heterojunctions: a comparative study of BTPT-4F and BTPPT-4F. <i>New Journal of Chemistry</i> , 2020, 44, 5224-5234.	1.4	12
5910	Type I photosensitizers based on phosphindole oxide for photodynamic therapy: apoptosis and autophagy induced by endoplasmic reticulum stress. <i>Chemical Science</i> , 2020, 11, 3405-3417.	3.7	182
5911	Substituent steric effect boosting phosphorescence efficiency of PtCu ₂ complexes. <i>Journal of Materials Chemistry C</i> , 2020, 8, 5174-5182.	2.7	8
5912	Comparison of the oxidation of halogenated phenols in UV/PDS and UV/H ₂ O ₂ advanced oxidation processes. <i>RSC Advances</i> , 2020, 10, 6464-6472.	1.7	7
5913	Chiral phosphoric acid catalyzed asymmetric arylation of indoles via nucleophilic aromatic substitution: mechanisms and origin of enantioselectivity. <i>Catalysis Science and Technology</i> , 2020, 10, 2277-2292.	2.1	9
5914	Efficient fluorescent OLEDs based on assistant acceptor modulated HLCT emissive state for enhancing singlet exciton utilization. <i>RSC Advances</i> , 2020, 10, 8866-8879.	1.7	25

#	ARTICLE	IF	CITATIONS
5915	Geometric and electronic structures of AlnCum (n=5, m=3) clusters: genetic algorithm combined with ab initio models. <i>Molecular Physics</i> , 2020, 118, e1726518.	0.8	0
5916	Structural Insights into the Dual-Phase Emission Mechanism of Naphthalene Derivatives with Scanning Tunneling Microscopy, X-ray Diffraction, and Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2020, 124, 5715-5722.	1.5	4
5917	Bond relaxation and electronic properties of two-dimensional Sb/MoSe2 and Sb/MoTe2 van der Waals heterostructures. <i>AIP Advances</i> , 2020, 10, .	0.6	8
5918	A Stable All-Thiophene-Based Core-Modified [38]Octaphyrin Diradicaloid: Conformation and Aromaticity Switch at Different Oxidation States. <i>Angewandte Chemie</i> , 2020, 132, 7484-7488.	1.6	6
5919	Probing the bent bonds in cyclopropane systems for gas storage and separation process: A computational study. <i>Journal of Computational Chemistry</i> , 2020, 41, 1271-1284.	1.5	4
5920	Guest-host complexes of 1-iodochlordecone and 1-iodo-pentachlorocyclohexane with cyclodextrins as radiotracers of organochlorine pesticides in polluted water. <i>Environmental Science and Pollution Research</i> , 2020, 27, 41105-41116.	2.7	7
5921	Critical comparison of R ^X -Y and R ^H -Y directionality in halogen and hydrogen bonds using modern computational chemistry methods. <i>Chemical Physics Letters</i> , 2020, 744, 137221.	1.2	10
5922	Understanding the effects of co-exposed facets on photocatalytic activities and fuel desulfurization performance in BiOCl singlet-crystalline sheets. <i>Journal of Hazardous Materials</i> , 2020, 391, 122198.	6.5	27
5923	Rapid degradation of tetracycline hydrochloride by heterogeneous photocatalysis coupling persulfate oxidation with MIL-53(Fe) under visible light irradiation. <i>Journal of Hazardous Materials</i> , 2020, 392, 122315.	6.5	150
5924	Carbohydrate-Binding Capability and Functional Conformational Changes of AbnE, an Arabino-oligosaccharide Binding Protein. <i>Journal of Molecular Biology</i> , 2020, 432, 2099-2120.	2.0	5
5925	Effect of 3d heterometallic ions on the magnetic properties of azido-Cu(II) with isonicotinic acid coligands: A theoretical perspective. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107562.	1.3	11
5926	Synthesis, experimental and computational characterizations of a new quinoline derived Schiff base and its Mn(II), Ni(II) and Cu(II) complexes. <i>Journal of Molecular Structure</i> , 2020, 1208, 127898.	1.8	25
5927	Fate of Dipole-Bound Anion States when Hydrated. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2064-2076.	1.1	14
5928	Theoretical Study on Deep Eutectic Solvents as Vehicles for the Delivery of Anesthetics. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1794-1805.	1.2	17
5929	Substantial Improvement of the Dielectric Strength of Cellulose-Liquid Composites: Effects of Traps at the Nanoscale Interface. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1881-1889.	2.1	32
5930	Microhydration of verbenone: how the chain of water molecules adapts its structure to the host molecule. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5855-5864.	1.3	11
5931	Cooperative effect of hetero-nuclear MnNi ⁺ cation enhancing C-H bond activation of cyclohexane: a theoretical study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	0
5932	A mechanistic insight into rhodium-doped gold clusters as a better hydrogenation catalyst. <i>Nanoscale</i> , 2020, 12, 5125-5138.	2.8	6

#	ARTICLE	IF	CITATIONS
5933	Absorptive Desulfurization of Model Biogas Stream Using Choline Chloride-Based Deep Eutectic Solvents. <i>Sustainability</i> , 2020, 12, 1619.	1.6	20
5934	A Raman study on the intracluster interactions of aminothiophenol-protected Ag 7 clusters-Photo-assisted Na ⁺ coupling reaction of the ligand. <i>Journal of Raman Spectroscopy</i> , 2020, 51, 764-773.	1.2	0
5935	Modeling Sensitivities of Energetic Materials using the Python Language and Libraries. <i>Propellants, Explosives, Pyrotechnics</i> , 2020, 45, 966-973.	1.0	12
5936	A diazabenzoperylene derivative as ratiometric fluorescent probe for cysteine with super large Stokes shift. <i>Analytical and Bioanalytical Chemistry</i> , 2020, 412, 2687-2696.	1.9	14
5937	The effect of edge termination on Li ⁺ ion adsorption of pristine and defected graphene sheets. <i>Journal of Materials Science</i> , 2020, 55, 5920-5937.	1.7	5
5938	Theoretical study on the effect of spacer groups on the nonlinear optical properties of polyvinyl carbazole molecular fragments. <i>Structural Chemistry</i> , 2020, 31, 1471-1479.	1.0	1
5940	Wavefunction analysis, charge transfer and molecular docking studies on famciclovir and entecavir: Potential anti-viral drugs. <i>Chemical Data Collections</i> , 2020, 26, 100353.	1.1	6
5941	Ultrathin Ag ₂ WO ₄ -coated P-doped g-C ₃ N ₄ nanosheets with remarkable photocatalytic performance for indomethacin degradation. <i>Journal of Hazardous Materials</i> , 2020, 392, 122355.	6.5	62
5942	Cyclic versus straight chain oligofuran as sensor: A detailed DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107569.	1.3	66
5943	Conductivity tuning of charged triazine and heptazine graphitic carbon nitride (g-C ₃ N ₄) quantum dots via nonmetal (B, O, S, P) doping: DFT calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 141, 109422.	1.9	46
5944	Gold(III) separation from acidic medium by amine-based ionic liquid. <i>Journal of Molecular Liquids</i> , 2020, 304, 112735.	2.3	24
5945	Spectroscopy characterization, theoretical study and antioxidant activities of the flavonoids-Pb(II) complexes. <i>Journal of Molecular Structure</i> , 2020, 1209, 127919.	1.8	22
5946	Vibrational and Hirshfeld surface analyses, quantum chemical calculations, and molecular docking studies of coumarin derivative 3-(1-m-toluidinoethylidene)-chromane-2,4-dione and its corresponding palladium(II) complex. <i>Journal of Molecular Structure</i> , 2020, 1209, 127935.	1.8	49
5947	Solvation-Dependent Excited-State Dynamics of Donor-Acceptor Molecules with Hybridized Local and Charge Transfer Character. <i>Journal of Physical Chemistry C</i> , 2020, 124, 5574-5582.	1.5	33
5948	Vanadyl Species Catalyzed 1,2-Oxidative Trifluoromethylation of Unactivated Olefins. <i>ACS Catalysis</i> , 2020, 10, 3676-3683.	5.5	21
5949	High- χ alternating copolymers for accessing sub-5 nm domains via simulations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5577-5583.	1.3	12
5950	Molecular engineering of acceptors to control aggregation for optimized nonfullerene solar cells. <i>Journal of Materials Chemistry A</i> , 2020, 8, 5458-5466.	5.2	45
5951	Mechanistic Study on Ag ^I -Catalyzed Oxidative Cross-Coupling/Cyclization between Terminal Alkynes and β -Enamino Esters under Base Conditions. <i>Journal of Organic Chemistry</i> , 2020, 85, 4408-4417.	1.7	5

#	ARTICLE	IF	CITATIONS
5952	The facile synthesis of zoledronate functionalized hydroxyapatite amorphous hybrid nanobiomaterial and its excellent removal performance on Pb ²⁺ and Cu ²⁺ . Journal of Hazardous Materials, 2020, 392, 122291.	6.5	42
5953	Theoretical investigation of intermolecular hydrogen bond induces fluorescence quenching phenomenon for Coumarin-1. Journal of Luminescence, 2020, 221, 117110.	1.5	23
5954	DFT investigations of linear Zn ³⁺ -type complex with compartmental N/O-donor Schiff base: Synthesis, characterizations, crystal structure, fluorescence and molecular docking. Journal of Molecular Structure, 2020, 1209, 127936.	1.8	26
5955	Halogen- π -halogen contacts in triiodide salts of pyridinium-derived cations: Theoretical and spectroscopic studies. Journal of Molecular Structure, 2020, 1209, 127949.	1.8	5
5956	The structures, electronic properties, and chemical bonding of binary alloy boron-aluminum clusters series B ₄ Al _n O ^{+/+} (n = 1-5). Materials Today Communications, 2020, 24, 100914.	0.9	4
5957	Temperature-dependent inhibition of PEG in acid copper plating: Theoretical analysis and experiment evidence. Materials Today Communications, 2020, 24, 100973.	0.9	13
5958	Theoretical Spectroscopic Studies on Chemical and Electronic Structures of Selenocysteine and Pyrrolysine. Journal of Physical Chemistry A, 2020, 124, 2215-2224.	1.1	3
5959	Theoretical insights into selective separation of trivalent actinide and lanthanide by ester and amide ligands based on phenanthroline skeleton. Dalton Transactions, 2020, 49, 4093-4099.	1.6	33
5960	Skillfully tuning 1-hydroxy-9H-fluoren-9-one forward-backward ESIPT processes by introducing electron-withdrawing groups: A theoretical exploration. Journal of Molecular Liquids, 2020, 303, 112627.	2.3	39
5961	The synthesis, experimental and theoretical characterization of a Pd(II) complex from diacetyl monoxime isobutyrohydrazone. Journal of Molecular Structure, 2020, 1209, 127950.	1.8	7
5962	Highly Efficient Phosphorescent Tetradentate Platinum(II) Complexes Containing Fused 6/5/6 Metallochromes. Inorganic Chemistry, 2020, 59, 3718-3729.	1.9	27
5963	The Dependence of Implicit Solvent Model Parameters and Electronic Absorption Spectra and Photoinduced Charge Transfer. Scientific Reports, 2020, 10, 3713.	1.6	11
5964	Effect of graphene between photoanode and sensitizer on the intramolecular and intermolecular electron transfer process. Physical Chemistry Chemical Physics, 2020, 22, 6391-6400.	1.3	32
5965	A TDDFT study on the hydrogen-bonding effect on ESIPT mechanism for [2,2'-bipyridyl]-3,3'-diol-(H ₂ O) _n (n = 1, 2) clusters: single or double?. Molecular Physics, 2020, 118, .	0.8	3
5966	Computational modeling of the kinetics and mechanism of tellurium-based glutathione peroxidase mimic. International Journal of Quantum Chemistry, 2020, 120, e26201.	1.0	9
5967	ROS reevaluation for degradation of 4-chloro-3,5-dimethylphenol (PCMX) by UV and UV/persulfate processes in the water: Kinetics, mechanism, DFT studies and toxicity evolution. Chemical Engineering Journal, 2020, 390, 124610.	6.6	43
5968	Adenine dimer on the pure and bimetallic nanosurfaces of Au and Ag metals: Hydrogen bonding on metal nanosurfaces. Computational Materials Science, 2020, 175, 109609.	1.4	2
5969	Molecular docking, quantum chemical computational and vibrational studies on bicyclic heterocycle α -nitro-2,3-dihydro-1,4-benzodioxine. Anti-cancer agent. Computational Biology and Chemistry, 2020, 86, 107226.	1.1	12

#	ARTICLE	IF	CITATIONS
5970	The effect of CF ₃ functional group substituent on bifunctional activation model and enantioselectivity for BINOL N-triflylphosphoramides catalyzed rearrangement reaction. <i>Journal of Catalysis</i> , 2020, 383, 230-238.	3.1	9
5971	Cyclic aliphatic amines: A critical analysis of the experimental enthalpies of formation by comparison with theoretical calculations. <i>Journal of Chemical Thermodynamics</i> , 2020, 145, 106092.	1.0	7
5972	A detailed analysis of the spin-crossover reaction of H ₂ S binding to heme and the six-coordinated FeP(Im)-HS ⁺ porphyrin complex. <i>Journal of Inorganic Biochemistry</i> , 2020, 206, 111049.	1.5	1
5973	A study on the modification of azole rings to regulate the transition dipole moment, MLCT and T1 structural distortion of 2-pyridyl-azole copper (I) complexes for high phosphorescence performance. <i>Organic Electronics</i> , 2020, 81, 105664.	1.4	5
5974	Theoretical investigation on the ESIPT mechanism and fluorescent sensing mechanism of 2-(2-hydroxyphenyl) thiazole-4-carboxaldehyde in methanol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 233, 118214.	2.0	19
5975	Stabilization of Open-Shell Single Bonds within Endohedral Metallofullerene. <i>Inorganic Chemistry</i> , 2020, 59, 3606-3618.	1.9	11
5976	Accurate Estimation of pK_b Values for Amino Groups from Surface Electrostatic Potential ($V_{S,min}$) Calculations: The Isoelectric Points of Amino Acids as a Case Study. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1445-1452.	2.5	23
5977	Probing Orientation-Specific Charge-Dipole Interactions between Hexafluoroisopropanol and Halides: A Joint Photoelectron Spectroscopy and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2036-2045.	1.1	17
5978	Aromaticity-Photovoltaic Property Relationship of Triphenylamine-Based D- π -A Dyes: Leads from DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3374-3385.	1.1	23
5979	Tuning the Trapping of Epoxides by Endo-Functionalized Molecular Tubes in an Aqueous Medium: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3589-3600.	1.5	10
5980	Structural Patterns and Stabilities of Hydrogen-Bonded Pairs Involving Ribonucleotide Bases and Arginine, Glutamic Acid, or Glutamine Residues of Proteins from Quantum Mechanical Calculations. <i>ACS Omega</i> , 2020, 5, 3612-3623.	1.6	11
5981	Directing the Simultaneous Conversion of Hemicellulose and Cellulose in Raw Biomass to Lactic Acid. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 4244-4255.	3.2	47
5982	Improvement of Antioxidative Activity of Apigenin by B ₁₂ N ₁₂ Nanocluster: Antioxidative Mechanism Analysis. <i>ChemistrySelect</i> , 2020, 5, 1829-1836.	0.7	7
5983	Intramolecular hydrogen bonding stabilizes trans-configuration in a mixed carbene/isocyanide PdII complexes. <i>Journal of Organometallic Chemistry</i> , 2020, 912, 121174.	0.8	27
5984	Electronic-level insight into the weak interactions of ion pairs in acetate anion-based ionic liquids. <i>Journal of Molecular Liquids</i> , 2020, 303, 112668.	2.3	10
5985	Physical mechanism of concentration-dependent fluorescence resonance energy transfer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 231, 118143.	2.0	6
5986	New Way for Probing Bond Strength. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1850-1860.	1.1	121
5987	Solution-phase vertical growth of aligned NiCo ₂ O ₄ nanosheet arrays on Au nanosheets with weakened oxygen-hydrogen bonds for photocatalytic oxygen evolution. <i>Nanoscale</i> , 2020, 12, 6195-6203.	2.8	23

#	ARTICLE	IF	CITATIONS
5988	The hydrogen transfer reaction between the substance of triplet state thioxanthone and alkane with sp ³ hybridization hydrogen. <i>Journal of Molecular Modeling</i> , 2020, 26, 56.	0.8	4
5989	Chitosan oligosaccharide derived polar host for lithium deposition in lithium metal batteries. <i>Sustainable Materials and Technologies</i> , 2020, 24, e00158.	1.7	10
5990	Crystal Engineering and Photophysical Properties of Phenyl-Pyrenimidazole Systems. <i>Crystal Growth and Design</i> , 2020, 20, 1681-1693.	1.4	4
5991	One- and Two-Dimensional Iodine-Rich Iodobismuthate(III) Complexes: Structure, Optical Properties, and Features of Halogen Bonding in the Solid State. <i>Inorganic Chemistry</i> , 2020, 59, 3290-3296.	1.9	62
5992	Theory meets experiment for elucidating the structure and stability of non-covalent complexes: water-amine interaction as a proof of concept. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5024-5032.	1.3	14
5993	Structure of Imidazolium-N-phthalolylglycinate Salt Hydrate: Combined Experimental and Quantum Chemical Calculations Studies. <i>Crystals</i> , 2020, 10, 91.	1.0	1
5994	Synthesis of Chromium(II) Complexes with Chelating Bis(alkoxide) Ligand and Their Reactions with Organoazides and Diazoalkanes. <i>Molecules</i> , 2020, 25, 273.	1.7	6
5995	Ru(II) water oxidation catalysts with 2,3-bis(2-pyridyl)pyrazine and tris(pyrazolyl)methane ligands: assembly of photo-active and catalytically active subunits in a dinuclear structure. <i>Dalton Transactions</i> , 2020, 49, 3341-3352.	1.6	7
5996	Towards cleaner wastewater treatment for special removal of cationic organic dye pollutants: A case study on application of supramolecular inclusion technology with β -cyclodextrin derivatives. <i>Journal of Cleaner Production</i> , 2020, 256, 120308.	4.6	29
5997	Spectroscopic and computational study of a new thiazolylazonaphthol dye 1-[(5-(3-nitrobenzyl)-1,3-thiazol-2-yl)diazanyl]naphthalen-2-ol. <i>Journal of Molecular Liquids</i> , 2020, 304, 112713.	2.3	16
5998	Principle of progressively and strongly immobilizing polysulfides on polyoxovanadate clusters for excellent Li-S batteries application. <i>Nano Energy</i> , 2020, 71, 104596.	8.2	15
5999	Structure-Performance Relationship in Thermally Stable Energetic Materials: Tunable Physical Properties of Benzopyridotetraazapentalene by Incorporating Amino Groups, Hydrogen Bonding, and π - π Interactions. <i>Crystal Growth and Design</i> , 2020, 20, 2106-2114.	1.4	43
6000	Deep Eutectic Solvents Formed by N-Methylacetamide and Heterocyclic Weak Acids for Highly Efficient and Reversible Chemical Absorption of Ammonia. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 2060-2067.	1.8	40
6001	B(C ₆ F ₅) ₃ /Chiral Phosphoric Acid Catalyzed Ketimine-ene Reaction of 2-aryls and α -methylstyrenes. <i>Angewandte Chemie</i> , 2020, 132, 4580-4586.	1.6	10
6002	Reactions of [Pt ₆ (CO) ₆ (SnX ₂) ₂ (SnX ₃) ₄] ₄ (X = Cl, Br) with Acids: Syntheses and molecular structures of [Pt ₁₂ (CO) ₁₀ (SnCl) ₂ (SnCl ₂) ₄ {Cl ₂ Sn($\frac{1}{4}$ -OH)SnCl ₂ }] ₂ and [Pt ₇ (CO) ₆ (SnBr ₂) ₄ {Br ₂ Sn($\frac{1}{4}$ -OH)SnBr ₂ }{Br ₂ Sn($\frac{1}{4}$ -Br)SnBr ₂ }] ₂ Platinum carbonyl clusters decorated by Sn(II)-Fragments. <i>Inorganica Chimica Acta</i> , 2020, 503, 119432.	1.2	3
6003	Modulation of opto-electronic properties of the functionalized hexagonal boron nitride nanosheets with tunable aryl alkyl ionic liquids (TAALs): Defect based analysis. <i>Journal of Molecular Liquids</i> , 2020, 304, 112696.	2.3	13
6004	DNA pyrimidine bases in water: Insights into relative reactivity, byproducts formation and combined toxicity during chlorination. <i>Science of the Total Environment</i> , 2020, 717, 137205.	3.9	7
6005	Isomorphous Series of Pd(II)-Containing Halogen-Bond Donors Exhibiting Cl/Br/I Triple Halogen Isostructural Exchange. <i>Crystal Growth and Design</i> , 2020, 20, 1975-1984.	1.4	19

#	ARTICLE	IF	CITATIONS
6006	Aromaticity as a Guide to Planarity in Conjugated Molecules and Polymers. <i>Journal of Physical Chemistry C</i> , 2020, 124, 5608-5612.	1.5	11
6007	Dihydrogen Bonds in Aqueous NaBD ₄ Solution by Neutron and X-ray Diffraction. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1622-1628.	2.1	11
6008	Second-generation 4,5,6,7-tetrahydrobenzo[<i>d</i>]thiazoles as novel DNA gyrase inhibitors. <i>Future Medicinal Chemistry</i> , 2020, 12, 277-297.	1.1	9
6009	Effect of N-doping on the catalytic decomposition of hydrogen iodide over activated carbon: Experimental and DFT studies. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 4511-4520.	3.8	10
6010	Multiple bonds of heavier group 14 compounds: H ₂ CYX ₂ and HXC ₂ YX ₂ (X = F, Cl, Br and I, Y = Si and Ge). <i>Inorganica Chimica Acta</i> , 2020, 503, 119430.	1.2	1
6011	Analysis of the structures and interactions between CL-20 and its formers. <i>Journal of Molecular Structure</i> , 2020, 1207, 127731.	1.8	4
6012	Theoretical Study of Iron Porphyrin Nitrene: Formation Mechanism, Electronic Nature, and Intermolecular C-H Amination. <i>Inorganic Chemistry</i> , 2020, 59, 1622-1632.	1.9	22
6013	Benchmark and performance of long-range corrected time-dependent density functional tight binding (LC-TD-DFTB) on rhodopsins and light-harvesting complexes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10500-10518.	1.3	36
6014	Competition and cooperativity of hydrogen-bonding and tetrel-bonding interactions involving triethylene diamine (DABCO), H ₂ O and CO ₂ in air. <i>New Journal of Chemistry</i> , 2020, 44, 2328-2338.	1.4	25
6015	Theoretical Study on the Sensing Mechanism of Novel Hydrazine Sensor TAPHP and Its ES IPT and ICT Processes. <i>Frontiers in Chemistry</i> , 2019, 7, 932.	1.8	24
6016	The common trends for the halogen, chalcogen, and pnictogen bonds via sorting principles and local bonding properties. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	20
6017	Diborane(6) and Its Analogues Stabilized by Mono-, Bi-, and Trinuclear Group 7 Templates: Combined Experimental and Theoretical Studies. <i>Inorganic Chemistry</i> , 2020, 59, 1917-1927.	1.9	16
6018	XCage: A Tricyclic Octacationic Receptor for Perylene Diimide with Picomolar Affinity in Water. <i>Journal of the American Chemical Society</i> , 2020, 142, 3165-3173.	6.6	54
6019	Molecular Simulation Elaborating the Mechanism of 1 ^H -Hydroxy Alantolactone Inhibiting Ubiquitin-Conjugating Enzyme UbcH5s. <i>Scientific Reports</i> , 2020, 10, 141.	1.6	11
6020	Molecular Design Strategy for High Redox Potential and Poorly Soluble n-Type Phenazine Derivatives as Cathode Materials for Lithium Batteries. <i>ChemSusChem</i> , 2020, 13, 2337-2344.	3.6	35
6021	Feasibility of pristine, Al-doped and Ga-doped Boron Nitride nanotubes for detecting SF ₄ gas: A DFT, NBO and QTAIM investigation. <i>Applied Surface Science</i> , 2020, 510, 145490.	3.1	63
6022	Theoretical and experimental study of the influence of cationic Eriochrome complexes on the BDD anodic oxidation of Eriochrome Black T solutions. <i>Electrochemistry Communications</i> , 2020, 112, 106668.	2.3	13
6023	Planarity does not always mean higher aromaticity – Intriguing metalloaromaticity of three Al ₁₃ + isomers. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107544.	1.3	3

#	ARTICLE	IF	CITATIONS
6024	Wave function and molecular reactivity study of char with different edges and the chemisorption properties of nitric oxide. <i>Journal of the Energy Institute</i> , 2020, 93, 1519-1526.	2.7	22
6025	Unveiling the effect of solvent polarity on the excited state intramolecular proton transfer mechanism of new 3-hydroxy-4-pyridylisoquinoline compound. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 232, 118082.	2.0	7
6026	An Application Exploiting Auophilic Bonding and iClick to Produce White Light Emitting Materials. <i>Inorganic Chemistry</i> , 2020, 59, 1893-1904.	1.9	22
6027	Boron-Doped Polycyclic Aromatic Hydrocarbons: A Molecular Set Revealing the Interplay between Topology and Singlet Fission Propensity. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1390-1396.	2.1	21
6028	Sensing mechanism of a ratiometric near-infrared fluorescent chemosensor for cysteine hydrosulfide: Intramolecular charge transfer. <i>Scientific Reports</i> , 2020, 10, 711.	1.6	7
6029	A single-molecule conformation modulating crystalline polymorph of a physical " pyrene dimer: blue and green emissions of a pyrene excimer. <i>Journal of Materials Chemistry C</i> , 2020, 8, 3367-3373.	2.7	46
6030	Design of single-porphyrin donors toward high open-circuit voltage for organic solar cells via an energy level gradient-distribution screening strategy of fragments: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4015-4022.	1.3	7
6031	Efficient donor-acceptor emitter based nonsymmetrical connection for organic emitting diodes with improving exciton utilization. <i>RSC Advances</i> , 2020, 10, 4002-4013.	1.7	8
6032	Are Heterometallapentalenes Aromatic or Not? A DFT Investigation. <i>Chemistry - A European Journal</i> , 2020, 26, 5381-5387.	1.7	4
6033	Theoretical studies of infrared signatures of proton-bound amino acid dimers with homochiral and heterochiral moieties. <i>Chirality</i> , 2020, 32, 359-369.	1.3	8
6034	Electron-donor substituents on the dppz-based ligands to control luminescence from dark to bright emissive state in Ir(III) complexes. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26167.	1.0	6
6035	First-principles study of AuSn (2-7) clusters: structural, electronic, magnetic, spectral properties, and adsorption properties with O ₂ and H ₂ O. <i>Journal of Nanoparticle Research</i> , 2020, 22, 1.	0.8	2
6036	Computational mechanistic study on Pd-catalyzed stereoselective synthesis of Z-1,3- and E-1,4-enynes from ligand-controlled regiodivergent hydroalkynylations of allenamides. <i>Molecular Catalysis</i> , 2020, 483, 110765.	1.0	1
6037	Intermolecular forces in pyrrolidones + 1,2-alkanediol liquid mixtures. <i>Journal of Molecular Liquids</i> , 2020, 302, 112539.	2.3	2
6038	Experimental and DFT studies on the molecular structure, spectroscopic properties, and molecular docking of 4-phenylpiperazine-1-ium dihydrogen phosphate. <i>Journal of Molecular Structure</i> , 2020, 1207, 127762.	1.8	90
6039	A tetrachlorocobaltate(II) salt with 2-amino-5-picolinium: Synthesis, theoretical and experimental characterization. <i>Journal of Molecular Structure</i> , 2020, 1207, 127781.	1.8	49
6040	Theoretical investigation into coordination and selectivity of uranyl-unilateral benzotriazole salophens (X = O/S) for R ₃ S-triadimefons. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5486.	1.7	6
6041	Evidence for Genuine Bimetallic Frustrated Lewis Pair Activation of Dihydrogen with Gold(I)/Platinum(0) Systems. <i>Chemistry - A European Journal</i> , 2020, 26, 5982-5993.	1.7	37

#	ARTICLE	IF	CITATIONS
6042	Computational study of inclusion complex of l-Glutamine/beta-Cyclodextrin: Electronic and intermolecular interactions investigations. <i>Journal of Molecular Structure</i> , 2020, 1206, 127740.	1.8	20
6043	Insights into the Luminescence Thermo-chromism of a Triarylboron Derivative: The Role of Intramolecular Group Interaction. <i>Journal of Physical Chemistry A</i> , 2020, 124, 889-897.	1.1	1
6044	η ³ -Coordinating Chiral Primary Amine/Palladium Synergistic Catalysis for Asymmetric Allylic Alkylation. <i>Journal of the American Chemical Society</i> , 2020, 142, 3184-3195.	6.6	65
6045	Unravelling the mechanism of the organocatalyzed aminolytic kinetic resolution of $\hat{\pm}$ -nitroepoxides: a theoretical study. <i>Catalysis Science and Technology</i> , 2020, 10, 1422-1430.	2.1	3
6046	Synergistic degradation of methylparaben on CuFe ₂ O ₄ -rGO composite by persulfate activation. <i>Journal of Alloys and Compounds</i> , 2020, 823, 153757.	2.8	40
6047	Insights on aggregation induced room temperature phosphorescence properties: A QM/MM study. <i>Journal of Luminescence</i> , 2020, 221, 117046.	1.5	11
6048	A Cornucopia of Iridium Nitrogen Compounds Produced from Laser-Abated Iridium Atoms and Dinitrogen. <i>Chemistry - A European Journal</i> , 2020, 26, 7384-7394.	1.7	10
6049	Computational study of HCl adsorption on stoichiometric and oxygen vacancy PuO ₂ {111}, {110} and {100} surfaces. <i>Journal of Nuclear Materials</i> , 2020, 530, 151951.	1.3	11
6050	Photovoltaic properties of the flavonoid-based photosensitizers: Molecular-scale perspective on the natural dye solar cells. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26171.	1.0	13
6051	Investigating the electronic and nonlinear optical properties of fullerene by substituting N, P, As, and Sb in the lattice structure: a DFT study. <i>Applied Physics A: Materials Science and Processing</i> , 2020, 126, 1.	1.1	2
6052	Quantum-chemical calculations on graphitic carbon nitride (g-C ₃ N ₄) single-layer nanostructures: polymeric slab vs. quantum dot. <i>Structural Chemistry</i> , 2020, 31, 1137-1148.	1.0	22
6053	The photophysical properties of three [M(phen) ₂ dppz] ₂ ⁺ (M=Ru and Zn) derivatives for two-photon photodynamic therapy: Insights from theoretical investigations. <i>Dyes and Pigments</i> , 2020, 176, 108244.	2.0	9
6054	Photogenerated charge collection on diamond electrodes with covalently linked chromophore monolayers. <i>Electrochimica Acta</i> , 2020, 337, 135762.	2.6	7
6055	Solvation structure and molecular interactions of ibuprofen with ethanol and water: A theoretical study. <i>Fluid Phase Equilibria</i> , 2020, 510, 112454.	1.4	20
6056	Ionization of adenine in the presence of Na ⁺ in the gas phase and water. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 392, 112404.	2.0	0
6057	A Computational Strategy for the Design of Photochromic Derivatives Based on Diarylethene and Nickel Dithiolene with Large Contrast in Nonlinear Optical Properties. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4221-4241.	1.5	23
6058	A sixteen-valence-electron carbon-group 13 family with global penta-atomic planar tetracoordinate carbon: an ionic strategy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3975-3982.	1.3	12
6059	Mechanistic insights into the lignin dissolution behaviors of a recyclable acid hydrotrope, deep eutectic solvent (DES), and ionic liquid (IL). <i>Green Chemistry</i> , 2020, 22, 1378-1387.	4.6	94

#	ARTICLE	IF	CITATIONS
6060	Fluorine-Substituted Phenanthro[9,10-d]imidazole Derivatives with Optimized Charge-Transfer Characteristics for Efficient Deep-Blue Emitters. <i>Organic Materials</i> , 2020, 02, 011-019.	1.0	9
6061	Amorphous polymerization of nitrogen in compressed cupric azide. <i>Journal of Computational Chemistry</i> , 2020, 41, 1026-1033.	1.5	2
6062	A newly synthesized nitrogen-rich derivative of bicyclic quinoxaline—Structural and conceptual DFT reactivity study. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4055.	0.9	19
6063	Insight into the Expanded Mislinked Porphyrins with High Second Order Nonlinear Optical Response. <i>Journal of Physical Chemistry A</i> , 2020, 124, 955-965.	1.1	18
6064	Effects of a Central Atom and Peripheral Substituents on Photoinduced Electron Transfer in the Phthalocyanine—Fullerene Donor—Acceptor Solution-Processable Dyads. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4010-4023.	1.5	27
6065	DFT study on the mechanism of bimetallic Pd—Zn-catalyzed cycloaddition of alkynyl aryl ethers with internal alkynes. <i>Dalton Transactions</i> , 2020, 49, 2914-2923.	1.6	1
6066	Bifunctional polymer-of-intrinsic-microporosity membrane for flexible Li/Na—H ₂ O ₂ batteries with hybrid electrolytes. <i>Journal of Materials Chemistry A</i> , 2020, 8, 3491-3498.	5.2	8
6067	Exploring the Mechanism of the Palladium-Catalyzed 3-Butene-2-ol Amination Reaction: A DFT Study. <i>Frontiers in Chemistry</i> , 2020, 8, 48.	1.8	2
6068	Tuning Solid-State Luminescence in Conjugated Organic Materials: Control of Excitonic and Excimeric Contributions through π -Stacking and Halogen Bond Driven Self-Assembly. <i>ChemPhysChem</i> , 2020, 21, 616-624.	1.0	23
6069	GIAO versus GIPAW: Comparison of Methods To Calculate ¹¹ B NMR Shifts of Icosahedral <i>closo</i> -Heteroboranes toward Boron-Rich Borides. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2173-2185.	1.1	6
6070	A novel colorimetric and fluorometric probe for the detection of CN [•] with high selectivity in aqueous media. <i>Dyes and Pigments</i> , 2020, 176, 108224.	2.0	24
6071	Alkoxyphenyl or alkylphenyl side-chained Thieno[2,3-f]benzofuran polymer for efficient non-fullerene solar cells. <i>Materials Today Energy</i> , 2020, 16, 100381.	2.5	4
6072	Pentacoordinated silver(I) complex featuring 8-phenylquinoline ligands: Interplay of coordination bonds, semicoordination, and stacking interactions. <i>Inorganica Chimica Acta</i> , 2020, 504, 119453.	1.2	5
6073	Design Rules for Improving the Cycling Stability of High-Performance Donor—Acceptor-Type Electrochromic Polymers. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 7529-7538.	4.0	26
6074	Selective Hydrogenation of Acetylene Catalysed by a B ₁₂ N ₁₂ Cluster Doped with a Single Nickel Atom: A DFT Study. <i>Catalysts</i> , 2020, 10, 115.	1.6	7
6075	Complexes of helium with neutral molecules: Progress toward a quantitative scale of bonding character. <i>Journal of Computational Chemistry</i> , 2020, 41, 1000-1011.	1.5	10
6076	Dynamic fluxionality of ternary Mg ₂ BeB ₈ cluster: a nanocompass. <i>Journal of Molecular Modeling</i> , 2020, 26, 30.	0.8	6
6077	Speciation of thioarsenicals through application of coffee ring effect on gold nanofilm and surface-enhanced Raman spectroscopy. <i>Analytica Chimica Acta</i> , 2020, 1106, 88-95.	2.6	13

#	ARTICLE	IF	CITATIONS
6078	Theoretical and experimental spectroscopic studies of monomeric and dimeric structures of 4-hydroxybenzamide. <i>Journal of Molecular Structure</i> , 2020, 1206, 127742.	1.8	2
6079	Metal-Organic Frameworks of Cu(II) Constructed from Functionalized Ligands for High Capacity H ₂ and CO ₂ Gas Adsorption and Catalytic Studies. <i>Inorganic Chemistry</i> , 2020, 59, 1810-1822.	1.9	25
6080	Tuning Second-Order Nonlinear Optical Properties of Cross-Linked Carbon Nanotube via External Electric Field. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3778-3783.	1.5	10
6081	Achieving remarkable and reversible mechanochromism from a bright ionic AIEgen with high specificity for mitochondrial imaging and secondary aggregation emission enhancement for long-term tracking of tumors. <i>Materials Chemistry Frontiers</i> , 2020, 4, 941-949.	3.2	65
6082	NiCo ₂ O ₄ nanoparticles: an efficient and magnetic catalyst for Knoevenagel condensation. <i>Journal of Zhejiang University: Science A</i> , 2020, 21, 74-84.	1.3	10
6083	Effects of intramolecular hydrogen bonds on phosphorescence emission: A theoretical perspective. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5527.	1.7	3
6084	A simple method of identifying π orbitals for non-planar systems and a protocol of studying π electronic structure. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	171
6085	Giant enhancement of the nonlinear optical properties of [2.2]paracyclophanes by an donor-bridge-acceptor. <i>Optik</i> , 2020, 203, 163988.	1.4	0
6086	Modification on the Indacenodithieno[3,2- <i>b</i>]thiophene Core to Achieve Higher Current and Reduced Energy Loss for Nonfullerene Solar Cells. <i>Chemistry of Materials</i> , 2020, 32, 1297-1307.	3.2	46
6087	Local Aromaticity: An Important Indicator of the Surface Active Sites of Heterocyclic Nanostructures. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2583-2590.	1.5	4
6088	Theoretical study on the microscopic mechanism of lignin solubilization in Keggin-type polyoxometalate ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2878-2886.	1.3	20
6089	B(C ₆ F ₅) ₃ /Chiral Phosphoric Acid Catalyzed Ketimine Ene Reaction of 2-Arylindoles and α -Methylstyrenes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 4550-4556.	2.59	40
6090	Tautomeric effect of guanine on stability, spectroscopic and absorbance properties in cytosine-guanine base pairs: a DFT and TD-DFT perspective. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	3
6091	Insights into the reaction mechanism of criegee intermediate with NO radical. <i>Computational and Theoretical Chemistry</i> , 2020, 1175, 112731.	1.1	3
6092	The influence on properties with different conjugated direction of phenoxazine and phenothiazine-based chromophores for organic nonlinear optical materials. <i>Dyes and Pigments</i> , 2020, 176, 108219.	2.0	17
6093	Chemically tunable DILs: Physical properties and highly efficient capture of low-concentration SO ₂ . <i>Separation and Purification Technology</i> , 2020, 240, 116572.	3.9	27
6094	Heterometallic Triply Bridging Bis-Borylene Complexes. <i>Chemistry - an Asian Journal</i> , 2020, 15, 780-786.	1.7	13
6095	Theoretical study on the stability of the complexes A ₂ BX ₃ [A = CH ₃ NH ₃ ⁺ , NH ₂ CHNH ₂ ⁺ , NH ₂ CHOH ⁺ ; B = Sn ²⁺ , Pb ²⁺ ; X = F ⁻ , Cl ⁻ , Br ⁻ , I ⁻]. <i>Journal of Molecular Modeling</i> , 2020, 26, 46.	0.8	9

#	ARTICLE	IF	CITATIONS
6096	Tuning the mechanical performance efficiently of various LLM-105 based PBXs via bioinspired interfacial reinforcement of polydopamine modification. <i>Composites Part B: Engineering</i> , 2020, 186, 107824.	5.9	23
6097	Cyanide-free silver immersion deposition involving 3-mercapto-1-propanesulfonic acid for copper finishing. <i>Materials Chemistry and Physics</i> , 2020, 244, 122671.	2.0	9
6098	Theoretical study of adsorption of ethanol and acetone molecules by perfect and defected h-BN nanosheet. <i>Superlattices and Microstructures</i> , 2020, 139, 106403.	1.4	2
6099	Phosphorescent Iridium(III) Complexes with Acyclic Diaminocarbene Ligands as Chemosensors for Mercury. <i>Inorganic Chemistry</i> , 2020, 59, 2209-2222.	1.9	37
6100	Enhanced Reverse Saturable Absorption in Substituted Twistacenes from Visible to Near-Infrared: Modulation of Terminal Twisted π -Conjugated Units. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4701-4708.	1.5	10
6101	Mechanistic Investigation of Isonitrile Formation Catalyzed by the Nonheme Iron/Fe-KG-Dependent Decarboxylase (ScoE). <i>ACS Catalysis</i> , 2020, 10, 2942-2957.	5.5	29
6102	The structure optimization of phenanthroimidazole based isomers with external quantum efficiency approaching 7% in non-doped deep-blue OLEDs. <i>Journal of Materials Chemistry C</i> , 2020, 8, 2975-2984.	2.7	35
6103	Theoretical investigation on rotaxanes containing a pyridyl-acyl hydrazone moiety: chemical $Z \rightarrow E$ and photochemical $E \rightarrow Z$ isomerizations. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	7
6104	Relationship between the Electrical Characteristics of Molecules and Fast Streamers in Ester Insulation Oil. <i>International Journal of Molecular Sciences</i> , 2020, 21, 974.	1.8	16
6105	DFT-Assisted Spectroscopic Studies on the Coordination of Small Ligands to Palladium: From Isolated Ions to Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4781-4790.	1.5	4
6106	Heteroleptic $[Cu(NN)P_2]^{+}$ type cuprous complexes and their structural modulation on phosphorescent color: Synthesis, structural characterization, properties, and theoretical calculations. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5561.	1.7	11
6107	Chlorotellurate(IV) supramolecular associates with π -trapped Br_2 : features of non-covalent halogen-halogen interactions in crystalline phases. <i>CrystEngComm</i> , 2020, 22, 1985-1990.	1.3	16
6108	Atmospheric implication of synergy in methanesulfonic acid-base trimers: a theoretical investigation. <i>RSC Advances</i> , 2020, 10, 5173-5182.	1.7	18
6109	Xe-chalcogen aerogen bond. Effect of substituents and size of chalcogen atom. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4115-4121.	1.3	11
6110	Ionic-caged heterometallic bismuth-platinum complex exhibiting electrocatalytic CO_2 reduction. <i>Dalton Transactions</i> , 2020, 49, 2652-2660.	1.6	9
6111	Synthesis, molecular docking studies, and larvicidal activity evaluation of new fluorinated neonicotinoids against <i>Anopheles darlingi</i> larvae. <i>PLoS ONE</i> , 2020, 15, e0227811.	1.1	12
6112	Competition between Intra and Intermolecular Triel Bonds. Complexes between Naphthalene Derivatives and Neutral or Anionic Lewis Bases. <i>Molecules</i> , 2020, 25, 635.	1.7	20
6113	N-doped Graphdiyne Coating for Dendrite-free Lithium Metal Batteries. <i>Chemistry - A European Journal</i> , 2020, 26, 5434-5440.	1.7	22

#	ARTICLE	IF	CITATIONS
6114	Achieving High-Performance Pure-Red Electrophosphorescent Iridium(III) Complexes Based on Optimizing Ancillary Ligands. <i>Chemistry - A European Journal</i> , 2020, 26, 4410-4418.	1.7	11
6115	Blue iridium(III) complexes with high internal quantum efficiency based on 4-(pyridin-3-yl)pyrimidine derivative and their electroluminescent properties. <i>Dyes and Pigments</i> , 2020, 177, 108257.	2.0	9
6116	Exploring the Role of Strong Intramolecular Coordination of the 2-(2'-pyridyl)phenyl Group in Heavy Main Group Halides: Insights from Synthesis, Structural, and Bonding Analyses. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 2143-2152.	1.0	5
6117	Complexation and enantioselectivity of sulfur/selenium-substituted uranyl-salophens with R/S-chiral lactone for RRS/SSR-3, 5-Dimethyl-2-(3-fluorophenyl)-2-morpholinols. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2020, 324, 993-1006.	0.7	7
6118	Designing of benzothiazole based non-fullerene acceptor (NFA) molecules for highly efficient organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020, 1181, 112833.	1.1	94
6119	UV365 induced elimination of contaminants of emerging concern in the presence of residual nitrite: Roles of reactive nitrogen species. <i>Water Research</i> , 2020, 178, 115829.	5.3	42
6120	Reaction Mechanisms on [3 + 2] Cycloaddition of Azides with Metal Carbyne Complexes: Significant Effects of Aromaticity, Substituent, and Metal Center. <i>Inorganic Chemistry</i> , 2020, 59, 7318-7324.	1.9	7
6121	A Comparative Experimental and Computational Study of Heterometallic Fe-M (M = Cu, Ag, Au) Carbonyl Clusters Containing N-Heterocyclic Carbene Ligands. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 2191-2202.	1.0	14
6122	π-Stacking effects on acid capacity of p-aminobenzoic acid. <i>Structural Chemistry</i> , 2020, 31, 1707-1716.	1.0	1
6123	Experimental and theoretical spectroscopic analysis, hydrogen bonding, reduced density gradient and antibacterial activity study on 2-Phenyl quinoline alkaloid. <i>Chemical Physics</i> , 2020, 536, 110827.	0.9	19
6124	Intermolecular weak interactions of crystalline purine and uric acid investigated by terahertz spectroscopy and theoretical calculation. <i>Journal of Luminescence</i> , 2020, 223, 117198.	1.5	24
6125	How the atomic electron-accepting ability affect the double ESIPT process of 2,5-bis(benzoxazol-2-yl)thiophene-3,4-diol?. <i>Journal of Luminescence</i> , 2020, 225, 117329.	1.5	28
6126	Density functional theory based studies on the adsorption of rare-earth ions from hydrated nitrate salt solutions on g-C ₃ N ₄ monolayer surface. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107577.	1.3	16
6127	U ₂ O@C ₇₆ : Non-Isolated-Pentagon-Rule Cages Preval with the U ₂ O Configuration Determined by Cage Shape and Dominated by Multicenter Bonds. <i>Inorganic Chemistry</i> , 2020, 59, 7039-7048.	1.9	10
6128	Multicolored Cathodically Coloring Electrochromism and Electrofluorochromism in Regioisomeric Star-Shaped Carbazole Dibenzofurans. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 24156-24164.	4.0	31
6129	Study of the aggregation behaviour of three primary reactive dyes via molecular dynamics simulations. <i>Molecular Simulation</i> , 2020, 46, 627-637.	0.9	8
6130	A theoretical/experimental probe to locate hydrogen(s) while constructing hierarchically structured cellulose-zinc oxide composite. <i>Cellulose</i> , 2020, 27, 5135-5147.	2.4	8
6131	Phosphorene defects for high-quality detection of nitric oxide and carbon monoxide: A periodic density functional study. <i>Chemical Engineering Journal</i> , 2020, 396, 125247.	6.6	36

#	ARTICLE	IF	CITATIONS
6132	Excited-state hydrogen bonding: Detecting ammonia using an HHTP-DPB covalent organic framework. <i>Chemical Physics</i> , 2020, 536, 110822.	0.9	5
6133	A DFT study on the metal ion selectivity of deferiprone complexes. <i>Computational Biology and Chemistry</i> , 2020, 86, 107267.	1.1	15
6134	Nitrogen and sulfur codoped micro-mesoporous carbon sheets derived from natural biomass for synergistic removal of chromium(VI): adsorption behavior and computing mechanism. <i>Science of the Total Environment</i> , 2020, 730, 138930.	3.9	64
6135	Metal-Ligand Cooperativity in Titanium-Catalyzed Anti-Markovnikov Hydroamination. <i>ACS Catalysis</i> , 2020, 10, 7100-7111.	5.5	12
6136	Revealing electronic features governing hydrolysis of cephalosporins in the active site of the L1 metallo- β -lactamase. <i>RSC Advances</i> , 2020, 10, 8664-8676.	1.7	9
6137	On the Stability of Interactions between Pairs of Anions $MCl_3^{\cdot-}$ Complexes of $M=Be, Mg, Ca, Sr, Ba$ with Pyridine and $CN^{\cdot-}$. <i>ChemPhysChem</i> , 2020, 21, 870-877.	1.0	25
6138	Formation of brown carbon on Fe-bearing clay from volatile phenol under simulated atmospheric conditions. <i>Atmospheric Environment</i> , 2020, 228, 117427.	1.9	10
6139	Observation of triplet $n\pi^*$ state in ultrafast intersystem crossing of 6-azathymine. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 396, 112491.	2.0	8
6140	The theory of cysteine two-photon fluorescence probes of coumarinocoumarin derivatives and kinetics of ICT and PET mechanisms of probe molecules. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 397, 112525.	2.0	11
6141	Investigation of the spectroscopic features along with the media polarity effect in some symmetrical disc-shaped liquid crystals. <i>Journal of Molecular Liquids</i> , 2020, 309, 113226.	2.3	3
6142	Quantum computational, spectroscopic and molecular docking studies on 2-acetylthiophene and its bromination derivative. <i>Journal of Molecular Structure</i> , 2020, 1212, 128129.	1.8	29
6143	Unexpected Trends in the Stability and Dissociation Kinetics of Lanthanide(III) Complexes with Cyclen-Based Ligands across the Lanthanide Series. <i>Inorganic Chemistry</i> , 2020, 59, 8184-8195.	1.9	15
6144	A mechanistic study of the activation of small molecules (H_2 and C_2H_2) by group 14 analogues of selenophene. <i>New Journal of Chemistry</i> , 2020, 44, 8922-8936.	1.4	0
6145	Structural and electronic properties of nanosize semiconductor $HfSiO_3/2^{\cdot-}$ ($n=6$) material: a double-hybrid density functional theory investigation. <i>Journal of Molecular Modeling</i> , 2020, 26, 85.	0.8	4
6146	Highly fluorescence emissive 5, 5'-distyryl-3, 3'-bithiophenes: Synthesis, crystal structure, optoelectronic and thermal properties. <i>Dyes and Pigments</i> , 2020, 179, 108396.	2.0	6
6147	Zinc(II) and Cadmium(II) complexes containing imidazole ring: Structural, spectroscopic, antibacterial, DFT calculations and Hirshfeld surface analysis. <i>Inorganica Chimica Acta</i> , 2020, 507, 119610.	1.2	19
6148	Solid-state fluorescent 1,2,4-triazole zinc(II) complexes: Self-organization via bifurcated (N H) $2^{\cdot-}$ Cl contacts. <i>Inorganica Chimica Acta</i> , 2020, 510, 119660.	1.2	3
6149	Phototuning Energy Transfer in Self-Organized Luminescent Helical Superstructures for Photonic Applications. <i>Advanced Optical Materials</i> , 2020, 8, 2000107.	3.6	73

#	ARTICLE	IF	CITATIONS
6150	Judicious Choice of Nâ€Heterocycles for the Realization of Skyâ€Blueâ€to Greenâ€Emitting Carbazolygold(III) C^C^N Complexes and Their Applications for Organic Lightâ€Emitting Devices. <i>Angewandte Chemie</i> , 2020, 132, 9771-9779.	1.6	6
6151	Influence of Hydration on the Structure and Interactions of Ethaline Deepâ€Eutectic Solvent: A Spectroscopic and Computational Study. <i>ChemPhysChem</i> , 2020, 21, 995-1005.	1.0	30
6152	Encapsulation of Mg₂ inside a C₆₀ cage forms an electride. <i>Journal of Computational Chemistry</i> , 2020, 41, 1645-1653.	1.5	20
6153	Revealing and comparing different excitedâ€state intramolecular proton transfer processes for 3â€(Tj ETQq1 1 0.784314 rgBT /Overlo 67, 1367-1373.	0.8	0
6154	In search of the smallest boroxolâ€type heterocyclic ring system: Planar hexagonal B 3 S 3 + cluster with double 6â€2if aromaticity. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26229.	1.0	1
6155	Theoretical study of a novel organic electride with large nonlinear optical responses. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26235.	1.0	3
6156	Experimental and DFT Studies on the FTâ€IR, NMR and UV/Vis Spectra of a Xanthene Derivative: The Case of 9â€benzoylâ€3,4,5,6,7,9â€hexahydroâ€1<i>h</i>â€xantheneâ€1,8(2<i>h</i>)â€dione. <i>ChemistrySelect</i> , 2020, 5, 3971-3980.	0.7	8
6157	Theoretical study on the activation of C-H bond in ethane by PdX+ (X = F, Cl, Br, H, and CH3) in the gas phase. <i>Journal of Molecular Modeling</i> , 2020, 26, 91.	0.8	0
6158	Theoretical study on noncovalent interaction of molecular tweezers by Zn(II) salphen-azo-crown ether triads receptor. <i>Journal of Molecular Modeling</i> , 2020, 26, 39.	0.8	8
6159	Computational modeling of the kinetics and mechanism of the new generation of glutathione peroxidase nanomimic: selenosubtilisin and telluros subtilisin. <i>Journal of the Iranian Chemical Society</i> , 2020, 17, 2119-2131.	1.2	1
6160	Bandgap engineering of polymetric carbon nitride copolymerized by 2,5,8-triamino-tri-s-triazine (melem) and barbituric acid for efficient nonsacrificial photocatalytic H2O2 production. <i>Applied Catalysis B: Environmental</i> , 2020, 271, 118917.	10.8	72
6161	Formation of atmospheric molecular clusters of methanesulfonic acidâ€Diethylamine complex and its atmospheric significance. <i>Atmospheric Environment</i> , 2020, 226, 117404.	1.9	16
6162	Modulating ESIPT behavior and fluorescent sensing mechanism of 2-(2â€hydroxyphenol)thiazole-4-carboxaldehyde derivatives: A theoretical study. <i>Chemical Physics Letters</i> , 2020, 747, 137342.	1.2	3
6163	Removal of thiophene sulfur model compound for coal by microwave with peroxyacetic acid. <i>Fuel</i> , 2020, 272, 117748.	3.4	28
6164	Kinetics, mechanism and toxicity of intermediates of solar light induced photocatalytic degradation of pindolol: Experimental and computational modeling approach. <i>Journal of Hazardous Materials</i> , 2020, 393, 122490.	6.5	14
6165	Mechanistic investigation of N-heterocyclic carbene and Na2CO3 cooperatively catalyzed C(sp3)-F bond activation reaction of fluoroenal. <i>Molecular Catalysis</i> , 2020, 489, 110944.	1.0	11
6166	Effect of side chain on the electrochemical performance of poly (ether ether ketone) based anion-exchange membrane: A molecular dynamics study. <i>Journal of Membrane Science</i> , 2020, 605, 118105.	4.1	42
6167	Extraction and mechanism exploration for separating cresols from coal tar by ionic liquid ethanolamine lactate. <i>Journal of Molecular Liquids</i> , 2020, 305, 112845.	2.3	29

#	ARTICLE	IF	CITATIONS
6168	Photophysical and theoretical studies on the solvatochromic effects and dipole moments evaluation of substituted 1-phenyl-3-naphthyl-5- (4-ethyl benzoate)-2-pyrazoline. Journal of Molecular Liquids, 2020, 307, 112967.	2.3	18
6169	Quantum chemical computational and spectroscopic (IR, Raman, NMR, and UV) studies on the 5-(5-methoxy-benzofuran-3-ylmethyl)-3H-[1, 3, 4] oxadiazole-2-thione. Journal of Molecular Structure, 2020, 1210, 128041.	1.8	19
6170	Molecular design of nitro-oxide-substituted cycloalkane derivatives for high-energy-density materials. Journal of Molecular Structure, 2020, 1212, 128128.	1.8	7
6171	Theoretical crystal structure prediction of aminosalicic acid: Charge density topological and electrostatic analyses. Journal of Molecular Structure, 2020, 1213, 128139.	1.8	5
6172	The effect of the heteroatom (X=P, As, Si and Ge) on the geometrical and electronic properties of $\hat{I}\pm$ -Keggin polyoxometalates (M=Mo, W and Nb) – A DFT investigation. Journal of Molecular Structure, 2020, 1213, 128159.	1.8	12
6173	Crystal engineering and electrostatic properties of co-crystals of pyrimethamine with benzoic acid and gallic acid. Journal of Molecular Structure, 2020, 1214, 128183.	1.8	8
6174	Experimental, computational, and in silico analysis of (C ₈ H ₁₄ N ₂) ₂ [CdCl ₆] compound. Journal of Molecular Structure, 2020, 1213, 128186.	1.8	58
6175	Noncovalent interaction stabilizes the 2,4-Dinitrophenylhydrazone Derivatives over g-C ₃ N ₄ surface to enhance optical properties: Synthesis, characterization, and DFT investigation. Journal of Molecular Structure, 2020, 1214, 128192.	1.8	12
6176	2-Methyltetrol sulfate ester-initiated nucleation mechanism enhanced by common nucleation precursors: A theory study. Science of the Total Environment, 2020, 723, 137987.	3.9	11
6177	Noncovalent Sulfoxide–Nitrile Coupling Involving Four-Center Heteroleptic Dipole–Dipole Interactions between the Sulfinyl and Nitrile Groups. Crystal Growth and Design, 2020, 20, 3417-3428.	1.4	17
6178	Exploring the Nature of Interaction and Stability between Water-Soluble Arsenic Pollutants and Metal–Phosphorene Hybrids: A Density Functional Theory Study. Journal of Physical Chemistry A, 2020, 124, 3662-3671.	1.1	9
6179	Second Near-Infrared Aggregation-Induced Emission Fluorophores with Phenothiazine Derivatives as the Donor and 6,7-Diphenyl-[1,2,5]Thiadiazolo[3,4-g]Quinoxaline as the Acceptor for In Vivo Imaging. ACS Applied Materials & Interfaces, 2020, 12, 20281-20286.	4.0	36
6180	Imidazo[1,2- <i>b</i>]pyridazine as Building Blocks for Host Materials for High-Performance Red-Phosphorescent Organic Light-Emitting Devices. ACS Applied Materials & Interfaces, 2020, 12, 19701-19709.	4.0	23
6181	Solubility and Stability Advantages of a New Cocrystal of Berberine Chloride with Fumaric Acid. ACS Omega, 2020, 5, 8283-8292.	1.6	46
6182	Excited-State Turn-On of Auophilicity and Tunability of Relativistic Effects in a Series of Digold Triazolates Synthesized via iClick. Journal of the American Chemical Society, 2020, 142, 8331-8341.	6.6	26
6183	Cp ₂ Ti(^η 2-BuNCN)Bu: A Complex with an Unusual ^η 2 Coordination Mode of a Heterocumulene Featuring a Free Carbene. Journal of the American Chemical Society, 2020, 142, 8006-8018.	6.6	24
6184	High-performance particulate matter including nanoscale particle removal by a self-powered air filter. Nature Communications, 2020, 11, 1653.	5.8	108
6185	Applying the Jellium model to octacarbonyl metal complexes. Communications Chemistry, 2020, 3, .	2.0	2

#	ARTICLE	IF	CITATIONS
6186	Unravelling the kinetics and molecular mechanism of the degenerate Cope rearrangement of bullvalene. <i>New Journal of Chemistry</i> , 2020, 44, 6543-6552.	1.4	8
6187	An anthracene-pendant ruthenium(II) complex conjugated to a biotin anchor, an essential handle for photo-induced anti-cancer activity. <i>New Journal of Chemistry</i> , 2020, 44, 6610-6622.	1.4	9
6188	Effect of number and different types of proton donors on excited-state intramolecular single and double proton transfer in bipyridine derivatives: theoretical insights. <i>New Journal of Chemistry</i> , 2020, 44, 8018-8031.	1.4	15
6189	Merging Cu-catalysed C-H functionalisation and intramolecular annulations: computational and experimental studies on an expedient construction of complex fused heterocycles. <i>Organic Chemistry Frontiers</i> , 2020, 7, 1235-1242.	2.3	6
6190	Theoretical study of the mechanism behind the site- and enantio-selectivity of C-H functionalization catalysed by chiral dirhodium catalyst. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9561-9572.	1.3	5
6191	Prediction of Binding Stability of Pu(IV) and PuO ₂ (VI) by Nitrogen Tridentate Ligands in Aqueous Solution. <i>International Journal of Molecular Sciences</i> , 2020, 21, 2791.	1.8	5
6192	New Eco-Friendly Xanthate-Based Flotation Agents. <i>Minerals (Basel, Switzerland)</i> , 2020, 10, 350.	0.8	6
6193	Arylaminopropanone Derivatives as Potential Cholinesterase Inhibitors: Synthesis, Docking Study and Biological Evaluation. <i>Molecules</i> , 2020, 25, 1751.	1.7	3
6194	Theoretical Investigation of Energetic Salts with Pentazolate Anion. <i>Molecules</i> , 2020, 25, 1783.	1.7	8
6195	Are Heterometallapentalenes Aromatic or Not? A DFT Investigation. <i>Chemistry - A European Journal</i> , 2020, 26, 5307-5307.	1.7	1
6196	A molecular electron density theory study to understand the interplay of theory and experiment in nitrene-enone cycloaddition. <i>Journal of Chemical Sciences</i> , 2020, 132, 1.	0.7	13
6197	Manganese Telluride Carbonyl Complexes: Facile Syntheses and Exotic Properties—Reversible Transformations, Hydrogen Generation, Paramagnetic, and Semiconducting Properties. <i>Inorganic Chemistry</i> , 2020, 59, 6923-6941.	1.9	7
6198	B ₁₃ + is a Tri-Spoke Wheel: A New Revelation through Electronic Structure Analysis. <i>ChemistrySelect</i> , 2020, 5, 3906-3916.	0.7	1
6199	Substituent control of photophysical properties for excited-state intramolecular proton transfer (ESIPT) of o-LHBDI derivatives: a TD-DFT investigation. <i>Journal of Molecular Modeling</i> , 2020, 26, 108.	0.8	12
6200	Nontoxic Black Phosphorus Quantum Dots Inhibit Insulin Amyloid Fibrillation at an Ultralow Concentration. <i>IScience</i> , 2020, 23, 101044.	1.9	13
6201	Copper(I)/Ganphos catalysis: enantioselective synthesis of diverse spirooxindoles using iminoesters and alkyl substituted methyleneindolinones. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 3740-3746.	1.5	20
6202	Hexagonal boron nitride induces anion trapping in a polyethylene oxide based solid polymer electrolyte for lithium dendrite inhibition. <i>Journal of Materials Chemistry A</i> , 2020, 8, 9579-9589.	5.2	81
6203	Computational Prediction of Chiral Iron Complexes for Asymmetric Transfer Hydrogenation of Pyruvic Acid to Lactic Acid. <i>Molecules</i> , 2020, 25, 1892.	1.7	3

#	ARTICLE	IF	CITATIONS
6204	Strong proton-shared hydrogen bonding in a methyl imidazole ⁺ HCl complex: evidence from matrix isolation infrared spectroscopy and ab initio computations. <i>New Journal of Chemistry</i> , 2020, 44, 7116-7128.	1.4	7
6205	Protic vs aprotic ionic liquid for CO ₂ fixation: A simulation study. <i>Green Energy and Environment</i> , 2020, 5, 183-194.	4.7	49
6206	Investigation of intermolecular interactions in inclusion complexes of pyroquilon with cucurbit[n]urils (n=7,8) using DFT-D3 correction dispersion. <i>Journal of Molecular Liquids</i> , 2020, 309, 113233.	2.3	23
6207	Adamantane based alkaline earthsides with excellent nonlinear optical response and ultraviolet transparency. <i>Optics and Laser Technology</i> , 2020, 129, 106298.	2.2	46
6208	Zwitterionic polymer chain-assisted lysozyme imprinted core-shell carbon microspheres with enhanced recognition and selectivity. <i>Talanta</i> , 2020, 217, 121085.	2.9	26
6209	Water Promotes the Oxidation of SO ₂ by O ₂ over Carbonaceous Aerosols. <i>Environmental Science & Technology</i> , 2020, 54, 7070-7077.	4.6	28
6210	Electronic Structure of Multicomponent Organic Molecular Materials: Evaluation of Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3712-3719.	2.3	20
6211	UV-Catalyzed Persulfate Oxidation of an Anthraquinone Based Dye. <i>Catalysts</i> , 2020, 10, 456.	1.6	20
6212	Structural, Spectroscopic, and Chemical Bonding Analysis of Zn(II) Complex [Zn(sal)](H ₂ O): Combined Experimental and Theoretical (NBO, QTAIM, and ELF) Investigation. <i>Crystals</i> , 2020, 10, 259.	1.0	13
6213	Photocatalytic dye degradation under sunlight irradiation using cerium ion adsorbed two-dimensional graphitic carbon nitride. <i>Journal of Environmental Chemical Engineering</i> , 2020, 8, 103942.	3.3	33
6214	BP[dG]-induced distortions to DNA polymerase and DNA duplex: A detailed mechanism of BP adducts blocking replication. <i>Food and Chemical Toxicology</i> , 2020, 140, 111325.	1.8	8
6215	Fullerene's ring: A new strategy to improve the performance of fullerene organic solar cells. <i>Organic Electronics</i> , 2020, 83, 105747.	1.4	19
6216	Eutectics and Salt of Dapsone With Hydroxybenzoic Acids: Binary Phase Diagrams, Characterization and Evaluation. <i>Journal of Pharmaceutical Sciences</i> , 2020, 109, 2224-2236.	1.6	12
6217	Pagoda[4]arene and <i>i</i> -Pagoda[4]arene. <i>Journal of the American Chemical Society</i> , 2020, 142, 8262-8269.	6.6	129
6218	Antioxidant Properties of Lapachol and Its Derivatives and Their Ability to Chelate Iron (II) Cation: DFT and QTAIM Studies. <i>Bioinorganic Chemistry and Applications</i> , 2020, 2020, 1-10.	1.8	2
6219	Anticrystal Engineering of Ketoprofen and Ester Local Anesthetics: Ionic Liquids or Deep Eutectic Mixtures?. <i>Pharmaceutics</i> , 2020, 12, 368.	2.0	18
6220	B-doped graphitic porous biochar with enhanced surface affinity and electron transfer for efficient peroxydisulfate activation. <i>Chemical Engineering Journal</i> , 2020, 396, 125119.	6.6	148
6221	What are the effects of cucurbit[n]uril on CTMS loading? Insights from QM calculations and MD simulations. <i>Computational Materials Science</i> , 2020, 181, 109751.	1.4	5

#	ARTICLE	IF	CITATIONS
6222	Computational insights of two-dimensional infrared spectroscopy under electric fields in phosphorylcholine. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26169.	1.0	3
6223	Investigation of Resveratrol Adsorption on Pine Pollen Grains: A First-Principles Study. <i>ChemistrySelect</i> , 2020, 5, 4307-4311.	0.7	3
6224	Unique electronic structure of Tri- $\frac{1}{4}$ -oxido-[bis(porphyrinato)niobium(V)]: Spontaneous symmetry breaking mechanism of the special coordination skeleton. <i>Computational and Theoretical Chemistry</i> , 2020, 1181, 112832.	1.1	3
6225	Theoretical study on the sensing mechanism of an ON1-OFF-ON2 type fluoride fluorescent chemosensor. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 237, 118397.	2.0	18
6226	Fast and efficient removal of Cr(VI) to ppb level together with Cr(III) sequestration in water using layered double hydroxide intercalated with diethyldithiocarbamate. <i>Science of the Total Environment</i> , 2020, 727, 138701.	3.9	32
6227	E π -Z photoinduced isomerization and hydrogen bonding in the peri-acetamido substituted (1H-pyrrol-2-ylmethylene)benzocycloalkanones. <i>Tetrahedron</i> , 2020, 76, 131202.	1.0	7
6228	Theoretical Study on the Reduction Mechanism of Np(VI) by Hydrazine Derivatives. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3720-3729.	1.1	6
6229	Computational Study of sp^x ($x=1-3$) Hybridized Be \sim Be Bonds Stabilized by Amidinate Ligands. <i>Chemistry - A European Journal</i> , 2020, 26, 10891-10895.	1.7	7
6230	Evidence for Genuine Bimetallic Frustrated Lewis Pair Activation of Dihydrogen with Gold(I)/Platinum(0) Systems. <i>Chemistry - A European Journal</i> , 2020, 26, 5915-5915.	1.7	11
6231	Anion \cdots anion Attraction in Complexes of MCl_3 ($M=Zn, Cd, Hg$) with CN^{\sim} . <i>ChemPhysChem</i> , 2020, 21, 1119-1125.	1.0	31
6232	Mechanism and Origins of Regio- and Mono/Di-selectivity in Rh(III)-Catalyzed α -meta-C-H Alkenylation with Alkynes. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 3294-3302.	1.2	2
6233	Mechanistic details of metal-free cyclization reaction of organophosphorus oxide with alkynes mediated by 2,6-lutidine and Tf_2O . <i>Journal of Computational Chemistry</i> , 2020, 41, 1709-1717.	1.5	5
6234	A density functional theory exploration on the Zn catalyst for acetylene hydration. <i>Journal of Molecular Modeling</i> , 2020, 26, 105.	0.8	9
6235	A conceptual DFT analysis of the plausible mechanism of some pericyclic reactions. <i>Structural Chemistry</i> , 2020, 31, 1745-1756.	1.0	8
6236	Computational study of 3-thiophene acetic acid: Molecular docking, electronic and intermolecular interactions investigations. <i>Computational Biology and Chemistry</i> , 2020, 86, 107268.	1.1	38
6237	C $_2$ CO $_2$ Li $_3^+$: A superalkali cation with planar pentacoordinate carbon. <i>Computational and Theoretical Chemistry</i> , 2020, 1180, 112824.	1.1	4
6238	Structuring of sunflower oil by stearic acid derivatives: Experimental and molecular modelling studies. <i>Food Chemistry</i> , 2020, 324, 126801.	4.2	15
6239	Effective blockage of chloride ion quenching and chlorinated by-product generation in photocatalytic wastewater treatment. <i>Journal of Hazardous Materials</i> , 2020, 396, 122670.	6.5	31

#	ARTICLE	IF	CITATIONS
6240	pH-Dependent adsorption of aromatic compounds on graphene oxide: An experimental, molecular dynamics simulation and density functional theory investigation. Journal of Hazardous Materials, 2020, 395, 122680.	6.5	48
6241	Activation of peroxymonosulfate by cobalt-impregnated biochar for atrazine degradation: The pivotal roles of persistent free radicals and ecotoxicity assessment. Journal of Hazardous Materials, 2020, 398, 122768.	6.5	100
6242	Density functional theory study of emerging pollutants removal from water by covalent triazine based framework. Journal of Molecular Liquids, 2020, 309, 113008.	2.3	25
6243	Interaction of supported ionic liquids phases onto copper nanoparticles: A DFT study. Journal of Molecular Liquids, 2020, 310, 113089.	2.3	11
6244	FT-IR and FT-Raman investigation, quantum chemical studies, molecular docking study and antimicrobial activity studies on novel bioactive drug of		

#	ARTICLE	IF	CITATIONS
6258	Rate-Limiting Steps in the Intramolecular C-H Activation of Ruthenium N-Heterocyclic Carbene Complexes. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3609-3617.	1.1	7
6259	Computational Evidence for Homonuclear Ge ^I Ge ^I Dative Bonds. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3795-3804.	1.1	3
6260	Quantum Chemical Support on the Two-Dimensional Assembly of Porphyrin Rings in the Application of Energy-Storage Devices. <i>Journal of Physical Chemistry C</i> , 2020, 124, 9712-9723.	1.5	7
6261	Balancing the Seesaw: Investigation of a Separator to Grasp Polysulfides with Diatomic Chemisorption. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 20596-20604.	4.0	12
6262	The First Quantitative Synthesis of a Closed Three-Link Chain (6 ₁ ³) Using Coordination and Noncovalent Interactions-Driven Self-Assembly. <i>Journal of the American Chemical Society</i> , 2020, 142, 9327-9336.	6.6	35
6263	Hypervalent Iodine(III) Compounds as Biaxial Halogen Bond Donors. <i>Journal of the American Chemical Society</i> , 2020, 142, 8633-8640.	6.6	67
6264	A DFT study to probe homo-conjugated norbornylogous bridged spacers in dye-sensitized solar cells: an approach to suppressing agglomeration of dye molecules. <i>RSC Advances</i> , 2020, 10, 15307-15319.	1.7	16
6265	A designer 32-electron superatomic CBe ₈ H ₁₂ cluster: core-shell geometry, octacoordinate carbon, and cubic aromaticity. <i>New Journal of Chemistry</i> , 2020, 44, 7286-7292.	1.4	9
6266	Enabling dynamic ultralong organic phosphorescence in molecular crystals through the synergy between intramolecular and intermolecular interactions. <i>Journal of Materials Chemistry C</i> , 2020, 8, 7384-7392.	2.7	27
6267	HERFD-XANES probes of electronic structures of iron ^{II/III} carbene complexes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9067-9073.	1.3	6
6268	Computational insight into the halogen bonded self-assembly of hexa-coordinated metalloporphyrins. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11558-11566.	1.3	13
6269	Appraising spin-state energetics in transition metal complexes using double-hybrid models: accountability of SOS0-PBESCAN0-2(a) as a promising paradigm. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9388-9404.	1.3	10
6270	Ligand conformations and spin states in sandwich-type complexes of the split (3+2) five-electron donor hydrocarbon ligand bicyclo[3.2.1]octa-2,6-dien-4-yl (bcod). <i>New Journal of Chemistry</i> , 2020, 44, 6902-6915.	1.4	4
6271	Ultrafast broadband nonlinear optical properties and excited-state dynamics of two bis-chalcone derivatives. <i>RSC Advances</i> , 2020, 10, 15199-15205.	1.7	15
6272	Theoretical calculation of total electron-impact ionization cross section of C ₆ F ₁₂ O. <i>AIP Advances</i> , 2020, 10, 035217.	0.6	9
6273	Substitutional doping of black phosphorene with boron, nitrogen, and arsenic for sulfur trioxide detection: a theoretical perspective. <i>Journal of Sulfur Chemistry</i> , 2020, 41, 399-420.	1.0	27
6274	A density functional theory study of the stereoselectivity of Cu(OTf) ₂ -catalyzed [3+2] cycloaddition of trifluoromethylated <i>N</i> -acylhydrazones and isoprene: A concerted asynchronous mechanism. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26236.	1.0	1
6275	Cysteine dioxygenase catalyzed C-F bond cleavage: An in silico approach. <i>Chemical Physics Letters</i> , 2020, 750, 137449.	1.2	4

#	ARTICLE	IF	CITATIONS
6276	Cascade Chromogenic System with Exponential Signal Amplification for Visual Colorimetric Detection of Acetone. <i>Analytical Chemistry</i> , 2020, 92, 6548-6554.	3.2	19
6277	Luminescent organic dyes containing a phenanthro[9,10- <i>D</i>]imidazole core and [Ir(N ^C)(N ^N)] ⁺ complexes based on the cyclometalating and diimine ligands of this type. <i>Dalton Transactions</i> , 2020, 49, 6751-6763.	1.6	19
6278	Gene reconstruction spandex with intrinsic antimicrobial activity. <i>Chemical Engineering Journal</i> , 2021, 404, 125152.	6.6	14
6279	Interatomic Interactions in Heterometallic Cubane-Type Clusters with {Mo ₃ S ₄ M} (M = Cu, Ni, Pd) Core. <i>Journal of Cluster Science</i> , 2021, 32, 415-421.	1.7	5
6280	Identification of new potential cyclooxygenase-2 inhibitors: insight from high throughput virtual screening of 18 million compounds combined with molecular dynamic simulation and quantum mechanics. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 1717-1734.	2.0	9
6281	Insight into the CO ₂ photoreduction mechanism over 9-hydroxyphenal-1-one (HPHN) carbon quantum dots. <i>Journal of Energy Chemistry</i> , 2021, 52, 269-276.	7.1	9
6282	Predicting reactivity to drug metabolism: beyond P450s modelling FMOs and UGTs. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 541-555.	1.3	13
6283	Kinetic and mechanistic investigation into odorant haloanisoles degradation process by peracetic acid combined with UV irradiation. <i>Journal of Hazardous Materials</i> , 2021, 401, 123356.	6.5	28
6284	Catalytic oxidation of dimethyl phthalate over titania-supported noble metal catalysts. <i>Journal of Hazardous Materials</i> , 2021, 401, 123274.	6.5	15
6285	Effect of polyethylene particles on dibutyl phthalate toxicity in lettuce (<i>Lactuca sativa</i> L.). <i>Journal of Hazardous Materials</i> , 2021, 401, 123422.	6.5	70
6286	A DFT Study of the Reaction between Benzopyrene Epoxide and C ₆₀ Derivatives as Possible Anticancer Activity. <i>Polycyclic Aromatic Compounds</i> , 2021, 41, 593-603.	1.4	2
6287	Geometry-Directed Self-Assembly of Polymeric Molecular Frameworks. <i>Angewandte Chemie</i> , 2021, 133, 2052-2057.	1.6	1
6288	Study on carboxyl groups in direct liquefaction of lignite: Conjoint analysis of theoretical calculations and experimental methods. <i>Fuel</i> , 2021, 286, 119298.	3.4	9
6289	Enhanced linear and nonlinear optical response of superhalogen (Al ₇) doped graphitic carbon nitride (g-C ₃ N ₄). <i>Optik</i> , 2021, 226, 165923.	1.4	46
6290	Nitrile group as IR probe to detect the structure and hydrogen-bond properties of piperidinium/pyrrolidinium based ionic liquids and acetonitrile mixtures. <i>Journal of Molecular Liquids</i> , 2021, 322, 114548.	2.3	4
6291	Chiral phosphoric acid catalyzed atroposelective C-H amination of arenes: mechanisms, origin and influencing factors of enantioselectivity. <i>Organic Chemistry Frontiers</i> , 2021, 8, 61-76.	2.3	3
6292	Influence of zinc and copper on the electronic, linear, and nonlinear optical properties of organometallic complexes with phenalenyl radical: a computational study. <i>Structural Chemistry</i> , 2021, 32, 835-845.	1.0	1
6293	Application of a 2D-QSAR with a sine normalization method for the biodegradation of fluoroquinolones to poison cyanobacteria. <i>Environmental Science and Pollution Research</i> , 2021, 28, 11302-11316.	2.7	6

#	ARTICLE	IF	CITATIONS
6294	A mechanism study on effects of bromide ion on mercury re-emission in WFGD slurry. <i>Chemical Engineering Journal</i> , 2021, 406, 127010.	6.6	6
6295	The theoretical study of excited-state intramolecular proton transfer of N, N,-bis (salicylidene)-(2-(3,4-diaminophenyl) benzothiazole). <i>Journal of Luminescence</i> , 2021, 230, 117741.	1.5	62
6296	Synthesis, structure, quantum computational and biological studies of novel thiophene derivatives. <i>Journal of Molecular Structure</i> , 2021, 1229, 129587.	1.8	5
6297	Strain-Driven Dyotropic Rearrangement: A Unified Ring-Expansion Approach to β -Methylene- γ -butyrolactones. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 4221-4230.	7.2	21
6298	Theoretical studies on how to tune the σ -hole pnictogen bonds by substitution and cooperative effects. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26531.	1.0	7
6299	Mechanistic insight into the degradation of ibuprofen in UV/H ₂ O ₂ process via a combined experimental and DFT study. <i>Chemosphere</i> , 2021, 267, 128883.	4.2	31
6300	Theoretical predictions of the spectroscopic properties of BODIPY dyes: Effects of the fused aromatic and heteroaromatic rings at the b, g bonds. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 247, 119125.	2.0	2
6301	Understanding the unique reactivity patterns of nickel/JoSPOphos manifold in the nickel-catalyzed enantioselective C-H cyclization of imidazoles. <i>Chemical Science</i> , 2021, 12, 718-729.	3.7	19
6302	High contrast temperature-responsive luminescence materials from purely organic molecule with persistent room-temperature phosphorescence. <i>Journal of Luminescence</i> , 2021, 230, 117731.	1.5	5
6303	Theoretical prediction of the SO ₂ absorption by hollow silica based porous ionic liquids. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 103, 107788.	1.3	18
6304	A new CuII-dinuclear paddlewheel complex. Structural and electronic properties. <i>Journal of Molecular Structure</i> , 2021, 1224, 129172.	1.8	5
6305	A Stable [4,3]Pericyclic Diradicaloid: Synthesis, Structure, and Electronic Properties. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 4464-4469.	7.2	45
6306	Applying a novel advanced oxidation process of activated peracetic acid by CoFe ₂ O ₄ to efficiently degrade sulfamethoxazole. <i>Applied Catalysis B: Environmental</i> , 2021, 280, 119422.	10.8	145
6307	FT-IR and FT-Raman investigation, quantum chemical analysis and molecular docking studies of <i>Journal of Molecular Structure</i> , 2021, 1225, 129070.	1.8	14
6308	Structural and computational analyses of a 2-propanolammonium-chlorocadmate(II) assembly: Pivotal role of hydrogen bonding and H-H interactions. <i>Journal of Molecular Structure</i> , 2021, 1223, 128998.	1.8	14
6309	pysisyphus: Exploring potential energy surfaces in ground and excited states. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26390.	1.0	29
6310	Quantum computational, spectroscopic investigations on ampyra (4-aminopyridine) by dft/td-dft with different solvents and molecular docking studies. <i>Journal of Molecular Structure</i> , 2021, 1224, 129021.	1.8	42
6311	Molecular spectroscopic investigation, quantum chemical, molecular docking and biological evaluation of 2-(4-Chlorophenyl)-1-[3-(4-chlorophenyl)-5-[4-(propan-2-yl) phenyl]-3, 5-dihydro-1H-pyrazole-yl] ethanone. <i>Journal of Molecular Structure</i> , 2021, 1224, 129010.	1.8	6

#	ARTICLE	IF	CITATIONS
6312	Structure, bonding and spectroscopic characterization of yttrium (III) octanoyl-aminocarboxylates complexes: A DFT study. <i>Journal of Molecular Structure</i> , 2021, 1224, 129022.	1.8	1
6313	Synthesis, spectral characteristics, weak interactions, electronic properties and biological activity of (E)-1-(4-hydroxybenzylidene)-4-(3-isopropylphenyl)thiosemicarbazone: An experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2021, 1224, 129044.	1.8	6
6314	Disentangling Multiple Effects on Excited State Intramolecular Charge Transfer among Asymmetrical Tripartite PPIâ€”TPA/PCz Triads. <i>Chemistry - A European Journal</i> , 2021, 27, 1337-1345.	1.7	12
6315	Bimetallic Feâ€”Ir and Trimetallic Feâ€”Irâ€”Au Carbonyl Clusters Containing Hydride and/or Phosphine Ligands: Syntheses, Structures and DFT Studies. <i>Journal of Cluster Science</i> , 2021, 32, 743-753.	1.7	2
6316	Theoretical studies on the heterogeneous ozonolysis of syringol on graphene: Mechanism, kinetics and ecotoxicity assessment. <i>Chemical Engineering Journal</i> , 2021, 404, 126484.	6.6	13
6317	Identifying and explaining the regioselectivity of alkylation of 1,2,4-triazole-3-thiones using NMR, GIAO and DFT methods. <i>Journal of Molecular Structure</i> , 2021, 1223, 128973.	1.8	17
6318	The coplanar family of bis(nitrotriazoles) tetrazine and oxides based as energetic compounds. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26364.	1.0	2
6319	Highly efficient capture of odorous sulfur-based VOCs by ionic liquids. <i>Journal of Hazardous Materials</i> , 2021, 402, 123507.	6.5	20
6320	Revelation of ESIPT mechanism for the novel fluorescent system HNIBT in toluene and methanol solvents: A TDDFT study. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 59-66.	0.8	2
6321	Decomposition of 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105): From thermodynamics to kinetics. <i>International Journal of Chemical Kinetics</i> , 2021, 53, 242-249.	1.0	2
6322	Insight into incident photon to current conversion efficiency in chlorophylls. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26483.	1.0	5
6323	Synthesis of the Three Mixed-ligand Metal Complexes and One Organic Salt of 3,5-Dinitrobenzoic Acid for Biopharmaceutical Optimization Through Monoethanolamine: Structures and DFT Studies of Complexes. <i>Journal of Chemical Crystallography</i> , 2021, 51, 405-417.	0.5	4
6324	Visible light absorption by perylene diimide for synergistic persulfate activation towards efficient photodegradation of bisphenol A. <i>Applied Catalysis B: Environmental</i> , 2021, 282, 119579.	10.8	97
6325	Structural effects on thermodynamic behavior and hydrogen bond interactions of waterâ€”ionic liquid systems. <i>Chemical Engineering Science</i> , 2021, 230, 116186.	1.9	23
6326	Rapid electrochemical reduction of a typical chlorinated organophosphorus flame retardant on copper foam: degradation kinetics and mechanisms. <i>Chemosphere</i> , 2021, 264, 128515.	4.2	13
6327	Phenolic matrix effect on aroma formation of terpenes during simulated wine fermentation â€” Part I: Phenolic acids. <i>Food Chemistry</i> , 2021, 341, 128288.	4.2	28
6328	Effects of zwitterionic surfactant adsorption on the component distribution in the crude oil droplet: A molecular simulation study. <i>Fuel</i> , 2021, 283, 119252.	3.4	36
6329	Synthesis, experimental and computational study of a non-centrosymmetric material 3-methylbenzylammonium trioxonitrate. <i>Journal of Molecular Structure</i> , 2021, 1225, 129132.	1.8	35

#	ARTICLE	IF	CITATIONS
6330	Orthogonal hydrogen and halogen bonding facilitate intermolecular charge transfer between barbutaric acid and molecular halogens over g-C ₃ N ₄ nanosheet: A comparative experimental and DFT calculations. <i>Journal of Molecular Structure</i> , 2021, 1223, 129211.	1.8	7
6331	Synthesis of 1-aryl-3-methylsulfanyl-5-amino-1,2,4-triazoles and their analysis by spectroscopy, X-ray crystallography and theoretical calculations. <i>Journal of Molecular Structure</i> , 2021, 1226, 129317.	1.8	14
6332	Theoretical determination of a reaction intermediate: Fukui function analysis, dual reactivity descriptor and activation energy. <i>Journal of Molecular Structure</i> , 2021, 1227, 129369.	1.8	33
6333	Substituent effect on ESIPT and hydrogen bond mechanism of N-(8-Quinoly) salicylaldimine: A detailed theoretical exploration. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 245, 118937.	2.0	11
6334	Sensing mechanism of fluorogenic urea with fluoride in solvent media: A new fluorescence quenching mechanism. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 118992.	2.0	6
6335	Investigations of adsorption behavior and anti-inflammatory activity of glycine functionalized Al ₁₂ N ₁₂ and Al ₁₂ ON ₁₁ fullerene-like cages. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 119023.	2.0	23
6336	A high potential biphenol derivative cathode: toward a highly stable air-insensitive aqueous organic flow battery. <i>Science Bulletin</i> , 2021, 66, 457-463.	4.3	31
6337	Activation of peroxymonosulfate by CoFeNi layered double hydroxide/graphene oxide (LDH/GO) for the degradation of gatifloxacin. <i>Separation and Purification Technology</i> , 2021, 255, 117685.	3.9	53
6338	The interplay between anion-π and H-bonding interactions in X ⁿ⁺ -Triazine ⁿ⁺ ·(HF) _n (HCl) _{3-n} (X = F, Cl) J. ETQqO	0.8	0
6339	Study on the mechanism of catalytic synthesis of dimethyldichlorosilane by AlCl ₃ /MIL-53(Al)@β-Al ₂ O ₃ . <i>Applied Organometallic Chemistry</i> , 2021, 35, .	1.7	8
6340	Magnesium of bare and halides encapsulated B40 fullerenes for their potential application as promising anode materials for Mg-ion batteries. <i>Applied Surface Science</i> , 2021, 538, 148060.	3.1	27
6341	Pentavalent P=O phosphorus bonding with associated Cl=O halogen bonding in influencing the geometry of POCl ₃ -Phenylacetylene heterodimers: Evidence from matrix isolation infrared spectroscopy and ab initio computations. <i>Journal of Molecular Structure</i> , 2021, 1224, 129288.	1.8	8
6342	Analysis of supramolecular interactions directing crystal packing of a combination of XRD, MEP, NBO, QTAIM, and NCI analyses. <i>Journal of Molecular Structure</i> , 2021, 1228, 129438.	1.8	3
6343	Pyridone Modified Cellulosic Adsorbent for Selective Segregation of Organic Dyes from Aqueous Solution. <i>Australian Journal of Chemistry</i> , 2021, 74, 230.	0.5	1
6344	Shedding light on the factors controlling the mechanism, selectivity and reactivity of the Diels-Alder reactions between substituted pyridinones and ethylenes: a MEDT study. <i>Molecular Physics</i> , 2021, 119, e1828635.	0.8	4
6345	Kinetics and column adsorption study of diclofenac and heavy-metal ions removal by amino-functionalized lignin microspheres. <i>Journal of Industrial and Engineering Chemistry</i> , 2021, 93, 302-314.	2.9	38
6346	Switchable and adjustable AIE activity of Pt(II) complexes achieving swift-responding and highly sensitive oxygen sensing. <i>Sensors and Actuators B: Chemical</i> , 2021, 326, 128987.	4.0	20
6347	Microwave Detection of Wet Triacetone Triperoxide (TATP): Non-Covalent Forces and Water Dynamics. <i>Chemistry - A European Journal</i> , 2021, 27, 1680-1687.	1.7	10

#	ARTICLE	IF	CITATIONS
6348	On the Role of Alkali-Metal-Like Superatom Al ₁₂ P in Reduction and Conversion of Carbon Dioxide. <i>Chemistry - A European Journal</i> , 2021, 27, 1039-1045.	1.7	14
6349	The adsorption of bromochlorodifluoromethane on pristine and Ge-doped silicon carbide nanotube: a PBC-DFT, NBO, and QTAIM study. <i>Structural Chemistry</i> , 2021, 32, 481-494.	1.0	27
6350	Exploration of adsorption mechanism of 2-phosphonobutane-1,2,4-tricarboxylic acid onto kaolinite and montmorillonite via batch experiment and theoretical studies. <i>Journal of Hazardous Materials</i> , 2021, 403, 123810.	6.5	94
6351	Synthesis, spectra, electronic structure, molecular docking and cytotoxicity investigation on 2-(piperidin-1-ylmethyl)-isoindoline-1,3-dione – A Mannich base system. <i>Journal of Molecular Structure</i> , 2021, 1224, 129151.	1.8	5
6352	A novel ratiometric fluorescent probe for selective detection and imaging of H ₂ S. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 118959.	2.0	29
6353	Cyclo[18]carbon as an ultra-elastic molecular O-ring with unique mechanical properties. <i>Carbon</i> , 2021, 171, 96-103.	5.4	40
6354	Intermolecular interaction characteristics of the all-carboatomic ring, cyclo[18]carbon: Focusing on molecular adsorption and stacking. <i>Carbon</i> , 2021, 171, 514-523.	5.4	333
6355	MEDT study of the 1,3-DC reaction of diazomethane with Psilostachyin and investigation about the interactions of some pyrazoline derivatives with protease (Mpro) of nCoV-2. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 102, 107763.	1.3	20
6356	The nonlinear optics property of heterodinuclear (Li and Na) sexipyridine helix: A density functional theory study. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26478.	1.0	2
6357	Photoexcited single metal atom catalysts for heterogeneous photocatalytic H ₂ O ₂ production: Pragmatic guidelines for predicting charge separation. <i>Applied Catalysis B: Environmental</i> , 2021, 282, 119589.	10.8	74
6358	Structures and non-covalent interaction behaviours of binary systems containing the ionic liquid 1-(2-hydroxyethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)imide and chloroform. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 244, 118843.	2.0	1
6359	Nature of the bond, reduction potential, and solvation properties of ruthenium nitrosyl complexes of the type <i>trans</i> -[Ru(NH ₃) ₃ (L)(NO)] ^{2+/3+} and [Ru(salen)(L)(NO)] ^{2+/3+} in different charge and spin states. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26476.	1.0	3
6360	Mechanistic insights into the reaction Cp ₂ Nb(CO)H (Cp ⁻ =η ⁻⁵ -C ₅ H ₅) with acetylenedicarboxylic acid (ADCA): DFT studies. <i>Inorganica Chimica Acta</i> , 2021, 514, 119990.	1.2	0
6361	Facile synthesis of solar light-driven Z-scheme Ag ₂ CO ₃ /TNS-001 photocatalyst for the effective degradation of naproxen: Mechanisms and degradation pathways. <i>Separation and Purification Technology</i> , 2021, 254, 117598.	3.9	21
6362	The adsorption of bromochlorodifluoromethane on pristine, Al, Ga, P, and As-doped boron nitride nanotubes: A study involving PBC-DFT, NBO analysis, and QTAIM. <i>Computational and Theoretical Chemistry</i> , 2021, 1193, 113047.	1.1	22
6363	Noncovalent functionalization of graphene through physisorption of 1,1-diamino-2,2-dinitroethene: Impacts of and cooperativity between hydrogen bond and π-π interaction. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 148, 109736.	1.9	4
6364	Dithieno[<i>a</i>], [<i>e</i>]pentalenes: Highly Antiaromatic Yet Stable π-Electron Systems without Bulky Substituents. <i>Chemistry - A European Journal</i> , 2021, 27, 1638-1647.	1.7	30
6365	Temozolomide binding to Cucurbit[7]uril: QTAIM, NCI-RDC and NBO analyses. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2021, 99, 61-77.	0.9	16

#	ARTICLE	IF	CITATIONS
6366	The direct evidence for ESPT route and ICT emission of N6-Methyladenine in aqueous solution. <i>Journal of Luminescence</i> , 2021, 229, 117698.	1.5	26
6367	A molecular electron density theory study of polar Diels-Alder reaction between 2,4-dimethyl-5-ethoxyoxazole and ethyl 4,4-trifluorocrotonate. <i>Structural Chemistry</i> , 2021, 32, 805-817.	1.0	2
6368	Triazine-cored covalent organic framework for ultrasensitive detection of polybrominated diphenyl ethers from real samples: Experimental and DFT study. <i>Journal of Hazardous Materials</i> , 2021, 403, 123917.	6.5	34
6369	Structural, physico-chemical landscapes, ground state and excited state properties in different solvent atmosphere of Avapritinib and its ultrasensitive detection using SERS/GERS on self-assembly formation with graphene quantum dots. <i>Journal of Molecular Liquids</i> , 2021, 322, 114555.	2.3	28
6370	Chloroquine and hydroxychloroquine inhibitors for COVID-19 sialic acid cellular receptor: Structure, hirshfeld atomic charge analysis and solvent effect. <i>Journal of Molecular Structure</i> , 2021, 1228, 129459.	1.8	6
6371	Complexes of Fe(III)-organic pollutants that directly activate Fenton-like processes under visible light. <i>Applied Catalysis B: Environmental</i> , 2021, 283, 119663.	10.8	87
6372	Amino, nitro, chloro, hydroxyl and methyl substitutions may inhibit the binding of PAHs with DNA. <i>Environmental Pollution</i> , 2021, 268, 115798.	3.7	13
6373	Significantly promoted SO ₂ uptake by the mixture of N-methylated ethylene imine polymer and 1-ethyl-3-methylimidazolium tetrazolate. <i>Journal of Hazardous Materials</i> , 2021, 404, 124101.	6.5	11
6374	DFT computational investigation of the reaction behavior of polyamidoamine dendrimer as nanocarrier for delivery of melphalan anticancer drug. <i>Journal of Molecular Liquids</i> , 2021, 323, 114625.	2.3	8
6375	Role of imidazole edge to edge supramolecular interaction in the crystal packing of Cu(II)(SCN ⁻) ₂ (imidazole) ₂ complex: A novel variety of supramolecular interaction revealed by CCDC database analysis and explored through DFT computational studies. <i>Journal of Molecular Structure</i> , 2021, 1227, 129513.	1.8	3
6376	Two dinuclear copper (II) and nickel (II) complexes based on 4-(diethylamino)salicylaldehyde: X-ray structures, spectroscopic, electrochemical, antibacterial, Hirshfeld surfaces analyses, and time-dependent density functional theory calculations. <i>Applied Organometallic Chemistry</i> , 2021, 35, .	1.7	15
6377	Roles of defects and linker exchange in phosphate adsorption on UiO-66 type metal organic frameworks: Influence of phosphate concentration. <i>Chemical Engineering Journal</i> , 2021, 405, 126681.	6.6	61
6378	Pyridoxal derived AIEgen as a fluorescent pH sensor. <i>Dyes and Pigments</i> , 2021, 184, 108844.	2.0	35
6379	Effect of positional isomerism on electron-transfer photochromism and photoluminescence of two pyromellitic diimide-based organic molecules. <i>Dyes and Pigments</i> , 2021, 186, 108941.	2.0	16
6380	β-Cyclodextrin functionalized SBA-15 via amide linkage as a super adsorbent for rapid removal of methyl blue. <i>Journal of Colloid and Interface Science</i> , 2021, 583, 100-112.	5.0	40
6381	A new mixed-ligand lanthanum(III) complex with salicylic acid and 1,10-phenanthroline: Synthesis, characterization, antibacterial activity, and underlying mechanism. <i>Journal of Molecular Structure</i> , 2021, 1225, 129096.	1.8	23
6382	An analysis of structural, spectroscopic, quantum chemical and in silico studies of ethyl 3-[(pyridin-2-yl)amino]propanoate: A potential thrombin inhibitor. <i>Journal of Molecular Structure</i> , 2021, 1226, 129378.	1.8	4
6383	Triazolotriazine-based thermally activated delayed fluorescence materials for highly efficient fluorescent organic light-emitting diodes (TSF-OLEDs). <i>Science Bulletin</i> , 2021, 66, 441-448.	4.3	40

#	ARTICLE	IF	CITATIONS
6402	A novel approach for efficient extraction and enrichment of phytochemicals with CO ₂ -based switchable-solvent from pigeon pea leaves. <i>Journal of Cleaner Production</i> , 2021, 284, 124629.	4.6	8
6403	Removal of metal-cyanide complexes and recovery of Pt(II) and Pd(II) from wastewater using an alkali-tolerant metal-organic resin. <i>Journal of Hazardous Materials</i> , 2021, 406, 124315.	6.5	27
6404	Surface modification of graphene by coupling with electron deficient radicals. <i>Journal of Solid State Chemistry</i> , 2021, 294, 121851.	1.4	15
6405	Fractionation of lignin using organic solvents: A combined experimental and theoretical study. <i>International Journal of Biological Macromolecules</i> , 2021, 168, 792-805.	3.6	39
6406	The ratiometric detection and mechanism of three typical phosphonates by quercetin-based fluorescent probe with low detection limits. <i>Journal of Luminescence</i> , 2021, 231, 117778.	1.5	6
6407	Effects of solvent polarity on excited state behaviors for the two intramolecular proton-transfer-site 4,4'-((hydrazine-1,2-diylidene-bis(methanylylidene))-bis(3-hydroxybenzoic acid) compound. <i>Journal of Luminescence</i> , 2021, 232, 117800.	1.5	43
6408	Spacer group-controlled luminescence and response of C ₃ -symmetric triphenylamine derivatives towards force stimuli. <i>CrystEngComm</i> , 2021, 23, 202-209.	1.3	9
6409	Isomers of B ₂ N-Fused Dibenzoazaacenes: How B ₂ N Affects Optoelectronic Properties and Device Behaviors?. <i>Chemistry - A European Journal</i> , 2021, 27, 4364-4372.	1.7	22
6410	Exploring the interaction of amino acid-based ionic liquids in water and organic solvents: Insight from MD simulations and QM calculations. <i>Journal of Molecular Liquids</i> , 2021, 327, 114867.	2.3	2
6411	When are two hydrogen bonds better than one? Accurate first-principles models explain the balance of hydrogen bond donors and acceptors found in proteins. <i>Chemical Science</i> , 2021, 12, 1147-1162.	3.7	17
6412	Self-aggregating cationic-chains enable alkaline stable ion-conducting channels for anion-exchange membrane fuel cells. <i>Journal of Materials Chemistry A</i> , 2021, 9, 327-337.	5.2	116
6413	Quasi-planar B5O sheet as a potential molecular sensor for NO ₂ : A DFT study. <i>Materials Chemistry and Physics</i> , 2021, 260, 124104.	2.0	4
6414	Towards H ₂ O catalyzed N ₂ -fixation over TiO ₂ doped Ru clusters (<i>n</i> = 5, 6): a mechanistic and kinetic approach. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1527-1538.	1.3	17
6415	Structural basis for tailor-made selective PI3K $\hat{\pm}$ / $\hat{\beta}$ inhibitors: a computational perspective. <i>New Journal of Chemistry</i> , 2021, 45, 373-382.	1.4	4
6416	The hydrogen-bond configuration modulates the energy transfer efficiency in helical protein nanotubes. <i>Nanoscale</i> , 2021, 13, 991-999.	2.8	6
6417	Interplay of Hückel and Möbius Aromaticity in Metal-Metal Quintuple Bonded Complexes of Cr, Mo, and W with Amidinate Ligand: Ab-initio DFT and Multireference Analysis*. <i>ChemPhysChem</i> , 2021, 22, 298-311.	1.0	3
6418	Studies on the photofading of alizarin, the main component of madder. <i>Dyes and Pigments</i> , 2021, 185, 108940.	2.0	28
6419	Insights into quaternary ammonium-based ionic liquids series with tetrafluoroborate anion for CO ₂ capture. <i>Journal of Molecular Liquids</i> , 2021, 327, 114857.	2.3	12

#	ARTICLE	IF	CITATIONS
6420	Structural characterization, DFT calculations, ADMET studies, antibiotic potentiating activity, evaluation of efflux pump inhibition and molecular docking of chalcone (E)-1-(2-hydroxy-3,4,6-trimethoxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one. Journal of Molecular Structure, 2021, 1227, 129692.	1.8	12
6421	Computational Screening of Multicomponent Solid Forms of 2-Aryl-Propionate Class of NSAID, Zaltoprofen, and Their Experimental Validation. Crystal Growth and Design, 2021, 21, 449-461.	1.4	13
6422	Effective corrosion inhibition of mild steel by eco-friendly thiourea functionalized glucosamine derivatives in acidic solution. Journal of Colloid and Interface Science, 2021, 585, 355-367.	5.0	42
6423	Molecular structure, spectroscopic (FT-IR, FT-Raman, NMR), HOMO-LUMO, chemical reactivity, AIM, ELF, LOL and Molecular docking studies on 1-Benzyl-4-(N-Boc-amino)piperidine. Journal of Molecular Structure, 2021, 1230, 129657.	1.8	72
6424	Chaetolactam A, an Azaphilone Derivative from the Endophytic Fungus <i>Chaetomium</i> sp. g1. Journal of Organic Chemistry, 2021, 86, 475-483.	1.7	13
6425	Extended gate-type organic transistor functionalized by molecularly imprinted polymer for taurine detection. Nanoscale, 2021, 13, 100-107.	2.8	22
6426	Corrosion inhibitor in CO ₂ -O ₂ -containing environment: Inhibition effect and mechanisms of Bis(2-ethylhexyl) phosphate for the corrosion of carbon steel. Corrosion Science, 2021, 179, 109173.	3.0	32
6427	Embedded Cluster Study of the Co-Adsorption of HCl and H ₂ O on PuO ₂ Surfaces. Journal of Nuclear Materials, 2021, 545, 152623.	1.3	4
6428	In Situ Observation of Non-Classical 2-Norbornyl Cation in Confined Zeolites at Ambient Temperature. Angewandte Chemie - International Edition, 2021, 60, 4581-4587.	7.2	16
6429	A molecular electron density theory study for [3+2] cycloaddition reactions of 1-pyrroline oxide with disubstituted acetylenes leading to bicyclic 4-isoxazolines. International Journal of Quantum Chemistry, 2021, 121, e26503.	1.0	11
6430	Effects of Different Ring-Expanded Strategies for Nonfullerene Acceptors in Organic Photovoltaics under Donor and Acceptor Excitation. Solar Rrl, 2021, 5, 2000615.	3.1	8
6431	An acylhydrazone coumarin as chemosensor for the detection of Ni ²⁺ with excellent sensitivity and low LOD: Synthesis, DFT calculations and application in real water and living cells. Inorganica Chimica Acta, 2021, 516, 120144.	1.2	12
6432	Assessment of the inhibitive behavior of a triazole based Schiff base compound in acidic media; an experimental and theoretical approach. Journal of Molecular Structure, 2021, 1227, 129700.	1.8	11
6433	Experimental and theoretical study on removal of organic contaminants with various function groups via suspension freezing separation. Separation and Purification Technology, 2021, 259, 118176.	3.9	5
6434	Synthesis of Dihydroquinolines as Scaffolds for Fluorescence Sensing of Hydroxyl Radical. Organic Letters, 2021, 23, 135-139.	2.4	17
6435	Theoretical investigation on the mechanism and enantioselectivity of organocatalytic asymmetric Povarov reactions of anilines and aldehydes. International Journal of Quantum Chemistry, 2021, 121, e26574.	1.0	5
6436	Hydrogen abstraction of alkyl radicals from polycyclic aromatic hydrocarbons and heterocyclic aromatic hydrocarbons. Chemical Engineering Science, 2021, 232, 116342.	1.9	7
6437	Efficient self-photo-degradation of cationic textile dyes involved triethylamine and degradation pathway. Chemosphere, 2021, 266, 129209.	4.2	19

#	ARTICLE	IF	CITATIONS
6438	Structure, conformational dynamics, quantum mechanical studies and potential biological activity analysis of multiple sclerosis medicine ozanimod. <i>Journal of Molecular Structure</i> , 2021, 1227, 129685.	1.8	37
6439	Density, Viscosity, and Electrical Conductivity of 1-Alkyl-3-methylimidazolium Dicyanamide Ionic Liquids. <i>Journal of Chemical & Engineering Data</i> , 2021, 66, 480-493.	1.0	20
6440	Cascade Hydrogenation&Cyclization of Levulinic Acid into Î³-Valerolactone Catalyzed by Half-Sandwich Iridium Complexes: A Mechanistic Insight from Density Functional Theory. <i>Journal of Organic Chemistry</i> , 2021, 86, 674-682.	1.7	7
6441	Efficient Cu Decorated Inorganic B ₁₂ P ₁₂ Nanoclusters for Sensing Toxic COCl ₂ Gas: A Detailed DFT Study. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 85-97.	1.0	36
6442	Theoretical design and exploration of low-valent uranium metallocenes via manipulating cyclopentadienyl substituent. <i>Computational and Theoretical Chemistry</i> , 2021, 1195, 113107.	1.1	6
6443	Refined standards for simulating UV&vis absorption spectra of acceptors in organic solar cells by TD-DFT. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 407, 113087.	2.0	9
6444	Possible Mechanisms and Origin of Selectivities for Phosphine&Catalyzed [2+n] (n=3, 4) Annulations of Saturated Amines and Î&Acetoxy Allenates. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 619-625.	1.3	10
6445	An Insight into Non&Covalent Interactions on the Bicyclo[1.1.1]pentane Scaffold. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 1113-1122.	1.2	8
6446	Contributions of alanine and serine to sulfuric acid-based homogeneous nucleation. <i>Atmospheric Environment</i> , 2021, 246, 118139.	1.9	2
6447	Tricyclic nitrogen-rich cation salts based on 1,2,3-triazole: Chemically stable and insensitive candidates for novel gas generant. <i>Chemical Engineering Journal</i> , 2021, 408, 128021.	6.6	15
6448	Structural and electronic properties of Pt _n Si ₁₂ (n=1&4) clusters: Quantum chemical calculations. <i>Computational and Theoretical Chemistry</i> , 2021, 1195, 113091.	1.1	1
6449	Elucidating the co-transport of bisphenol A with polyethylene terephthalate (PET) nanoplastics: A theoretical study of the adsorption mechanism. <i>Environmental Pollution</i> , 2021, 270, 116192.	3.7	37
6450	Inclusion complexation of chloroquine with Î± and Î²-cyclodextrin: Theoretical insights from the new B97-3c composite method. <i>Journal of Molecular Structure</i> , 2021, 1227, 129696.	1.8	21
6451	The spectral-shapes of absorption, emission, ECD and CPL of a fluorene-fused [7]helicene: Vibronic effect and solvent inhomogenous broadening. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 249, 119293.	2.0	3
6452	Unusual Reactivity and Photophysical Properties of Platinum(II) Pincer Complexes Containing 6,6'-Diphenyl&2,2'-bipyridine Ligands. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 117-125.	1.0	1
6453	Atomic insights into the sintering process of polycyclic aromatic hydrocarbon clusters. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 1181-1188.	2.4	9
6454	Binding properties of cucurbit[7]uril to neutral and protonated amino acids: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26491.	1.0	5
6455	Probing the halogen bond donation ability of multivalent At-center in AtX _n (X=Cl, Br, I; n=1, 3). <i>Tj ETQq1 1 0.784314 rgBT /Over</i>	1.1	11

#	ARTICLE	IF	CITATIONS
6456	Perspective on ultramicroporous carbon as sulphur host for Li-S batteries. <i>Journal of Energy Chemistry</i> , 2021, 59, 242-256.	7.1	40
6457	Reactivity and mechanism between OH and phenolic pollutants: Efficiency and DFT calculation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 407, 113025.	2.0	12
6458	Degradation of odorous sulfide compounds by different oxidation processes in drinking water: Performance, reaction kinetics and mechanism. <i>Water Research</i> , 2021, 189, 116643.	5.3	13
6459	Ultra-Fast Computation of Excited-States Spectra for Large Systems: Ultraviolet and Fluorescence Spectra of Proteins. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2021, 13, 140-146.	2.2	2
6460	A molecular dynamics study of the binding effectiveness between undoped conjugated polymer binders and tetra-sulfides in lithium-sulfur batteries. <i>Composites Part B: Engineering</i> , 2021, 206, 108531.	5.9	9
6461	Activated carbon synthesized from Sargassum (sp) for adsorption of caffeine: Understanding the adsorption mechanism using molecular modeling. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 104795.	3.3	27
6462	Theoretical design and characterization of D-A1-A based organic dyes for efficient DSSC by altering promising acceptor (A1) moiety. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 407, 113048.	2.0	28
6463	Spontaneous assembly of microbial extracellular polymeric substances into microcapsules involved in trapping and immobilizing degradation-resistant oxoanions. <i>Science of the Total Environment</i> , 2021, 758, 143651.	3.9	5
6464	Similar but Not the Same: Difference in the Ability to Form Cocrystals between Nimesulide and the Pyridine Analogues. <i>Crystal Growth and Design</i> , 2021, 21, 287-296.	1.4	8
6465	Spectroscopic calculations, Hirshfeld surface analysis, and molecular docking studies of anticancer 6-(4-Aminophenyl)-4-(4-methoxyphenyl)-2-methoxynicotinonitrile. <i>Spectroscopy Letters</i> , 2021, 54, 51-64.	0.5	3
6466	Strain-Driven Dyotropic Rearrangement: A Unified Ring-Expansion Approach to β -Methylene- γ -butyrolactones. <i>Angewandte Chemie</i> , 2021, 133, 4267-4276.	1.6	2
6467	Stabilization mechanism of arsenic-sulfide slag by density functional theory calculation of arsenic-sulfide clusters. <i>Journal of Hazardous Materials</i> , 2021, 410, 124567.	6.5	9
6468	Coordination-promoted photoluminescence induced by configuration twisting regulation. <i>Journal of Luminescence</i> , 2021, 231, 117783.	1.5	2
6469	Insight of organic molecule dissolution and diffusion in cross-linked polydimethylsiloxane using molecular simulation. <i>Journal of Membrane Science</i> , 2021, 620, 118863.	4.1	24
6470	A DFT study of the adsorption of deep eutectic solvents onto graphene and defective graphene nanoflakes. <i>Journal of Molecular Liquids</i> , 2021, 327, 114850.	2.3	16
6471	A novel interaction mechanism in lignin pyrolysis: Phenolics-assisted hydrogen transfer for the decomposition of the β -O-4 linkage. <i>Combustion and Flame</i> , 2021, 225, 395-405.	2.8	44
6472	Mechanism of transition metal cluster catalysts for hydrogen evolution reaction. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 3484-3492.	3.8	17
6473	Computational investigation of vanillin- β -cyclodextrin inclusion complex: Electronic and intermolecular analysis. <i>Journal of Molecular Liquids</i> , 2021, 321, 114839.	2.3	11

#	ARTICLE	IF	CITATIONS
6474	Radical Cyclic [3]Daisy Chains. <i>CheM</i> , 2021, 7, 174-189.	5.8	26
6475	A dendrite-free composite Li metal anode enabled by lithiophilic Co, N codoped porous carbon nanofibers. <i>Journal of Power Sources</i> , 2021, 483, 229188.	4.0	26
6476	Theoretical insight into the hydrogenolysis mechanism of lignin dimer compounds based on experiments. <i>Renewable Energy</i> , 2021, 163, 1831-1837.	4.3	33
6477	Syntheses, formation mechanisms and structures of a series of linear diborazanes. <i>CrystEngComm</i> , 2021, 23, 404-410.	1.3	2
6478	Predicting the origin of selectivity in NHC-catalyzed ring opening of formylcyclopropane: a theoretical investigation. <i>Catalysis Science and Technology</i> , 2021, 11, 332-337.	2.1	28
6479	Vibrational Spectra and Molecular Vibrational Behaviors of All-Carboatomic Rings, cyclo[18]carbon and Its Analogues. <i>Chemistry - an Asian Journal</i> , 2021, 16, 56-63.	1.7	50
6480	Investigation and comparison of pristine/doped BN, AlN, and CN nanotubes as drug delivery systems for Tegafur drug: a theoretical study. <i>Structural Chemistry</i> , 2021, 32, 1019-1037.	1.0	14
6481	Theoretical investigation of phenol adsorption on functionalized graphene using DFT calculations for effective removal of organic contaminants from wastewater. <i>Journal of Molecular Liquids</i> , 2021, 324, 114777.	2.3	27
6482	A iridium(III) complex-based "turn-on" fluorescent probe with two recognition site for rapid detection of thiophenol and its application in water samples and human serum. <i>Tetrahedron</i> , 2021, 77, 131738.	1.0	7
6483	A theoretical investigation on decarboxylation mechanism of antibiotic para-aminosalicylic acid to highly toxic form meta-aminophenol. <i>Structural Chemistry</i> , 2021, 32, 1053-1060.	1.0	4
6484	Ni-BTC metal-organic framework loaded on MCM-41 to promote hydrodeoxygenation and hydrocracking in jet biofuel production. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 3898-3908.	3.8	21
6485	Ionic liquid-multi walled carbon nanotubes composite tablet for continuous adsorption of tetracyclines and heavy metals. <i>Journal of Cleaner Production</i> , 2021, 286, 124937.	4.6	36
6486	Structural features of nickel(II) mixed ligand complexes with mefenamic acid and nitrogen donor ligands. <i>Journal of Molecular Structure</i> , 2021, 1230, 129632.	1.8	5
6487	Molecular design of dibenzo[g,p]chrysene-based hole-transporting materials for perovskite solar cells: A theoretical study. <i>Synthetic Metals</i> , 2021, 271, 116631.	2.1	13
6488	On differences in substituent effects in substituted ethene and acetylene derivatives and their boranyl analogs. <i>Structural Chemistry</i> , 2021, 32, 285-296.	1.0	3
6489	Synthesis and comprehensive spectroscopic (X-ray, NMR, FTIR, UV-Vis), quantum chemical and molecular docking investigation of 3-acetyl-4-hydroxy-2-oxo-2H-chromen-7-yl acetate. <i>Journal of Molecular Structure</i> , 2021, 1225, 129256.	1.8	31
6490	A novel quinoxalinedione-bicapped tri-ruthenium carbonyl cluster [Ru ₃ (η -H) ₂ (CO) ₆ (η -3-HDCQX) ₂]: synthesis, characterization, anticancer activity and theoretical investigation of Ru-Ru and Ru-Ligand bonding interactions. <i>Polyhedron</i> , 2021, 193, 114889.	1.0	0
6491	Carboxyl-Dominant Oxygen Rich Carbon for Improved Sodium Ion Storage: Synergistic Enhancement of Adsorption and Intercalation Mechanisms. <i>Advanced Energy Materials</i> , 2021, 11, .	10.2	133

#	ARTICLE	IF	CITATIONS
6492	Investigation on a series of 3-nitro-1,2,4-triazol-5-one based energetic derivatives: Molecular design and screening. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26542.	1.0	1
6493	Construction of novel trimeric π -interaction subphthalocyanine-sensitized titanium dioxide for highly efficient photocatalytic degradation of organic pollutants. <i>Journal of Alloys and Compounds</i> , 2021, 855, 157458.	2.8	11
6494	Structural aspects, conformational preference and other physico-chemical properties of Artesunate and the formation of self-assembly with graphene quantum dots: A first principle analysis and surface enhancement of Raman activity investigation. <i>Journal of Molecular Liquids</i> , 2021, 325, 114810.	2.3	33
6495	Understanding endohedral behaviors of ten-electron atomic and cluster system inside C ₆₀ from first-principles. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 127, 114532.	1.3	7
6496	Theoretical and experimental findings regarding the electroanalysis of dienestrol in natural waters using a silver nanoparticles/single-walled carbon nanotubes-based amperometric sensor. <i>Journal of Electroanalytical Chemistry</i> , 2021, 880, 114821.	1.9	3
6497	Investigation on the preparation of 2,2-difluoroethylamine by amination of 1-halo-2,2-difluoroethane. <i>Journal of Fluorine Chemistry</i> , 2021, 242, 109690.	0.9	1
6498	Computational study on the metabolic activation mechanism of PeCDD by Cytochrome P450 1A1. <i>Journal of Hazardous Materials</i> , 2021, 405, 124276.	6.5	7
6499	A Stable [4,3]Pentacene Diradicaloid: Synthesis, Structure, and Electronic Properties. <i>Angewandte Chemie</i> , 2021, 133, 4514-4519.	1.6	12
6500	New N-heterocyclic mono- and disilavinylidene iron complexes by density functional theory. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4148.	0.9	0
6501	Effects of the atomic number of alkali atom and pore size of graphyne on the second-order nonlinear optical response of superalkali salts of graphynes OM 3 + @ GYs (M = Li, Na, and K). <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26477.	1.0	11
6502	Insight into the binding mode of HIF-2 agonists through molecular dynamic simulations and biological validation. <i>European Journal of Medicinal Chemistry</i> , 2021, 211, 112999.	2.6	7
6503	A DFT study of fulvic acid binding with bivalent metals: Cd, Cu, Mg, Ni, Pb, Zn. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 102, 107800.	1.3	18
6504	Theoretical study on the photocyclization reactivity mechanism in a diarylethene derivative with multicolour fluorescence modulation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 406, 113024.	2.0	3
6505	Rhodium-catalyzed C-H olefination of aromatic acids with unactivated olefins to achieve branched vinylated or linear allylated product: A theoretical investigation. <i>Molecular Catalysis</i> , 2021, 499, 111295.	1.0	4
6506	Structural investigations, quantum mechanical studies on proton and metal affinity and biological activity predictions of selpercatinib. <i>Journal of Molecular Liquids</i> , 2021, 325, 114765.	2.3	18
6507	Argentophilic interactions in argentine chalcogenides: First principles calculations and topological analysis of electron density. <i>Journal of Computational Chemistry</i> , 2021, 42, 242-247.	1.5	7
6508	Cisplatin under oriented external electric fields: A deeper insight into electrochemotherapy at the molecular level. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26578.	1.0	4
6509	Excited-state conformation capture by supramolecular chains towards triplet-involved organic emitters. <i>Chinese Chemical Letters</i> , 2021, 32, 1669-1674.	4.8	8

#	ARTICLE	IF	CITATIONS
6510	İ€-Conjugated polymeric light emitting diodes with sky-blue emission by employing thermally activated delayed fluorescence mechanism. <i>Chemical Engineering Journal</i> , 2021, 417, 128089.	6.6	24
6511	Dissociation of ZnO ring from Zn ₃ O ₃ cluster by CASSCF. <i>Chemical Physics</i> , 2021, 542, 111077.	0.9	1
6512	Design strategy for blue thermally activated delayed fluorescence: Position and methyl substitutions. <i>Chemical Physics Letters</i> , 2021, 764, 138260.	1.2	6
6513	Theoretical study on thienothiophene core hole-transporting materials in perovskite solar cells: S atom position effect. <i>Chemical Physics Letters</i> , 2021, 764, 138264.	1.2	15
6514	Contribution of methyl hydroperoxide to sulfuric acid-based new particle formation in the atmosphere. <i>Chemical Physics Letters</i> , 2021, 766, 138266.	1.2	2
6515	Imidazoporphyrins with appended polycyclic aromatic hydrocarbons: To conjugate or not to conjugate?. <i>Dyes and Pigments</i> , 2021, 186, 109042.	2.0	6
6516	Novel 2,5-bis(6-(trimethylammonium)hexyl)-3,6-diaryl-1,4-diketopyrrolo[3,4-c]pyrrole pigments as levelers for efficient electroplating applications. <i>Dyes and Pigments</i> , 2021, 186, 109064.	2.0	14
6517	Reaction activity and mechanism of R ³ -CH structure oxidation in coal self-heating. <i>Fuel</i> , 2021, 290, 119797.	3.4	22
6518	The validation of molecular interaction among dimer chitosan with urea and creatinine using density functional theory: In application for hemodialysis membrane. <i>International Journal of Biological Macromolecules</i> , 2021, 168, 339-349.	3.6	17
6519	Boosting electrochemical performance of activated carbon by tuning effective pores and synergistic effects of active species. <i>Journal of Colloid and Interface Science</i> , 2021, 587, 290-301.	5.0	30
6520	Theoretical studies on photocatalytic application of GO-ZnO nanocomposite for the reduction of methylene blue dye. <i>Materials Today: Proceedings</i> , 2021, 44, 4451-4456.	0.9	2
6521	Computational investigation on the chiral differentiation of D- and L-penicillamine by β -cyclodextrin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 248, 119277.	2.0	11
6522	A detailed computational study on binding of kinase inhibitors into β -cyclodextrin: inclusion complex formation. <i>Molecular Systems Design and Engineering</i> , 2021, 6, 80-92.	1.7	14
6523	An Ultimate Investigation on the Adsorption of Amantadine on Pristine and Decorated Fullerenes C ₅₉ X (X=Si, Ge, B, Al, Ga, N, P, and As): A DFT, NBO, and QTAIM Study. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 23-39.	1.0	28
6524	In Situ Observation of Nonclassical α -Norbornyl Cation in Confined Zeolites at Ambient Temperature. <i>Angewandte Chemie</i> , 2021, 133, 4631-4637.	1.6	2
6525	Enhanced photodegradation of sulfadimidine via PAA/g-C ₃ N ₄ -FeO polymeric catalysts under visible light. <i>Chemical Engineering Journal</i> , 2021, 413, 127456.	6.6	20
6526	Precisely regulating the Brønsted acidity and catalytic reactivity of novel allylic C-H acidic catalysts. <i>Fuel</i> , 2021, 289, 119845.	3.4	1
6527	Efficient all-solution-processing deep-red polymer light-emitting diodes (PLEDs) based on [Ir(dpqx) ₂ (N ⁺ O)]-heteroleptic complexes with asymmetric N ⁺ O-ancillary İ€-donors. <i>Journal of Luminescence</i> , 2021, 232, 117843.	1.5	1

#	ARTICLE	IF	CITATIONS
6528	Purine derivatives as high efficient eco-friendly inhibitors for the corrosion of mild steel in acidic medium: Experimental and theoretical calculations. <i>Journal of Molecular Liquids</i> , 2021, 323, 114809.	2.3	10
6529	Superiority of Iridium Photocatalyst and Role of Quinuclidine in Selective $\text{C}(\text{sp}^3)\text{-H}$ Alkylation: Theoretical Insights. <i>Journal of Organic Chemistry</i> , 2021, 86, 484-492.	1.7	3
6530	Understanding the Dipole Moment of Liquid Water from a Self-Attractive Hartree Decomposition. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6-12.	2.1	14
6531	Functioning Water-insoluble Ferrocenes for Aqueous Organic Flow Battery via Host-Guest Inclusion. <i>ChemSusChem</i> , 2021, 14, 745-752.	3.6	37
6532	Theoretical research of second generation molecular motor with unidirectional rotary motion. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4175.	0.9	1
6533	Single Si-doped fullerene as a catalyst in the oxygen reduction reaction: A quantum chemical insight. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26565.	1.0	5
6534	A water-soluble, adhesive and 3D cross-linked polyelectrolyte binder for high-performance lithium-sulfur batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 2375-2384.	5.2	30
6535	1,2,3-Triazole with linear and branched catenated nitrogen chains – The role of regiochemistry in energetic materials. <i>Chemical Engineering Journal</i> , 2021, 410, 128148.	6.6	42
6536	Electronic structure modelling of the edge-functionalisation of graphene by Mn_xO_y particles. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 514-527.	1.3	2
6537	Long-range exciton diffusion in a non-fullerene acceptor: approaching the incoherent limit. <i>Journal of Materials Chemistry C</i> , 2021, 9, 1419-1428.	2.7	15
6538	Nonconventional $\text{C}(\text{sp}^3)\text{-Cl}$ halogen bond in complexes of alkyl carbanions. <i>Chemical Physics Letters</i> , 2021, 763, 138195.	1.2	3
6539	Effect of additives on the oxidative stability and corrosivity of biodiesel samples derived from babassu oil and residual frying oil: An experimental and theoretical assessment. <i>Fuel</i> , 2021, 289, 119939.	3.4	11
6540	An oxygen-passivated vanadium cluster $[\text{V}@V_{10}O_{15}]^{+}$ with metal-metal coordination produced by reacting Vn^{+} with O_2 . <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 921-927.	1.3	9
6541	The density functional theory study of 2D nonmetallic catalyst defective graphene for acetylene hydration. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26561.	1.0	1
6542	Excitation Wavelength-Dependent Charge Generation Dynamics in a Nonfullerene Organic Solar Cell Interface. <i>Solar Rrl</i> , 2021, 5, 2000719.	3.1	6
6543	Physical mechanism and electric-magnetic interaction in ECD and ROA: Visualization methods on chirality. <i>Chemical Physics Letters</i> , 2021, 763, 138206.	1.2	1
6544	Efficient all-solution-processed near-infrared (NIR) polymer light-emitting diode (PLED) based on the $[\text{Ir}(\text{C}^{\wedge}\text{N}1)_2(\text{C}^{\wedge}\text{N}2)]$ -heteroleptic Ir(III)-complex $[\text{Ir}(\text{iqbt})_2(\text{Br-ppy})]$. <i>Journal of Luminescence</i> , 2021, 231, 117770.	1.5	1
6545	New insights on the ESIPT process based on solid-state data and state-of-the-art computational methods. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1146-1155.	1.3	26

#	ARTICLE	IF	CITATIONS
6546	Highly Efficient Orange-Red Thermally Activated Delayed Fluorescence Compounds Comprising Dual Dicyano-Substituted Pyrazine/Quinoxaline Acceptors. <i>ChemPlusChem</i> , 2021, 86, 95-102.	1.3	2
6547	Computational study of phosphate adsorption on Mg/Ca modified biochar structure in aqueous solution. <i>Chemosphere</i> , 2021, 269, 129374.	4.2	29
6548	Theoretical insights into the ring structures and aromaticity of neutral and ionic $(\text{SiO})_0, \pm(n=2-4)$. <i>Chemical Physics</i> , 2021, 541, 111047.	0.9	6
6549	Study on the effect of substituents on the structure, volatility, and fluorescence of N-(Alkyl or Tj ETQq1 1 0.784314 rgBT /Overlock 121646.	0.8	3
6550	How the functional group substitution and solvent effects affect the antioxidant activity of (+)-catechin?. <i>Journal of Molecular Liquids</i> , 2021, 327, 114818.	2.3	14
6551	Liquid-liquid equilibria and mechanism exploration for the extraction of sulfides from FCC naphtha via organic solvent as extractant. <i>Journal of Molecular Liquids</i> , 2021, 327, 114821.	2.3	24
6552	Heteroatom Engineering of Hyper-Cross-Linked Polymers for Iodine Capture. <i>ACS Applied Polymer Materials</i> , 2021, 3, 209-215.	2.0	20
6553	Conformational changes in hydroxyl functional groups upon hydration: the case study of endo fenchol. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2179-2185.	1.3	13
6554	Theoretical prediction of Xe-containing polymer. <i>Molecular Physics</i> , 2021, 119, e1842532.	0.8	0
6555	Ultrastrong Regulation Effect of the Electric Field on the All-Carboatomic Ring Cyclo[18]Carbon**. <i>ChemPhysChem</i> , 2021, 22, 386-395.	1.0	62
6556	New Insight into the Aromaticity of $\langle i \rangle \text{cyclo} \langle /i \rangle \text{-N} \langle \text{sub} \rangle 5 \langle / \text{sub} \rangle \langle \text{sup} \rangle \hat{\text{c}} \langle / \text{sup} \rangle$ by Constructing 3D Arrays in Crystal Structures. <i>Crystal Growth and Design</i> , 2021, 21, 33-39.	1.4	7
6557	Investigating the Stabilizing Forces of Pentazolates Salts. <i>ACS Applied Energy Materials</i> , 2021, 4, 146-153.	2.5	17
6558	Enhancement of air-stability, π -stacking ability, and charge transport properties of fluoroalkyl side chain engineered n-type naphthalene tetracarboxylic diimide compounds. <i>RSC Advances</i> , 2021, 11, 57-70.	1.7	9
6559	Rotational spectrum and internal dynamics of the hydrogen-bonded pyrrole-pyridine aromatic pair. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 249, 119320.	2.0	1
6560	Coordination Environment Prevents Access to Intraligand Charge-Transfer States through Remote Substitution in Rhenium(I) Terpyridinedicarbonyl Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 1325-1333.	1.9	8
6561	Switching from an electride-like molecule to the molecular electride K-F6C6H6 driven by an oriented external electric field. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1443-1453.	1.3	7
6562	Dative $\langle i \rangle$ versus $\langle /i \rangle$ electron-sharing bonding in the isoelectronic argon compounds $\text{ArR} \langle \text{sup} \rangle + \langle / \text{sup} \rangle$ (R = $\text{CH} \langle \text{sub} \rangle 3 \langle / \text{sub} \rangle$, $\text{NH} \langle \text{sub} \rangle 2 \langle / \text{sub} \rangle$, OH, and F). <i>New Journal of Chemistry</i> , 2021, 45, 1363-1372.	1.4	1
6563	Quantum-chemical investigation of the phosphine ligand effects on the structure and electronic properties of a rhenabenzyne complex. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 776-784.	0.8	0

#	ARTICLE	IF	CITATIONS
6564	Antimony(III) Iodide Complexes with Pyridine: Structures and bonding via three pnictogen bonds. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2021, 647, 687-695.	0.6	5
6565	Chlorine drying with hygroscopic ionic liquids. <i>Green Energy and Environment</i> , 2021, 6, 350-362.	4.7	17
6566	Necessity of structural rearrangements for O O bond formation between O5 and W2 in photosystem II. <i>Journal of Energy Chemistry</i> , 2021, 57, 436-442.	7.1	7
6567	Excited state structure of isolated 4-cyanoindole from a combined Franck-Condon and rotational constants analysis. <i>Journal of Molecular Structure</i> , 2021, 1223, 129241.	1.8	5
6568	Sensitivity of ³¹ P NMR chemical shifts to hydrogen bond geometry and molecular conformation for complexes of phosphinic acids with pyridines. <i>Magnetic Resonance in Chemistry</i> , 2021, 59, 465-477.	1.1	4
6569	Highly Efficient InGaN Nanorods Photoelectrode by Constructing a Scheme Charge Transfer System for Unbiased Water Splitting. <i>Small</i> , 2021, 17, e2006666.	5.2	32
6570	TD-DFT Studies on sp- and sp ² -Hybridized Single Vacancy-Defected [60]Fullerene: Electronic Excitation and Nonlinear Optical Properties of C59 [9-4] and C59 [8-5] Isomers. <i>Journal of Physical Chemistry A</i> , 2021, 125, 106-114.	1.1	10
6571	Structurally Modelling the a Carboxylate Facial Triad with a Bulky N, O Phenolate Ligand. <i>Chemistry - A European Journal</i> , 2021, 27, 5191-5204.	1.7	8
6572	Sensing Mechanism of an Excited State Intermolecular Hydrogen Bond for Phthalimide: Indispensable Role of Dimethyl Sulfoxide. <i>Chinese Journal of Chemistry</i> , 2021, 39, 1113-1120.	2.6	3
6573	Synergistic effect of mesoporous graphitic carbon nitride and peroxydisulfate in visible light-induced degradation of atenolol: A combined experimental and theoretical study. <i>Chemical Engineering Journal</i> , 2021, 412, 127979.	6.6	18
6574	The spectroscopic and transition properties of phosphor selenium: MRCI+Q study including spin-orbit coupling. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021, 259, 107422.	1.1	2
6575	Theoretical investigation of adsorption mechanism of doxorubicin anticancer drug on the pristine and functionalized single-walled carbon nanotube surface as a drug delivery vehicle: A DFT study. <i>Journal of Molecular Liquids</i> , 2021, 322, 114890.	2.3	53
6576	Probing solvents effects on the absorption spectrum of oxo-centered carbonyl-triruthenium clusters. <i>Polyhedron</i> , 2021, 194, 114944.	1.0	2
6577	Heterogeneous activation of peroxymonosulfate by bimetallic MOFs for efficient degradation of phenanthrene: Synthesis, performance, kinetics, and mechanisms. <i>Separation and Purification Technology</i> , 2021, 259, 118217.	3.9	60
6578	Hydrophilic Sulfonated 2,9-Diamide-1,10-phenanthroline Endowed with a Highly Effective Ligand for Separation of Americium(III) from Europium(III): Extraction, Spectroscopy, and Density Functional Theory Calculations. <i>Inorganic Chemistry</i> , 2021, 60, 357-365.	1.9	34
6579	Revealing the biradicaloid nature inherited in the derivatives of thieno[3,4-c][1,2,5]thiadiazole: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1050-1061.	1.3	6
6580	Highly efficient solution processed OLEDs based on iridium complexes with steric phenylpyridazine derivative. <i>Inorganica Chimica Acta</i> , 2021, 516, 120100.	1.2	6
6581	Effects of microplastic on arsenic accumulation in <i>Chlamydomonas reinhardtii</i> in a freshwater environment. <i>Journal of Hazardous Materials</i> , 2021, 405, 124232.	6.5	39

#	ARTICLE	IF	CITATIONS
6582	Enhancement of air stability and photovoltaic performance in organic solar cells by structural modulation of bisamide-based donor-acceptor copolymers: A computational insight. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26524.	1.0	9
6583	Aldol Condensation-Polymerized <i>n</i> -Doped Conjugated Polyelectrolytes for High-Performance Nonfullerene Polymer Solar Cells. <i>Solar Rrl</i> , 2021, 5, .	3.1	12
6584	Cationic covalent organic framework for efficient removal of PFOA substitutes from aqueous solution. <i>Chemical Engineering Journal</i> , 2021, 412, 127509.	6.6	54
6585	A QSPR model for estimating Henry's law constant of H ₂ S in ionic liquids by ELM algorithm. <i>Chemosphere</i> , 2021, 269, 128743.	4.2	6
6586	Adsorption of sulfonamides on biochars derived from waste residues and its mechanism. <i>Journal of Hazardous Materials</i> , 2021, 406, 124291.	6.5	66
6587	DFT and QTAIM investigations of the adsorption of chlormethine anticancer drug on the exterior surface of pristine and transition metal functionalized boron nitride fullerene. <i>Journal of Molecular Liquids</i> , 2021, 323, 114627.	2.3	73
6588	A theoretical study describing the sensing mechanism of the novel triarylborane substituted naphthalimide molecule. <i>Journal of Molecular Structure</i> , 2021, 1228, 129443.	1.8	2
6589	Molecular structure, spectral (FT-IR, FT-Raman, Uv-Vis, and fluorescent) properties and quantum chemical analyses of azomethine derivative of 4-aminoantipyrine. <i>Journal of Molecular Structure</i> , 2021, 1227, 129512.	1.8	17
6590	Adsorption of greenhouse gases on the surface of covalent organic framework of porphyrin " An ab initio study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 126, 114448.	1.3	8
6591	Adsorption mechanism of decomposition gas of SF ₆ circuit breaker on MOF-505 analogue. <i>Vacuum</i> , 2021, 183, 109816.	1.6	15
6592	Geometry-Directed Self-Assembly of Polymeric Molecular Frameworks. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 2024-2029.	7.2	12
6593	The detailed electronic structure, spectroscopic features, and reactivity of dimethylanisoles. <i>Journal of Molecular Structure</i> , 2021, 1227, 129517.	1.8	4
6594	Similarities and Differences between Crystal and Enzyme Environmental Effects on the Electron Density of Drug Molecules. <i>Chemistry - A European Journal</i> , 2021, 27, 3407-3419.	1.7	10
6595	IRMOF α : Theoretical evaluation of aluminum doping on hydrogen, methane, and hydrogen sulfide adsorption. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26510.	1.0	6
6596	Theoretical designing and understanding of the performances of Bi π -H bridged organocatalysts by π -conjugated molecules in CO ₂ hydroboration. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26512.	1.0	3
6597	Stability of spherical molecular complexes: a theoretical study of self-assembled M12L24 nanoballs. <i>Structural Chemistry</i> , 2021, 32, 775-785.	1.0	2
6598	Defect-rich porous carbon with anti-interference capability for adsorption of bisphenol A via long-range hydrophobic interaction synergized with short-range dispersion force. <i>Journal of Hazardous Materials</i> , 2021, 403, 123705.	6.5	66
6599	Planar Tetracoordinate Silicon in Organic Molecules As Carbenoid-Type Amphoteric Centers: A Computational Study. <i>Chemistry - A European Journal</i> , 2021, 27, 1402-1409.	1.7	10

#	ARTICLE	IF	CITATIONS
6600	Structures and spectral properties of 5-phenyl-5H-benzo[b]phosphindole 5-oxide and its substituted derivatives: The substitutional effect study based on density functional theory calculations. <i>Journal of Molecular Structure</i> , 2021, 1226, 129401.	1.8	3
6601	Unraveling the effect of fluorine substitution on the hydrogen bonding interaction in the complexes of fluorosubstituted pyridines and acetic acid. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4151.	0.9	3
6602	The H ⁺ ions and static electric field effects on the adsorption and detection of cyanogen fluoride on the surface of boron nitride nanocage: a DFT, TD-DFT study. <i>Adsorption</i> , 2021, 27, 91-104.	1.4	6
6603	The effect of charge on the dihydrogen storage capacity of Sc ²⁺ @C ₆ H ₆ . <i>International Journal of Hydrogen Energy</i> , 2021, 46, 955-966.	3.8	7
6604	A new copper(II)-based layered coordination polymer: Crystal structure, topology, QTAIM analysis, experimental and theoretical magnetic properties based on DFT combined with broken-symmetry formalism (BS-DFT). <i>Polyhedron</i> , 2021, 193, 114881.	1.0	15
6605	Microsolvation of Co ²⁺ in water: Density functional theory calculations coupled with stochastic kicking method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 245, 118935.	2.0	8
6606	A computational investigation of the equilibrium geometries, energetics, vibrational frequencies, infrared intensities and Raman activities of C ₂ O _y (<i>y</i> = 3, 4) species. <i>Molecular Physics</i> , 2021, 119, e1837404.	0.8	1
6607	Theoretical investigation of aromaticity and charge transfer in emission process of triarylmethyl radicals as <i>scp</i> OLED materials. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26522.	1.0	6
6608	Photovoltaic and spectroscopic properties of bacteriochlorin-based photosensitizer: molecular approach. <i>Research on Chemical Intermediates</i> , 2021, 47, 1071-1085.	1.3	5
6609	Insight into the halogen-bonding interactions in the C ₆ F ₅ X- <i>Z</i> H ₃ (X = Cl, Br, I; Z = N, P, As) and C ₆ F ₅ I- <i>Z</i> (Ph) ₃ (Z = N, P, As) complexes. <i>Structural Chemistry</i> , 2021, 32, 767-774.	1.0	4
6610	Theoretical rationale for the role of the strong halogen bond in the design and synthesis of organic semiconductor materials. <i>Computational and Theoretical Chemistry</i> , 2021, 1194, 113074.	1.1	7
6611	Removal of malachite green dye from aqueous solution by adsorbents derived from polyurethane plastic waste. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 104704.	3.3	29
6612	Photophysical characteristics and photosensitizing abilities of thieno[3,2-b]thiophene-Based photosensitizers for photovoltaic and photocatalytic applications. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 406, 112979.	2.0	6
6613	Theoretical study on the detailed excited state triple proton transfer mechanism of cyclic 6-Azaindole trimer. <i>Chemical Physics Letters</i> , 2021, 762, 138137.	1.2	7
6614	Spectroscopy, lifetime, and charge-displacement of the methanol-noble gas complexes: An integrated experimental-theoretical investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 119049.	2.0	4
6615	Stabilization of the [cyclo ⁵ N] ⁻ anion by Lewis acid-base interactions. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26473.	1.0	0
6616	Reaction model and thermodynamic properties between sulfur-containing active groups and oxygen during coal self-heating. <i>Canadian Journal of Chemistry</i> , 2021, 99, 31-42.	0.6	4
6617	Crystal structure analysis of (E)-N-(3,5-dimethylphenyl)-2-(substituted benzylidene)thiosemicarbazone: Experimental and theoretical studies. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4138.	0.9	1

#	ARTICLE	IF	CITATIONS
6618	The magnetic binary lithium clusters W_2Li_n ($n = 15-19$): A theoretical prediction of superatomic molecules. International Journal of Quantum Chemistry, 2021, 121, e26434.	1.0	2
6619	Bacterial Cellulose Composite Solid Polymer Electrolyte With High Tensile Strength and Lithium Dendrite Inhibition for Long Life Battery. Energy and Environmental Materials, 2021, 4, 434-443.	7.3	58
6620	Interaction of hydrogen sulfide with the pristine and B&N-doped beryllium oxide nanotube: DFT study. Journal of Sulfur Chemistry, 2021, 42, 51-66.	1.0	4
6621	Growth behavior and properties of $(HF)_{16}$ clusters. Structural Chemistry, 2021, 32, 395-403.	1.0	6
6622	$Co_{13}O_8$ metalloxocubes: a new class of perovskite-like neutral clusters with cubic aromaticity. National Science Review, 2021, 8, nwaa201.	4.6	21
6623	Influence of Heavy Atom Effect on the Photophysics of Coinage Metal Carbene-Metal Amide Emitters. Advanced Functional Materials, 2021, 31, 2005438.	7.8	37
6624	Zinc oxide-quercetin nanocomposite as a smart nano-drug delivery system: Molecular-level interaction studies. Applied Surface Science, 2021, 536, 147741.	3.1	76
6625	Scandium doping of black phosphorene for enhanced sensitivity to hydrogen sulfide: Periodic DFT calculations. Journal of Physics and Chemistry of Solids, 2021, 148, 109765.	1.9	14
6626	Density functional theory studies on two novel polynitrogen compounds: $N_5 + N_3$ and $N_5 + N_5$. Journal of Physical Organic Chemistry, 2021, 34, e4135.	0.9	2
6627	Benchmark studies of hydrogen bond governing reactivity of cephalosporins in metallo- β -lactamase: Efficient and reliable QSPR equations. International Journal of Quantum Chemistry, 2021, 121, e26451.	1.0	3
6628	Living Long and Prosperous: Productive Intraligand Charge-Transfer States from a Rhenium(I) Terpyridine Photosensitizer with Enhanced Light Absorption. Inorganic Chemistry, 2021, 60, 1334-1343.	1.9	22
6629	Europium-linked structures and electronic properties of nanosize semiconductor $\langle EuSi_n \rangle_0^+$ ($n = 11-18$) clusters. International Journal of Quantum Chemistry, 2021, 121, e26457.	1.0	4
6630	A theoretical insight into the reducing properties of bicyclic dithia hydrocarbons and hetero-bicyclic dithiolopyrrolone compounds with rotation-restricted planar disulfide linkage. Structural Chemistry, 2021, 32, 107-113.	1.0	0
6631	Detection of CNX cyanogen halides ($X = F, Cl$) on metal-free defective phosphorene sensor: periodic DFT calculations. Molecular Physics, 2021, 119, e1819577.	0.8	17
6632	Alkali Metal Doping for Enhancement of Nonlinear Optical Properties of Dicyclopenta[4,3,2,1-gh:4,3,2,2,1-pqr]perylene: A New Bowl-Shaped Fragment of Fullerene C70. Journal of Inorganic and Organometallic Polymers and Materials, 2021, 31, 648-658.	1.0	2
6633	Improved photovoltaic performance of phosphonic acid-based sensitized solar cells via an electron-withdrawing moiety: A density of functional theory study. International Journal of Quantum Chemistry, 2021, 121, e26431.	1.0	5
6634	Gold at crossroads of radical generation and scavenging at density functional theory level: Nitrogen and oxygen free radicals versus their precursors in the face of nanogold. Journal of Physical Organic Chemistry, 2021, 34, .	0.9	1
6635	Two models to estimate the density of organic cocrystals. RSC Advances, 2021, 11, 12066-12073.	1.7	2

#	ARTICLE	IF	CITATIONS
6636	Exploiting the role of stereoelectronic effects to design the antagonists of the human complement C3a receptor. <i>New Journal of Chemistry</i> , 2021, 45, 9443-9455.	1.4	2
6637	How Do Ionic Liquids "Fold" Ionenenes? Computational and Experimental Analysis of Imidazolium Polymers Based on Ether and Alkyl Chain Variations Dissolved in an Ionic Liquid. <i>Macromolecules</i> , 2021, 54, 1611-1622.	2.2	4
6638	Effect of Polymerization on the Charge-Transfer Mechanism in the One (Two)-Photon Absorption Process of "A-Type Triphenylamine Derivatives. <i>Journal of Physical Chemistry A</i> , 2021, 125, 777-794.	1.1	11
6639	Understanding structural and molecular properties of complexes of nucleobases and Au ₁₃ golden nanocluster by DFT calculations and DFT-MD simulation. <i>Scientific Reports</i> , 2021, 11, 435.	1.6	19
6640	Conformational stability and structural analysis of methanethiol clusters: a revisit. <i>RSC Advances</i> , 2021, 11, 29207-29214.	1.7	8
6641	Triplet state (anti)aromaticity of some monoheterocyclic analogues of benzene, naphthalene and anthracene. <i>New Journal of Chemistry</i> , 2021, 45, 5060-5074.	1.4	6
6642	Synthesis and photophysical properties of donor-substituted phenyl-phosphochromones as potential TADF materials. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1747-1755.	2.3	1
6643	Mechanistic insights into the C-H activation of methane mediated by the unsupported and silica-supported VO ₂ OH and CrOOH: a DFT study. <i>RSC Advances</i> , 2021, 11, 11295-11303.	1.7	3
6644	Effect of multiple oxadiazole rings with nitro and nitramino functionalities on energetic properties: computational analysis of the structure-property relationship. <i>New Journal of Chemistry</i> , 2021, 45, 7368-7376.	1.4	8
6645	Interaction Between Microwave and Molecules. , 2021, , 105-149.		0
6646	Pseudo-octahedral nickel(II) complexes of strongly absorbing benzannulated pincer-type amido ligands: ligand-based redox and non-Aufbau electronic behaviour. <i>RSC Advances</i> , 2021, 11, 3547-3555.	1.7	3
6647	Mass spectral and theoretical investigations of the transient proton-bound dimers on the cleavage processes of the peptide GHK and its analogues. <i>RSC Advances</i> , 2021, 11, 4077-4086.	1.7	2
6648	Theoretical investigations about the effect of electron-withdrawing groups on properties of A-D-A type small molecules donor for organic solar cells. <i>Journal of Molecular Modeling</i> , 2021, 27, 54.	0.8	10
6649	Far-Red to Near Infrared Emissive Aqueous Nanoparticles Based on a New Organic Material with Three BODIPY Dyes at the Periphery of the Core: A Combined Experimental and Theoretical Study. <i>Electronic Materials</i> , 2021, 2, 24-38.	0.9	1
6650	Unveiling the high regioselectivity and stereoselectivity within the synthesis of spirooxindolenitropyrrolidine: A molecular electron density theory perspective. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4189.	0.9	21
6651	Metalloporphyrin immobilized CeO ₂ : <i>in situ</i> generation of active sites and synergistic promotion of photocatalytic water oxidation. <i>Catalysis Science and Technology</i> , 2021, 11, 2560-2569.	2.1	1
6652	Supramolecular salts assembled by melamine and two organic hydroxyl acids: synthesis, structure, hydrogen bonds, and luminescent property. <i>CrystEngComm</i> , 2021, 23, 2235-2248.	1.3	6
6653	A DFT study on the C-H oxidation reactivity of Fe(IV) "oxo species with N ₄ /N ₅ ligands derived from l-proline. <i>RSC Advances</i> , 2021, 11, 2293-2297.	1.7	2

#	ARTICLE	IF	CITATIONS
6654	Global aromaticity in 2D macrocyclic polyradicaloids and 3D fully conjugated molecular cages. , 2021, , 405-447.		0
6655	Structure–property relationship of novel supramolecular gels based on coumarins. <i>New Journal of Chemistry</i> , 2021, 45, 13369-13379.	1.4	2
6656	Quantum computational investigations and molecular docking studies on amentoflavone. <i>Heliyon</i> , 2021, 7, e06079.	1.4	22
6657	Sensing mechanism of a new fluorescent probe for hydrogen sulfide: photoinduced electron transfer and invalidity of excited-state intramolecular proton transfer. <i>RSC Advances</i> , 2021, 11, 22214-22220.	1.7	22
6658	Regioselectivity and stereoselectivity of intramolecular [2 + 2] photocycloaddition catalyzed by chiral thioxanthone: a quantum chemical study. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 1532-1540.	1.5	7
6659	Synthesis and supramolecular organization of the iodide and triiodides of a polycyclic adamantane-based diammonium cation: the effects of hydrogen bonds and weak π - π interactions. <i>CrystEngComm</i> , 2021, 23, 2384-2395.	1.3	11
6660	Tailoring long-range superlattice chirality in molecular self-assemblies <i>via</i> weak fluorine-mediated interactions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21489-21495.	1.3	2
6661	DFT and AFIR study on the copper(<i>scp</i>)-catalyzed mechanism of 5-enamine-trisubstituted-1,2,3-triazole synthesis <i>via</i> C–N cross-coupling and the origin of ring-opening of 2 <i>H</i> -azirines. <i>RSC Advances</i> , 2021, 11, 2744-2755.	1.7	4
6662	The design of anion– π interactions and hydrogen bonds for the recognition of chloride, bromide and nitrate anions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11455-11465.	1.3	5
6663	Sequence-selective recognition of cationic amphipathic tripeptides with similar structures in aqueous solutions by cucurbit[7]uril. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13724-13733.	1.3	4
6664	Crystal Structure, Experimental and DFT of (Z)-4-((4-Fluorophenyl)amino)pent-3-en-2-one. <i>Asian Journal of Chemistry</i> , 2021, 33, 1638-1644.	0.1	1
6665	Non-stoichiometric molybdenum sulfide clusters and their reactions with the hydrogen molecule. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 347-355.	1.3	11
6666	1,2,5-Oxadiazole-1,2,3,4-tetrazole-based high-energy materials: molecular design and screening. <i>Structural Chemistry</i> , 2021, 32, 1619-1628.	1.0	4
6667	Design of functionalized bridged 1,2,4-triazole <i>N</i> -oxides as high energy density materials and their comprehensive correlations. <i>RSC Advances</i> , 2021, 11, 27420-27430.	1.7	4
6668	Chemical structure stabilities of a Si_xF_y ($x \leq 6, y \leq 12$) series. <i>RSC Advances</i> , 2021, 11, 21832-21839.	1.7	4
6669	A computational study on second-order nonlinear optical properties based on bis-cyclometalated Ir(<i>scp</i>) complexes: redox and substituent effects. <i>New Journal of Chemistry</i> , 2021, 45, 10725-10734.	1.4	8
6670	Construction of a double-walled carbon nanoring. <i>Nanoscale</i> , 2021, 13, 4880-4886.	2.8	11
6671	Electrolytes and Interphases in Potassium Ion Batteries. <i>Advanced Materials</i> , 2021, 33, e2003741.	11.1	181

#	ARTICLE	IF	CITATIONS
6672	An electrolyte- and catalyst-free electrooxidative sulfonylation of imidazo[1,2- <i>a</i>]pyridines. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3110-3117.	2.3	21
6673	Unveiling the role of pyrylium frameworks on π -stacking interactions: a combined <i>ab initio</i> and experimental study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1965-1973.	1.3	1
6674	Iron- and zinc-mediated reductive coupling of styrenes and alkyl bromides: mechanistic investigation using DFT calculations. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3372-3380.	2.3	1
6675	A data-driven and DFT assisted theoretic guide for membrane design in flow batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 14545-14552.	5.2	9
6676	Exploring the non-covalent interactions behind the formation of amine-water complexes: the case of <i>N</i> -allylmethylamine monohydrate. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7368-7375.	1.3	5
6677	Multiple investigations of aqueous Eu(III) oxalate complexes: the reduction in coordination number and validation of spectral linear correlation. <i>Dalton Transactions</i> , 2021, 50, 9388-9398.	1.6	6
6678	Trinuclear molybdenum clusters with sulfide bridges as potential anionic receptors <i>via</i> chalcogen bonding. <i>CrystEngComm</i> , 2021, 23, 4607-4614.	1.3	6
6679	Site-Specific Electronic Properties of [Ag ₂₅ (SR) ₁₈] ⁺ Nanoclusters by X-Ray Spectroscopy. <i>Small</i> , 2021, 17, e2005162.	5.2	6
6680	Blue organic light-emitting diodes with hybridized local and charge-transfer excited state realizing high external quantum efficiency. <i>RSC Advances</i> , 2021, 11, 8606-8618.	1.7	23
6681	A color-tunable single-component luminescent molecule with multiple emission centers. <i>Chemical Science</i> , 2021, 12, 9201-9206.	3.7	32
6682	Contribution of nitrogen configurations to the adsorption of Cd(II) in nitrogen-enriched biochar. <i>New Journal of Chemistry</i> , 2021, 45, 12669-12677.	1.4	5
6683	The substituent effect on the photophysical and charge transport properties of non-planar dibenzo[<i>a,m</i>]rubicenes. <i>New Journal of Chemistry</i> , 2021, 45, 20556-20568.	1.4	2
6684	Electrochemical reduction of CO ₂ to CO and HCOO ⁻ using metal-cyclam complex catalysts: predicting selectivity and limiting potential from DFT. <i>Dalton Transactions</i> , 2021, 50, 11446-11457.	1.6	3
6685	Interfacial co-polymerization derived nitrogen-doped carbon enables high-performance carbon felt for vanadium flow batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 17300-17310.	5.2	15
6686	Density functional theory studies of boron clusters with exotic properties in bonding, aromaticity and reactivity. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24118-24124.	1.3	11
6687	Radical cations and dications of bis[1]benzothieno[1,4]thiazine isomers. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5744-5755.	2.3	2
6688	Energetic isomers of bridged oxadiazole nitramines: the effect of asymmetric heterocyclics on stability and energetic properties. <i>Dalton Transactions</i> , 2021, 50, 13286-13293.	1.6	22
6689	A combined experimental and computational study to decipher complexity in the asymmetric hydrogenation of imines with Ru catalysts bearing atropisomerizable ligands. <i>Catalysis Science and Technology</i> , 2021, 11, 2497-2511.	2.1	6

#	ARTICLE	IF	CITATIONS
6690	Classics Meet Classics: Theoretical and Experimental Studies of Halogen Bonding in Adducts of Platinum(II) 1,5-Cyclooctadiene Halide Complexes with Diiodine, Iodoform, and 1,4-Diiodotetrafluorobenzene. <i>Crystal Growth and Design</i> , 2021, 21, 974-987.	1.4	15
6691	Endohedral metallofullerene electrides of Ca ₁₂ O ₁₂ with remarkable nonlinear optical response. <i>RSC Advances</i> , 2021, 11, 1569-1580.	1.7	28
6692	Theoretical insight into the origins of chemo- and diastereo-selectivity in the palladium-catalysed (3 +) Tj ETQqO O 0,rgBT /Overlock 10 Tf	2.8	8
6693	Molecular modeling investigation of adsorption of Zolinda drug on surfaces of the B12N12 and Al12N12 nanocages. <i>Structural Chemistry</i> , 2021, 32, 1181-1196.	1.0	19
6694	Ground- and excited-state characteristics in photovoltaic polymer N2200. <i>RSC Advances</i> , 2021, 11, 20191-20199.	1.7	15
6695	Role of metcar on the adsorption and activation of carbon dioxide: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5559-5570.	1.3	10
6696	Insights into the kinetics and molecular mechanism of the Newmanâ€™Kwart rearrangement. <i>New Journal of Chemistry</i> , 2021, 45, 16978-16988.	1.4	2
6697	Hydrogen adsorption on inorganic benzenes decorated with alkali metal cations: theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5315-5324.	1.3	14
6698	A combination of heterogeneous catalysis and photocatalysis for the olefination of quinoxalin-2(1 <i>H</i>)-ones with ketones in water: a green and efficient route to (<i>Z</i>)-enaminones. <i>Green Chemistry</i> , 2021, 23, 2123-2129.	4.6	48
6699	Organic phosphorescent polymorphs induced by various halogen bonds with stimuli-responsive single/dual phosphorescence switching. <i>Journal of Materials Chemistry C</i> , 2021, 9, 2738-2743.	2.7	16
6700	Polarization-induced charge separation in conjugated microporous polymers for efficient visible light-driven C-3 selenocyanation of indoles. <i>Chemical Science</i> , 2021, 12, 5631-5637.	3.7	28
6701	Geometry transformation of ionic surfactants and adsorption behavior on water/n-decane-interface: calculation by molecular dynamics simulation and DFT study. <i>RSC Advances</i> , 2021, 11, 28286-28294.	1.7	6
6702	Hydrogen bonding interactions between arsenious acid and dithiothreitol/dithioerythritol at different pH values: a computational study with an explicit solvent model. <i>New Journal of Chemistry</i> , 2021, 45, 20181-20192.	1.4	4
6703	Transient absorption, femtosecond dynamics, vibrational coherence and molecular modelling of the photoisomerization of <i>N</i>-salicylidene-<i>o</i>-aminophenol in solution. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20989-21000.	1.3	1
6704	Stabilization of dichalcogenide ligands in the coordination sphere of a ruthenium system. <i>Dalton Transactions</i> , 2021, 50, 12990-13001.	1.6	3
6705	Formation of an air-stable diborane via a stepwise BH ₃ addition of pyrido[1,2- <i>a</i>]isoindole with H ₂ evolution. <i>Chemical Communications</i> , 2021, 57, 9882-9885.	2.2	1
6706	Chemisorption of CO ₂ by diamine-tetraamido macrocyclic motifs: a theoretical study. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 3873-3881.	1.5	5
6707	Detection of hydrogen peroxide and glucose with a novel fluorescent probe by the enzymatic reaction of amino functionalized MOF nanosheets. <i>Analytical Methods</i> , 2021, 13, 4228-4237.	1.3	5

#	ARTICLE	IF	CITATIONS
6708	Conversion of carbon dioxide to a novel molecule NCNBO ^{•-} mediated by NbBN ₂ ^{•-} anions at room temperature. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22613-22619.	1.3	2
6709	Metal- and halide-free, solid-state polymeric water vapor sorbents for efficient water-sorption-driven cooling and atmospheric water harvesting. <i>Materials Horizons</i> , 2021, 8, 1518-1527.	6.4	60
6710	Significant Roles of a Particularly Stable Two-Center Two-Electron Lu ^{II} -Lu ^{III} Bond in Lu ₂ @C ₈₆ : Electronic Structure of Lu and Radius of Lu ²⁺ . <i>Inorganic Chemistry</i> , 2021, 60, 2425-2436.	1.9	8
6711	Excess chemical potential of thiophene in [C4MIM] [BF ₄ , Cl, Br, CH ₃ COO] ionic liquids, determined by molecular simulations. <i>RSC Advances</i> , 2021, 11, 29394-29406.	1.7	2
6712	Photoinduced electron transfer in nano-Saturn complexes of fullerene. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2126-2133.	1.3	8
6713	Computational prediction of Au(ⁱ /scp) ⁺ Pb(ⁱⁱ /scp) bonding in coordination complexes and study of the factors affecting the formation of Au(ⁱ /scp) ⁺ E(ⁱⁱ /scp) (E = Ge, Sn, Pb) covalent bonds. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10174-10183.	1.3	2
6714	Pyrene-1,5,6,10-tetracarboxyl diimide: a new building block for high-performance electron-transporting polymers. <i>Journal of Materials Chemistry C</i> , 2021, 9, 7599-7606.	2.7	14
6715	Excited state character of Cibalackrot-type compounds interpreted in terms of H ^{1/4} ckel-aromaticity: a rationale for singlet fission chromophore design. <i>Chemical Science</i> , 2021, 12, 6159-6171.	3.7	30
6716	Calculation and analysis of interaction between characteristic functional group of persimmon tannin and metal ions. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, 70, 123101.	0.2	3
6717	Unusual molecular complexes of antimony fluoride dimers with acetonitrile and pyridine: structures and bonding. <i>Dalton Transactions</i> , 2021, 50, 13357-13367.	1.6	3
6718	A Heteropolynuclear Pt ^{II} -Ag System Having Cycloplatinated Rollover Bipyridyl Units. <i>Inorganic Chemistry</i> , 2021, 60, 1513-1522.	1.9	7
6719	3,5-difluoro-2,4,6-trinitroanisole: promising melt-cast insensitive explosives instead of TNT. <i>Journal of Energetic Materials</i> , 2022, 40, 206-217.	1.0	9
6720	Elucidating the mechanism and origins of selectivity on catalyst-dependent cyclization reactions to form polycyclic indolines from a theoretical study. <i>RSC Advances</i> , 2021, 11, 20622-20634.	1.7	1
6721	Intramolecular hydrogen bond and vibrational spectroscopic study of cellulose oligosaccharide using density functional theory. <i>AIP Conference Proceedings</i> , 2021, , .	0.3	1
6722	On the influence of water molecules on the outer electronic shells of R ⁺ SeH, R ⁺ Se(•) and R ⁺ SeOH fragments in the selenocysteine amino acid residue. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13965-13970.	1.3	2
6723	Designing an alkali-metal-like superatom Ca ₃ B for ambient nitrogen reduction to ammonia. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18908-18915.	1.3	7
6724	Synthesis and luminescence properties of two Ir(ⁱⁱⁱ /scp) complexes containing styrene-modified phenylpyridine ligands. <i>New Journal of Chemistry</i> , 2021, 45, 3311-3318.	1.4	5
6725	Photoelectron spectroscopy and theoretical study of Al _n C ₅ ⁺⁰ (<i>n</i> = 1-5) clusters: structural evolution, relative stability of star-like clusters, and planar tetracoordinate carbon structures. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1967-1975.	1.3	20

#	ARTICLE	IF	CITATIONS
6726	Study on the growth patterns and simulated photoelectron spectroscopy of double vanadium atoms doped silicon clusters V_2Si_n ($n=12$) and their anions. <i>Molecular Physics</i> , 2021, 119, e1864042.	0.8	2
6727	Electronic structures, chemical bonds, and stabilities of $Zr_nTa_{4-n}C_n$ ($n=1-4$) clusters: Anion photoelectron spectroscopy and theoretical calculations. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, 70, 023601-023601.	0.2	2
6728	Molecular polarizabilities of some energetic compounds. <i>Journal of Molecular Modeling</i> , 2021, 27, 51.	0.8	1
6729	Studies on chemoselective synthesis of 1,4- and 1,2-dihydropyridine derivatives by a Hantzsch-like reaction: a combined experimental and DFT study. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 3882-3892.	1.5	6
6730	High-energetic and low-sensitive 1,3,5-triamino 2,4,6-trinitrobenzene (TATB) crystal: first principles investigation and Hirshfeld surface analysis. <i>New Journal of Chemistry</i> , 2021, 45, 6136-6143.	1.4	9
6731	Tuning the first hyperpolarizability of hexaphyrins with different connections of mislinked pyrrole units: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8489-8499.	1.3	10
6732	Replacing the cyano ($C\equiv N$) group to design environmentally friendly fused-ring electron acceptors. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18085-18092.	1.3	5
6733	Synthesis, characterisation and DFT studies of [3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl](phenyl)methanone derivatives. <i>Results in Chemistry</i> , 2021, 3, 100165.	0.9	1
6734	Mechanism of zinc ejection by disulfiram in nonstructural protein 5A. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 12204-12215.	1.3	22
6735	Aggregation-enhanced emission in tetraphenylpyrazine-based luminogens: theoretical modulation and experimental validation. <i>Materials Chemistry Frontiers</i> , 2021, 5, 5012-5023.	3.2	10
6736	The influence of the shape and configuration of sensitizer molecules on the efficiency of DSSCs: a theoretical insight. <i>RSC Advances</i> , 2021, 11, 5556-5567.	1.7	7
6737	A bench-stable N -trifluoroacetyl nitrene equivalent for a simple synthesis of 2-trifluoromethyl oxazoles. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 6628-6632.	1.5	9
6738	Mechanism and regio- and stereoselectivity in an NHC-catalyzed Mannich/lactamization domino reaction. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6204-6212.	1.3	7
6739	Mechanistic understanding of the Cu(I)-catalyzed domino reaction constructing 1-aryl-1,2,3-triazole from electron-rich aryl bromide, alkyne, and sodium azide: a DFT study. <i>Catalysis Science and Technology</i> , 2021, 11, 3208-3216.	2.1	3
6740	Benzobisthiadiazole-based high-spin donor-acceptor conjugated polymers with localized spin distribution. <i>Materials Advances</i> , 2021, 2, 2943-2955.	2.6	10
6741	Origin of High-Efficiency Near-Infrared Organic Thermally Activated Delayed Fluorescence: The Role of Electronic Polarization. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1249-1255.	1.5	11
6742	A new perspective for evaluating the photoelectric performance of organic-inorganic hybrid perovskites based on the DFT calculations of excited states. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11548-11556.	1.3	23
6743	Metal-organic framework-derived carbon as a positive electrode for high-performance vanadium redox flow batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 5648-5656.	5.2	30

#	ARTICLE	IF	CITATIONS
6744	Enhancing functionalities of organic ultraviolet-visible phototransistors incorporating spiropyran-merocyanine photochromic materials. <i>Journal of Materials Chemistry A</i> , 2021, 9, 22522-22532.	5.2	9
6745	Quantum Computational, Spectroscopic and Molecular Docking Studies on N-(4-Hydroxyphenyl)picolinamide. <i>Asian Journal of Organic & Medicinal Chemistry</i> , 2021, 6, 186-203.	0.1	0
6746	Flame-retardant single-ion conducting polymer electrolytes based on anion acceptors for high-safety lithium metal batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 7692-7702.	5.2	33
6747	Halo-fluorescein for photodynamic bacteria inactivation in extremely acidic conditions. <i>Nature Communications</i> , 2021, 12, 526.	5.8	37
6748	Revealing the Specific Spatial Confinement in 8-membered Ring Cage-type Molecular Sieves via Solid-state NMR and Theoretical Calculations. <i>ChemCatChem</i> , 2021, 13, 1299-1305.	1.8	3
6749	Tuning the hyperconjugative aromaticity in Au(III)-substituted indoliums. <i>Dalton Transactions</i> , 2021, 50, 8096-8101.	1.6	6
6750	Push-pull effect to improve the electronic and optical properties of [7] circulene. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 959.	0.8	1
6751	A ratiometric photoelectrochemical microsensor based on a small-molecule organic semiconductor for reliable <i>in vivo</i> analysis. <i>Chemical Science</i> , 2021, 12, 12977-12984.	3.7	22
6752	From Antiaromatic Norcorrolato nickel(II) to Aromatic and Nonaromatic Zwitterions: Innocent Ligands with Unbalanced Charge of the Core. <i>Organic Letters</i> , 2021, 23, 1032-1037.	2.4	11
6753	Study of self-assembly system of norfloxacin molecularly imprinted polymers based on simulated design. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	6
6754	Combining machine learning and high-throughput experimentation to discover photocatalytically active organic molecules. <i>Chemical Science</i> , 2021, 12, 10742-10754.	3.7	52
6755	Positive impact of chromophore flexibility on the efficiency of red thermally activated delayed fluorescence materials. <i>Materials Horizons</i> , 2021, 8, 1297-1303.	6.4	41
6756	Comparison of Bifurcated Halogen with Hydrogen Bonds. <i>Molecules</i> , 2021, 26, 350.	1.7	12
6757	Coupling molecular rigidity and flexibility on fused backbones for NIR-II photothermal conversion. <i>Chemical Science</i> , 2021, 12, 5177-5184.	3.7	32
6758	Characterizing hydrogen and tetrel bonds in clusters of CO ₂ with carboxylic acids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16915-16922.	1.3	10
6759	Laser spectroscopic and computational insights into unexpected structural behaviours of sandwich complexes upon ionization. <i>Dalton Transactions</i> , 2021, 50, 10729-10736.	1.6	5
6760	A theoretical study of the hydroboration of α,β -unsaturated carbonyl compounds catalyzed by a metal-free complex and subsequent C-C coupling with acetonitrile. <i>New Journal of Chemistry</i> , 2021, 45, 14134-14140.	1.4	3
6761	Structural and electronic properties of FeCl ₃ and CrO ₃ interacting with GaP nanotubes from DFT calculations. <i>New Journal of Chemistry</i> , 2021, 45, 9483-9490.	1.4	1

#	ARTICLE	IF	CITATIONS
6762	A theoretical study on the excited-state deactivation paths for the A ⁵ FU dimer. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16089-16106.	1.3	3
6763	A Theoretical Study on Terpene-Based Natural Deep Eutectic Solvent: Relationship between Viscosity and Hydrogen Bonding Interactions. <i>Global Challenges</i> , 2021, 5, 2000103.	1.8	24
6764	Triazine-based porous organic polymers with enhanced electronegativity as multifunctional separator coatings in lithium-sulfur batteries. <i>Nanoscale</i> , 2021, 13, 12028-12037.	2.8	15
6765	Aromatic nature of neutral and dianionic 1,4-diaza-2,3,5,6-tetraborinine derivatives. <i>RSC Advances</i> , 2021, 11, 592-598.	1.7	2
6766	A rotational spectroscopic and <i>ab initio</i> study of <i>cis</i> - and <i>trans</i> -(α)-carveol: further insights into conformational dynamics in monoterpenes and monoterpenoids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15159-15168.	1.3	6
6767	Boosting the photoelectric conversion efficiency of DSSCs through graphene quantum dots: insights from theoretical study. <i>Materials Chemistry Frontiers</i> , 2021, 5, 5814-5825.	3.2	10
6768	DFT study of H ₂ adsorption at a Cu-SSZ-13 zeolite: a cluster approach. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9980-9990.	1.3	16
6769	J-Aggregation Enhanced Thermally Activated Delayed Fluorescence for Amplified Spontaneous Emission. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
6770	Experimental and Theoretical Studies of Dimers Stabilized by Two Chalcogen Bonds in the Presence of a N \cdots N Pnicogen Bond. <i>Journal of Physical Chemistry A</i> , 2021, 125, 657-668.	1.1	14
6771	Alkali metal doping of black phosphorus monolayer for ultrasensitive capture and detection of nitrogen dioxide. <i>Scientific Reports</i> , 2021, 11, 842.	1.6	9
6772	First Principle Analysis on Pyridine Amide Derivatives TM Adsorption Behavior on the Pt (111) Surface. <i>Crystals</i> , 2021, 11, 98.	1.0	2
6773	E \cdots E triple bonds (E = Group 13) promoted by charge transfer from alkali metals. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
6774	A novel highly sensitive dual-channel chemical sensor for sequential recognition of Cu ²⁺ and CN ⁻ in aqueous media and its bioimaging applications in living cells. <i>New Journal of Chemistry</i> , 2021, 45, 18421-18432.	1.4	6
6775	Metallocene: multi-layered molecular rotors. <i>Dalton Transactions</i> , 2021, 50, 14156-14162.	1.6	2
6776	Intramolecular aurophilic interactions in dinuclear gold(μ) complexes with twisted bridging 2,2'-bipyridine ligands. <i>Dalton Transactions</i> , 2021, 50, 12448-12456.	1.6	17
6777	Interactions of aromatic rings in the crystal structures of hybrid polyoxometalates and Ru clusters. <i>CrystEngComm</i> , 2021, 23, 6409-6417.	1.3	9
6778	On the role of steric and exchange correlation effects in halogenated complexes. <i>New Journal of Chemistry</i> , 2021, 45, 16254-16263.	1.4	1
6779	Molecular Dynamics Simulations of Self-Healing Topological Copolymers with a Comblike Structure. <i>Macromolecules</i> , 2021, 54, 1095-1105.	2.2	24

#	ARTICLE	IF	CITATIONS
6780	Synthesis and characterization of photochromic triethylene glycol-containing spiropyrans and their assembly in solution. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3047-3058.	2.3	7
6781	Electronic Transitions, Inter- and Intra-Bond Interactions of an Azabicyclic Single Crystal using DFT. <i>Asian Journal of Chemistry</i> , 2021, 33, 2365-2372.	0.1	0
6782	Ab initio study of spectroscopic properties at anharmonic force fields of LiNH ₂ . <i>Journal of Molecular Modeling</i> , 2021, 27, 33.	0.8	2
6783	Investigation of the thermal decomposition mechanism of glycerol: the combination of a theoretical study based on the Minnesota functional and experimental support. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20466-20477.	1.3	6
6784	A donor-acceptor liganded metal-organic framework showcases the hydrogen-bond-enhanced sensing of N-heterocyclic explosives. <i>Journal of Materials Chemistry C</i> , 2021, 9, 12086-12093.	2.7	6
6785	A combined experimental and theoretical investigation of the excited-state dynamics of 2,4,6-trinitrotoluene (TNT) in DMSO solvent. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20718-20723.	1.3	2
6786	Perspective of structural flexibility on selective inhibition towards CYP1B1 over CYP1A1 by $\hat{\pm}$ -naphthoflavone analogs. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20230-20246.	1.3	5
6787	Naphthobox: a selective molecular box for planar aromatic cations. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5265-5270.	2.3	6
6788	The size-dependent influence of palladium doping on the structures of cationic gold clusters. <i>Nanoscale Advances</i> , 2021, 3, 6197-6205.	2.2	3
6789	Theoretical study of the NHC-catalyzed C-S bond cleavage and reconstruction reaction: mechanism, stereoselectivity, and role of catalysts. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5352-5360.	2.3	16
6790	Insight into the adsorption of Cr(VI) on functionalized carboxymethyl cellulose-based sponge via experimental and theoretical calculations. <i>New Journal of Chemistry</i> , 2021, 45, 20280-20288.	1.4	3
6791	Synthesis and Electronic Properties of Diketopyrrolopyrrole-Based Polymers with and without Ring-Fusion. <i>Macromolecules</i> , 2021, 54, 970-980.	2.2	23
6792	Boron-nitrogen substituted planar cores: designing dopant-free hole-transporting materials for efficient perovskite solar cells. <i>Nanoscale</i> , 2021, 13, 4241-4248.	2.8	16
6793	The cooperative role of innocent ligand in N-heterocyclic carbene manganese catalyzed carbon dioxide hydrogenation. <i>Catalysis Science and Technology</i> , 2021, 11, 7189-7199.	2.1	5
6794	Activation of $\hat{2}$ -diketones for CO ₂ capture and utilization. <i>Reaction Chemistry and Engineering</i> , 2021, 6, 2364-2375.	1.9	4
6795	In acid-aminopyrimidine continuum: experimental and computational studies of furan tetracarboxylate-2-aminopyrimidinium salt. <i>RSC Advances</i> , 2021, 11, 21463-21474.	1.7	15
6796	Interfacial interactions and structures of protic ionic liquids on a graphite surface: A first-principles study and comparison with aprotic ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18338-18348.	1.3	8
6797	Theoretical insight on antioxidant potency of kanzakiflavone-2 and its derivatives. <i>Structural Chemistry</i> , 2021, 32, 1451-1458.	1.0	1

#	ARTICLE	IF	CITATIONS
6798	Modulating the carrier transport of PtAg ₂ heteronuclear complexes to attain highly efficient OLEDs with narrow-band emission. <i>Journal of Materials Chemistry C</i> , 2021, 9, 5403-5410.	2.7	6
6799	Theoretical assessment of calix[4]arene-N ² -ketoimine (n=1-4) derivatives: Conformational studies, optoelectronic, and sensing of Cu ²⁺ cation. <i>Journal of Molecular Modeling</i> , 2021, 27, 16.	0.8	1
6800	Ni and Zn N-confused porphyrin complexes as recyclable catalysts for high efficiency solvent-free CO ₂ fixation into cyclic carbonates. <i>Catalysis Science and Technology</i> , 2021, 11, 2144-2154.	2.1	17
6801	Nitrogen-rich Compounds with Multiple Azole Rings: Gas Generant, Enthalpy Enhancer and Applicable Cationic Component. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 421-427.	1.3	1
6802	A relativistic DFT probe for small-molecule activation mediated by low-valent uranium metallocenes. <i>New Journal of Chemistry</i> , 2021, 45, 4270-4279.	1.4	0
6803	Adjacent N-H and C-NH ₂ groups in a highly efficient amphoteric structure for energetic materials resulting from tautomerization proved by crystal engineering. <i>CrystEngComm</i> , 2021, 23, 1544-1549.	1.3	4
6804	Theoretical study on the molecular stacking interactions and charge transport properties of triazasumanene crystals from explanation to prediction. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4681-4689.	1.3	11
6805	A theoretical investigation into the cooperativity effect on the TNT melting point under external electric field. <i>Journal of Molecular Modeling</i> , 2021, 27, 4.	0.8	4
6806	Ultrafast channel I and channel II charge generation processes at a nonfullerene donor-acceptor PTB7:PDI interface is crucial for its excellent photovoltaic performance. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2097-2104.	1.3	4
6807	A Ni-doping-induced phase transition and electron evolution in cobalt hexacyanoferrate as a stable cathode for sodium-ion batteries. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2491-2499.	1.3	12
6808	Hydrogen abstraction/addition reactions in soot surface growth. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 3071-3086.	1.3	4
6809	The preparation of novel triphenylamine-based AIE-effect fluorescent probe for selectively detecting mercury(II) ion in aqueous solution. <i>New Journal of Chemistry</i> , 2021, 45, 5049-5059.	1.4	13
6810	A computational approach on the stereoselective binding of peptides from aqueous medium with <i>endo</i> -functionalized molecular tubes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22703-22717.	1.3	3
6811	Multiple "Hot exciton" channel molecular design in organic electroluminescence materials: a theoretical investigation. <i>Materials Advances</i> , 2021, 2, 1351-1357.	2.6	12
6812	Remarkable static and dynamic NLO response of alkali and superalkali doped macrocyclic [hexa]thiophene complexes; a DFT approach. <i>RSC Advances</i> , 2021, 11, 4118-4128.	1.7	35
6813	Halogen bonds as a tool in the design of high energetic materials: evidence from crystal structures and quantum chemical calculations. <i>CrystEngComm</i> , 2021, 23, 6915-6922.	1.3	7
6814	Nature and role of the weak intermolecular bond in enantiomeric conformations of H ₂ O ₂ -noble gas adducts: a chiral prototypical model. <i>New Journal of Chemistry</i> , 2021, 45, 8240-8247.	1.4	3
6815	Exploration of the cofactor specificity of wild-type phosphite dehydrogenase and its mutant using molecular dynamics simulations. <i>RSC Advances</i> , 2021, 11, 14527-14533.	1.7	3

#	ARTICLE	IF	CITATIONS
6816	Catalytic cycle of the partial oxidation of methane to methanol over Cu-ZSM-5 revealed using DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4963-4974.	1.3	16
6817	Acenes and phenacenes in their lowest-lying triplet states. Does kinked remain more stable than straight?. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13574-13582.	1.3	18
6818	Elastic orange emissive single crystals of 1,3-diamino-2,4,5,6-tetrabromobenzene as flexible optical waveguides. <i>Journal of Materials Chemistry C</i> , 2021, 9, 9465-9472.	2.7	15
6819	Physico-chemical properties of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK) diazonium ion: a theoretical investigation. <i>RSC Advances</i> , 2021, 11, 26750-26762.	1.7	0
6820	Synthesis, characterization, and theoretical studies of the photovoltaic properties of novel reactive azonitrobenzaldehyde derivatives. <i>RSC Advances</i> , 2021, 11, 28433-28446.	1.7	42
6821	Highly-efficient production of spherical co-agglomerates of drugs via an organic solvent-free process and a mechanism study. <i>Green Chemistry</i> , 2021, 23, 2710-2721.	4.6	22
6822	Computational investigation of the substituent effect in the [2+4] Diels-Alder cycloaddition reactions of $\text{HSi}(\text{Si})_3\text{C}_6\text{H}_4\text{X}$ with benzene. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 806-816.	0.8	5
6823	Weak covalent interactions and anionic charge-sharing polymerisation in cluster environments. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11596-11610.	1.3	4
6824	NICS "Nucleus-independent Chemical Shift. , 2021, , 99-154.		25
6825	Theoretical design of asymmetric D_{1h} - D_{2h} -A type non-fullerene acceptors for organic solar cells. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 12321-12328.	1.3	20
6826	Design, synthesis, and properties of a six-membered oligofuran macrocycle. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1775-1782.	2.3	12
6827	Theoretical studies on triplet formations in nitrobenzoxadiazole (NBD) derivatives: The impact of donor group and heteroatom substitution. <i>Results in Chemistry</i> , 2021, 3, 100116.	0.9	0
6828	Understanding H_2O -Induced Thermo-Oxidative Reclamation of Vulcanized Styrene Butadiene Rubber at Low Temperatures. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 2378-2387.	3.2	15
6829	Infrared photodissociation spectroscopic and theoretical study of HnC_4O^+ ($n=1, 2$) cation clusters in the gas phase. <i>Molecular Physics</i> , 2021, 119, e1879301.	0.8	0
6830	Selective Separation of HNO_3 and HCl by Extraction: The Investigation on the Noncovalent Interaction between Extractants and Acids by Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1214-1226.	1.2	6
6831	Anion Photoelectron Spectroscopy and Theoretical Studies of $\text{Al}_4\text{C}_6^{+}$: Global Minimum Triangle-Shaped Structures and Hexacoordinated Aluminum. <i>Journal of Physical Chemistry A</i> , 2021, 125, 302-307.	1.1	13
6832	$[\text{Bi}_6\text{Mo}_3(\text{CO})_9]^{4+}$: a multiple local \tilde{f} -aromatic cluster containing a distorted Bi_6 triangular prism. <i>Chemical Communications</i> , 2021, 57, 3656-3659.	2.2	15
6833	Post-synthetic modification of supramolecular assemblies of \hat{I}^2 -diketonato $\text{Cu}(\text{ii})$ complexes: comparing and contrasting the molecular topology by crystal structure and quantum computational studies. <i>CrystEngComm</i> , 2021, 23, 4344-4369.	1.3	14

#	ARTICLE	IF	CITATIONS
6834	Gaseous cyclodextrin- <i>closo</i> -dodecaborate complexes $\text{I}^{\pm}\text{CD}\text{A}\text{-B}_{12}\text{X}_{12}$ ($\text{I}^{\pm} = \text{I}^{\pm}, \text{I}^2, \text{and } \text{I}^3$; X = F, Cl, Br, and I): electronic structures and intramolecular interactions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13447-13457.	2.3	8
6835	DFT Study on the Chemical Absorption Mechanism of CO_2 in Diamino Protic Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1416-1428.	1.2	12
6836	Anti-electrostatic-halogen bonding in solution. <i>Chemical Science</i> , 2021, 12, 8246-8251.	3.7	20
6837	Halogen Bonds Stabilised by an Electronic Exchange Channel. <i>ChemistrySelect</i> , 2021, 6, 680-684.	0.7	3
6838	A new isostructural halogenated chalcone with optical properties. <i>Journal of Molecular Modeling</i> , 2021, 27, 52.	0.8	3
6839	One-pot atmospheric pressure synthesis of $[\text{H}_3\text{Ru}_4(\text{CO})_{12}]^+$. <i>Dalton Transactions</i> , 2021, 50, 9610-9622.	1.6	9
6840	Coordination-induced emission enhancement in copper(i) iodide coordination polymers supported by 2-(alkylsulfanyl)pyrimidines. <i>Dalton Transactions</i> , 2021, 50, 9317-9330.	1.6	17
6841	Influence of the Pd%:Bi ratio on Pd-Bi/Al ₂ O ₃ catalysts: structure, surface and activity in glucose oxidation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14889-14897.	1.3	4
6842	Stereoselective rhodium-catalyzed 2-C ^H 1,3-dienylation of indoles: dual functions of the directing group. <i>Chemical Science</i> , 2021, 12, 11330-11337.	3.7	13
6843	Study on hydrodeoxygenation mechanism of anisole over Ni (111) by first-principles calculation. <i>Molecular Catalysis</i> , 2022, 523, 111402.	1.0	18
6844	Simulation of Elastic and Fatigue Properties of Epoxy/SiO ₂ Particle Composites through Molecular Dynamics. <i>CMES - Computer Modeling in Engineering and Sciences</i> , 2021, 128, 339-357.	0.8	3
6845	Mechanistic insights into the I^{\pm} -branched amine formation with pivalic acid assisted C ^H bond activation catalysed by Cp [*] Rh complexes. <i>Dalton Transactions</i> , 2021, 50, 12888-12895.	1.6	1
6846	Silver-catalyzed desulfurizative annulation of 1,2-benzisothiazoles with ynamides to construct multi-substituted isoquinolines. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5446-5453.	2.3	3
6847	Halogenated sodium/lithium monocarba- <i>closo</i> -decaborates: syntheses, characterization, and solid-state ionic conductivity. <i>Materials Chemistry Frontiers</i> , 2021, 5, 8037-8046.	3.2	4
6848	Directed transforming of coke to active intermediates in methanol-to-olefins catalyst to boost light olefins selectivity. <i>Nature Communications</i> , 2021, 12, 17.	5.8	55
6849	Theoretical calculation of regioselectivity and solvation effects on C ^H activation of <i>closo</i> -carborane guided by directing group. <i>Dalton Transactions</i> , 2021, 50, 10291-10298.	1.6	2
6850	Coordination-driven assembly of actinide-organic polyrotaxanes involving crown ether macrocycles. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3686-3694.	2.3	2
6851	Unveiling the Unexpected Reactivity of Electrophilic Diazoalkanes in [3+2] Cycloaddition Reactions within Molecular Electron Density Theory. <i>Chemistry</i> , 2021, 3, 74-93.	0.9	9

#	ARTICLE	IF	CITATIONS
6852	Strategy of regulating the electrophilic/nucleophilic ability by ionic ratio in poly(ionic liquid)s to control the coupling reaction of epoxide. <i>Catalysis Science and Technology</i> , 2021, 11, 6498-6506.	2.1	12
6853	Local structure and NO adsorption/desorption property of Pd ²⁺ cations at different paired Al sites in CHA zeolite. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22273-22282.	1.3	15
6854	From helices to superhelices: hierarchical assembly of homochiral van der Waals 1D coordination polymers. <i>Chemical Science</i> , 2021, 12, 12619-12630.	3.7	9
6855	A comparative study on the coordination of diglycolamide isomers with Nd(III): extraction, third phase formation, structure, and computational studies. <i>RSC Advances</i> , 2021, 11, 27969-27977.	1.7	5
6856	External electric field effects on the σ -hole and lone-pair hole interactions of group V elements: a comparative investigation. <i>RSC Advances</i> , 2021, 11, 4022-4034.	1.7	14
6857	Introducing methoxy or fluorine substitutions on the conjugated side chain to reduce the voltage loss of organic solar cells. <i>Journal of Materials Chemistry C</i> , 2021, 9, 11163-11171.	2.7	10
6858	Rhodium(<i>rac</i>)/bisoxazolinephosphine-catalyzed regio- and enantioselective amination of allylic carbonates: a computational study. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3320-3331.	2.3	7
6859	Complexation and Separation of Trivalent Actinides and Lanthanides by a Novel DGA Derived from Macrocyclic Crown Ether: Synthesis, Extraction, and Spectroscopic and Density Functional Theory Studies. <i>ACS Omega</i> , 2021, 6, 2156-2166.	1.6	11
6860	Achieving visible-light-excited organic room-temperature phosphorescence by manipulating π - π^* conjugation. <i>Journal of Materials Chemistry C</i> , 2021, 9, 14623-14627.	2.7	8
6861	A Biomimetic Transpiration Textile for Highly Efficient Personal Drying and Cooling. <i>Advanced Functional Materials</i> , 2021, 31, 2008705.	7.8	98
6862	Elucidating the chemiexcitation of dioxetanones by replacing the peroxide bond with S-S, N-N and C-C bonds. <i>New Journal of Chemistry</i> , 2021, 45, 18518-18527.	1.4	6
6863	Lone-pair stabilized channels and blocked transport in apatite-related structures. <i>Dalton Transactions</i> , 2021, 50, 13232-13235.	1.6	0
6864	Solvent effect on xylose-to-furfural reaction in biphasic systems: combined experiments with theoretical calculations. <i>Green Chemistry</i> , 2021, 23, 8510-8518.	4.6	41
6865	Rational design of near-infrared fluorophores with a phenolic D-A type structure and construction of a fluorescent probe for cysteine imaging. <i>New Journal of Chemistry</i> , 2021, 45, 18528-18537.	1.4	9
6866	Experimental and theoretical investigation of conformational states and noncovalent interactions in crystalline sulfonamides with a methoxyphenyl moiety. <i>CrystEngComm</i> , 2021, 23, 6137-6162.	1.3	13
6867	Inter-ligand charge-transfer interactions in a photochromic and redox active zinc-organic framework. <i>CrystEngComm</i> , 2021, 23, 5982-5988.	1.3	7
6868	Revealing the optical properties of polycyclic aromatic hydrocarbon clusters with surface formyl groups. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 1207-1215.	2.4	5
6869	Charge-Transfer Resonance and Electromagnetic Enhancement Synergistically Enabling MXenes with Excellent SERS Sensitivity for SARS-CoV-2 S Protein Detection. <i>Nano-Micro Letters</i> , 2021, 13, 52.	14.4	137

#	ARTICLE	IF	CITATIONS
6870	Donor-acceptor based two-dimensional covalent organic frameworks for near-infrared photothermal conversion. <i>Materials Chemistry Frontiers</i> , 2021, 5, 6575-6581.	3.2	17
6871	Theoretical model for N-heterocyclic carbene-catalyzed decarboxylation reactions. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3268-3273.	2.3	19
6872	Pyrazolo[1,5-a]pyrimidine with similar amino-nitro-amino arrangement characteristics to TATB: a novel heat-resistant explosive with fused structure. <i>CrystEngComm</i> , 2021, 23, 2801-2808.	1.3	17
6873	State-crossing from a Locally Excited to an Electron Transfer State(SLEET) Model Rationalizing the Aggregation-induced Emission Mechanism of (Bi)piperidylanthracenes. <i>Chemical Research in Chinese Universities</i> , 2021, 37, 157-161.	1.3	9
6874	Tuning Transition Electric and Magnetic Dipole Moments: [7]Helicenes Showing Intense Circularly Polarized Luminescence. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 686-695.	2.1	107
6875	Hydrogen-Bond-Assisted Exciplex Emitters Realizing Improved Efficiencies and Stabilities in Organic Light Emitting Diodes. <i>Advanced Functional Materials</i> , 2021, 31, 2010100.	7.8	23
6876	A systematic investigation on the impact of the level of oxidation at sulfur and the configuration of R-S-sulfoxide on the solid structure. <i>CrystEngComm</i> , 2021, 23, 4181-4193.	1.3	1
6877	Mpro-SARS-CoV-2 Inhibitors and Various Chemical Reactivity of 1-Bromo- and 1-Chloro-4-vinylbenzene in [3 + 2] Cycloaddition Reactions. <i>Organics</i> , 2021, 2, 1-16.	0.6	16
6878	Novel cocrystals of the potent 1,2,4-thiadiazole-based neuroprotector with carboxylic acids: virtual screening, crystal structures and solubility performance. <i>New Journal of Chemistry</i> , 2021, 45, 3034-3047.	1.4	13
6879	A predictive toolset for the identification of effective lignocellulosic pretreatment solvents: a case study of solvents tailored for lignin extraction. <i>Green Chemistry</i> , 2021, 23, 7269-7289.	4.6	22
6880	Unfolding the Extraction and Complexation Behaviors of Trivalent f-Block Elements by a Tetradentate N,O-Hybrid Phenanthroline Derived Phosphine Oxide Ligand. <i>Inorganic Chemistry</i> , 2021, 60, 2805-2815.	1.9	31
6881	Unusual C-H interactions directed by the $[(C_6H_6)Ru]_2W_8O_{30}(OH)_2$ hybrid anion. <i>CrystEngComm</i> , 2021, 23, 4125-4135.		
6882	Electrostatic repulsion-controlled regioselectivity in nitrene-mediated allylic C-H amidations. <i>Organic Chemistry Frontiers</i> , 0, , .	2.3	11
6883	Antiaromaticity-aromaticity transition of cyclo[16]carbon upon metal encapsulation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8817-8824.	1.3	17
6884	Insights into the existing form of glycolaldehyde in methanol solution: an experimental and theoretical investigation. <i>New Journal of Chemistry</i> , 2021, 45, 8149-8154.	1.4	2
6885	Construction and mechanistic understanding of high-performance all-air-processed perovskite solar cells via mixed-cation engineering. <i>Materials Chemistry Frontiers</i> , 2021, 5, 4244-4253.	3.2	7
6886	Theoretical prediction of chiral actinide endohedral borospherenes. <i>New Journal of Chemistry</i> , 2021, 45, 6803-6810.	1.4	4
6887	Competitive and cooperative n-π* and π-π* interactions in benzaldehyde-formaldehyde: rotational characterization. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8778-8783.	1.3	9

#	ARTICLE	IF	CITATIONS
6888	Intramolecular CH ₃ -migration-controlled cation reactions in the VUV photochemistry of 2-methyl-3-buten-2-ol investigated by synchrotron photoionization mass spectrometry and theoretical calculations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10456-10467.	1.3	4
6889	Supramolecular self-assembly and perfected <i>in vitro</i> / <i>in vivo</i> property of 5-fluorouracil and ferulic acid on the strength of double optimized strategy: the first 5-fluorouracil-phenolic acid nutraceutical cocrystal with synergistic antitumor efficacy. <i>Analyst</i> , 2021, 146, 2506-2519.	1.7	14
6890	Hydrogen versus tetrel bonds in complexes of 3-oxetanone with water and formaldehyde. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7295-7301.	1.3	8
6891	Selective separation of lactic, malic, and tartaric acids based on the hydrophobic deep eutectic solvents of terpenes and amides. <i>Green Chemistry</i> , 2021, 23, 5866-5874.	4.6	25
6892	Reaction mechanisms of cyclo[18]carbon and triplet oxygen. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17545-17552.	1.3	11
6893	Theoretical assessments on the interaction between amino acids and the g-Mg ₃ N ₂ monolayer: dispersion corrected DFT and DFT-MD simulations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17440-17452.	1.3	43
6894	Reactivity of dicationic N-heterocyclic chalcogen carbene analogues with methane and ethene: a theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2419-2429.	1.3	1
6895	The mechanism of the selective binding ability between opiate metabolites and acyclic cucurbit[4]uril: an MD/DFT study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2186-2192.	1.3	1
6896	Polycentric binding in complexes of trimethylamine-N-oxide with dihalogens. <i>RSC Advances</i> , 2021, 11, 6131-6145.	1.7	1
6897	A new 3D Ag(<i>scp</i>) ₂ -based high-energy metal organic frameworks (HE-MOFs): synthesis, crystal structure and explosive performance. <i>New Journal of Chemistry</i> , 2021, 45, 3552-3558.	1.4	3
6898	Sandwich-like low-sensitive nitroamine explosives stabilized by hydrogen bonds and π-π stacking interactions. <i>CrystEngComm</i> , 2021, 23, 1953-1960.	1.3	10
6899	Squaraine Organic Crystals with Strong Dipole Effect Toward Stable Lithium-Organic Batteries. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
6900	Probing the anomeric effect and mechanism of isomerization of oxazinane rings by DFT methods. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 1066-1082.	1.5	8
6901	Designing high energy density flow batteries by tuning active-material thermodynamics. <i>RSC Advances</i> , 2021, 11, 5432-5443.	1.7	8
6902	Mechanistic study of the cooperative palladium/Lewis acid-catalyzed transfer hydrocyanation reaction: the origin of the regioselectivity. <i>Dalton Transactions</i> , 2021, 50, 1233-1238.	1.6	0
6903	Tuning the electronic and nonlinear optical properties of black phosphorus quantum dots by introducing electron-donating/withdrawing molecules (TTF/TCNQ). <i>New Journal of Chemistry</i> , 2021, 45, 12399-12407.	1.4	3
6904	The development of a highly selective fluorescent probe for the rapid detection of HClO in living cells and zebrafish. <i>New Journal of Chemistry</i> , 2021, 45, 12569-12575.	1.4	1
6905	Troubleshooting unstable molecules in chemical space. <i>Chemical Science</i> , 2021, 12, 5566-5573.	3.7	5

#	ARTICLE	IF	CITATIONS
6906	The effect of asymmetric external reorganization energy on electron and hole transport in organic semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15236-15244.	1.3	4
6907	Theoretical and Experimental Insights into the Self-Assembly and Ion Response Mechanisms of Tripodal Quinolinamido-Based Supramolecular Organogels. <i>ChemPlusChem</i> , 2021, 86, 146-154.	1.3	3
6908	Application of hard and soft acid base theory to uncover the destructiveness of Lewis bases to UiO-66 type metal organic frameworks in aqueous solutions. <i>Journal of Materials Chemistry A</i> , 2021, 9, 14868-14876.	5.2	27
6909	Interplay of halogen and hydrogen bonding in a series of heteroleptic iron(III) complexes. <i>CrystEngComm</i> , 2021, 23, 4069-4076.	1.3	6
6910	Microwave-initiated recombination of hydrogen bonds of a perylene diimide supramolecule for PPCP photodegradation. <i>Catalysis Science and Technology</i> , 2021, 11, 3787-3798.	2.1	6
6911	Quantum Computational, Spectroscopic, NHO and Molecular Docking Studies on 1-Methyl-nicotinamide (MNA): An Antithrombotic, Anti-inflammatory, Gastroprotective and Vasoprotective Compound. <i>Asian Journal of Organic & Medicinal Chemistry</i> , 2021, 6, 128-140.	0.1	0
6912	A new anthraquinone derivative as a near UV and visible light photoinitiator for free-radical, thiol-ene and cationic polymerizations. <i>Polymer Chemistry</i> , 2021, 12, 3299-3306.	1.9	15
6913	Catalytic sulfate formation mechanism influenced by important constituents of cloud water via the reaction of SO ₂ oxidized by hypobromic acid in marine areas. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15935-15949.	1.3	1
6914	One dimensional halogen bond design: Br-N versus I-N with fluoroarenes. <i>CrystEngComm</i> , 2021, 23, 6098-6106.	1.3	6
6915	Novel recognition mechanism based on oxidative addition of Pt(II) complex-based luminescent probes for hypochlorite ion detection. <i>Analyst</i> , 2021, 146, 5691-5703.	1.7	4
6916	Possible effects of fluxionality of a cavitand on its catalytic activity through confinement. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15817-15834.	1.3	5
6917	Boosting intermolecular interactions of fused cyclic explosives: the way to thermostable and insensitive energetic materials with high density. <i>New Journal of Chemistry</i> , 2021, 45, 9358-9367.	1.4	13
6918	Dual roles of the electronic effect on selectivity: pincer nickel-electrocatalyzed CO ₂ reduction. <i>Catalysis Science and Technology</i> , 2021, 11, 874-885.	2.1	6
6919	Photophysical properties of N-methyl and N-acetyl substituted alloxazines: a theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13734-13744.	1.3	4
6920	Tartrate-stabilized titanium-oxo clusters containing sulfonate chromophore ligands: synthesis, crystal structures and photochemical properties. <i>New Journal of Chemistry</i> , 2021, 45, 10930-10939.	1.4	2
6921	Superatomic Rydberg State Excitation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
6922	Use of Low Frequency Raman Bands to Identify Non-planar Deformation of Ni(II) Meso-tetraphenylporphyrin Induced by Axial Ligands. <i>Chinese Journal of Chemical Physics</i> , 0, , .	0.6	1
6923	A property-oriented adaptive design framework for rapid discovery of energetic molecules based on small-scale labeled datasets. <i>RSC Advances</i> , 2021, 11, 25764-25776.	1.7	2

#	ARTICLE	IF	CITATIONS
6942	Extraction and separation of Pd(II)/Pt(IV) by neutral sulfur-containing extractant from hydrochloric acid medium. <i>New Journal of Chemistry</i> , 2021, 45, 19467-19475.	1.4	7
6943	Novel thermally activated delayed fluorescence materials by high-throughput virtual screening: going beyond donor-acceptor design. <i>Journal of Materials Chemistry C</i> , 2021, 9, 3324-3333.	2.7	27
6944	Where is the best substitution position for amino groups on carbon dots: a computational strategy toward long-wavelength red emission. <i>Journal of Materials Chemistry C</i> , 2021, 9, 14444-14452.	2.7	9
6945	Mutually exclusive hole and electron transfer coupling in cross stacked acenes. <i>Chemical Science</i> , 2021, 12, 5064-5072.	3.7	14
6946	Structure and solvation dynamics of the hydroxide ion in ice-like water clusters: a CCSD(T) and carâ€parrinello molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18990-18998.	1.3	1
6947	Electronic structures and properties of dianionic pentacarbonyls $[\text{TM}(\text{CO})_5]^{2-}$ (TM = Cr, Mo, W). <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18640-18646.	1.3	1
6948	Inspiration for revival of old drugs: improving solubility and avoiding hygroscopicity of pipemidic acid by forming two pharmaceutical salts based on charge-assisted hydrogen bond recognitions. <i>New Journal of Chemistry</i> , 2021, 45, 19704-19713.	1.4	3
6949	Comparative study on the impact of through-space charge transfer over the electroluminescence performance of delayed fluorescence molecules. <i>Journal of Materials Chemistry C</i> , 2021, 9, 14808-14814.	2.7	15
6950	Endowing nitro-compounds with bright and stimuli-responsive luminescence based on propeller-like AIEgens. <i>Journal of Materials Chemistry C</i> , 2021, 9, 12177-12183.	2.7	8
6951	Highly efficient T-shaped deep-red thermally activated delayed fluorescence emitters: substitution position effect. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21883-21892.	1.3	20
6952	Replacing hybrid density functional theory: motivation and recent advances. <i>Chemical Society Reviews</i> , 2021, 50, 8470-8495.	18.7	80
6953	Cation- π dipole interaction that creates ordered ion channels in an anion exchange membrane for fast OH^- conduction. <i>AIChE Journal</i> , 2021, 67, e17133.	1.8	53
6954	Effects of anthocyanins on β -lactoglobulin glycooxidation: a study of mechanisms and structure-activity relationship. <i>Food and Function</i> , 2021, 12, 10550-10562.	2.1	8
6955	The effect of size, charge state and composition on the binding of propene to yttrium-doped gold clusters. <i>RSC Advances</i> , 2021, 11, 29186-29195.	1.7	6
6956	From mono-rings to bridged bi-rings to caged bi-rings: a promising design strategy for all-nitrogen high-energy-density materials N10 and N12. <i>New Journal of Chemistry</i> , 2021, 45, 6379-6385.	1.4	7
6957	Enhanced Solubility and Antitumor Activity of Curcumin via Breaking and Rebuilding of the Hydrogen Bond. <i>ACS Applied Bio Materials</i> , 2021, 4, 918-927.	2.3	16
6958	Characterizing the lone pair- π hole interaction in complexes of ammonia with perfluorinated arenes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9121-9129.	1.3	11
6959	Theoretical introduction and design of Si/N catalysts as efficient reducing agents in CO_2 hydroboration by planar Si/N π -conjugated molecules. <i>Structural Chemistry</i> , 2021, 32, 1327-1340.	1.0	2

#	ARTICLE	IF	CITATIONS
6960	Turning-on persistent luminescence out of chromium-doped zinc aluminate nanoparticles by instilling antisite defects under mild conditions. <i>Nanoscale</i> , 2021, 13, 8514-8523.	2.8	10
6961	Enantioseparation of 5,5-Dibromo-2,2-dichloro-3-selanyl-4,4-bipyridines on Polysaccharide-Based Chiral Stationary Phases: Exploring Chalcogen Bonds in Liquid-Phase Chromatography. <i>Molecules</i> , 2021, 26, 221.	1.7	17
6962	All-polymer solar cells with efficiency approaching 16% enabled using a dithieno[3,2- <i>b</i> :3,4- <i>b'</i> :5,6]benzo[1,2- <i>c</i>][1,2,5]thiadiazole (fDTBT)-based polymer donor. <i>Journal of Materials Chemistry A</i> , 2021, 9, 8975-8983.	1.4	54
6963	Supramolecular BODIPY based dimers: synthesis, computational and spectroscopic studies. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 8118-8127.	1.5	2
6964	Curled cation structures accelerate the dynamics of ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21042-21064.	1.3	14
6965	Structural and electronic analysis of the octarepeat region of prion protein with four Cu ²⁺ by polarizable MD and QM/MM simulations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21568-21578.	1.3	2
6966	Phenyl-triggered photophysical switching between normal fluorescence and delayed fluorescence in phthalonitrile-based luminophores. <i>Aggregate</i> , 2021, 2, 145-150.	5.2	16
6967	A rechargeable zinc-air battery based on zinc peroxide chemistry. <i>Science</i> , 2021, 371, 46-51.	6.0	551
6968	Origins of ligand-controlled diastereoselectivity in dirhodium-catalysed direct amination of aliphatic C(sp ³)-H bonds. <i>Catalysis Science and Technology</i> , 2021, 11, 6960-6964.	2.1	2
6969	A study on the rules of ligands in highly efficient Ru(II) amide/AC catalysts for acetylene hydrochlorination. <i>Catalysis Science and Technology</i> , 2021, 11, 7347-7358.	2.1	12
6970	Effects of lateral-chain thiophene fluorination on morphology and charge transport of BDT-T based small molecule donors: a study with multiscale simulations. <i>Journal of Materials Chemistry C</i> , 2021, 9, 14637-14647.	2.7	5
6971	Topological unraveling of the [3+2] cycloaddition (32CA) reaction between <i>N</i> -methylphenylnitrone and styrene catalyzed by the chromium tricarbonyl complex using electron localization function and catastrophe theory. <i>New Journal of Chemistry</i> , 2021, 45, 20342-20351.	1.4	6
6972	Rhodamine phenol-based fluorescent probe for the visual detection of GB and its simulant DCP. <i>New Journal of Chemistry</i> , 2021, 45, 7564-7570.	1.4	9
6973	Anti-electrostatic hydrogen bonding between anions of ionic liquids: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7426-7433.	1.3	8
6974	Electronic structure of polypyrrole composited with a low percentage of graphene nanofiller. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8557-8570.	1.3	8
6975	A novel photochemical sensor based on quinoline-functionalized phenazine derivatives for multiple substrate detection. <i>New Journal of Chemistry</i> , 2021, 45, 5040-5048.	1.4	5
6976	Ligands enhanced the Ac-C≡C triple bond. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10244-10250.	1.3	2
6977	Geometrical and energetic characteristics of Se-Se interactions in crystal structures of organoselenium molecules. <i>CrystEngComm</i> , 2021, 23, 3383-3390.	1.3	1

#	ARTICLE	IF	CITATIONS
6978	Crystal structure, DFT studies and thermal characterization of new luminescent stannate (IV) based inorganic-organic hybrid compound. <i>Journal of Molecular Structure</i> , 2021, 1224, 129266.	1.8	22
6979	Crystal Packing Studies, Thermal Properties and Hirshfeld Surface Analysis in the Zn(II) Complex of 3-Aminopyridine with Thiocyanate as Co-Ligand. <i>Open Journal of Inorganic Chemistry</i> , 2021, 11, 63-84.	0.7	2
6980	Synergistic Interplay between Asymmetric Backbone Conformation, Molecular Aggregation, and Charge-Carrier Dynamics in Fused-Ring Electron Acceptor-Based Bulk Heterojunction Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 2961-2970.	4.0	12
6981	Experimental and Theoretical Studies on Effects of Structural Modification of Tin Nanoclusters for Third-Order Nonlinear Optical Properties. <i>Inorganic Chemistry</i> , 2021, 60, 1885-1892.	1.9	21
6982	Molecular Mechanism and Absorption Performance Evaluation of CO ₂ Capture from the PCC Process by Monoethanolamine-Based Deep Eutectic Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 1483-1493.	1.8	20
6983	Triplet State Baird Aromaticity in Macrocycles: Scope, Limitations, and Complications. <i>Journal of Physical Chemistry A</i> , 2021, 125, 570-584.	1.1	10
6984	Optical Properties of the Atomically Precise C ₄ Core [Au ₉ (PPh ₃) ₈] ³⁺ Cluster Probed by Transient Absorption Spectroscopy and Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2033-2044.	1.5	8
6985	Through-Space Exciton Delocalization in Segregated HJ-Crystalline Molecular Aggregates. <i>Journal of Physical Chemistry A</i> , 2021, 125, 943-953.	1.1	7
6986	Computational study of 1,2,3-triazol-5-ylidenes with p-block element substituents. <i>New Journal of Chemistry</i> , 2021, 45, 4802-4809.	1.4	2
6987	Spectral analysis and density functional theory study of tert-butylhydroquinone. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, 70, 053102.	0.2	3
6988	Water distribution in confined space of single-wall carbon nanotube. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, .	0.2	2
6989	Broadening the Horizon of the Bell-Evans-Polanyi Principle towards Optically Triggered Structure Planarization. <i>Angewandte Chemie</i> , 2021, 133, 7281-7288.	1.6	4
6990	Enhancement in the Photovoltaic Properties of Hole Transport Materials by End-Capped Donor Modifications for Solar Cell Applications. <i>Bulletin of the Korean Chemical Society</i> , 2021, 42, 597-610.	1.0	49
6991	Molecular understanding of the LCST phase behaviour of P(MEO ₂ MA-b-OEGMA) block copolymers. <i>Molecular Simulation</i> , 2021, 47, 299-305.	0.9	2
6992	Sulfonated Reverse Osmosis Membrane Fabricated with Comonomer Having Excellent Scaling and Fouling Resistance. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 3095-3104.	1.8	12
6993	A DFT investigation of anion-π interactions between halogen oxyanions (XO ₃ ⁻ , X = Cl, Br, I) and aromatic π-systems (benzene and coronene). <i>IOP Conference Series: Materials Science and Engineering</i> , 2021, 1046, 012017.	0.3	0
6994	Prediction of azulene-based nanographene-like materials. <i>Diamond and Related Materials</i> , 2021, 112, 108235.	1.8	4
6995	Study on the growth behavior and photoelectron spectroscopy of neodymium-doped silicon nanoclusters NdSi _{0/1} (n = 0-20) with a double-hybrid density functional theory. <i>Journal of Molecular Modeling</i> , 2021, 27, 86.	0.8	2

#	ARTICLE	IF	CITATIONS
6996	On Close Parallels between the Zintl-Based Superatom Ge ₉ Be and Chalcogen Elements. <i>Inorganic Chemistry</i> , 2021, 60, 3196-3206.	1.9	8
6997	Cefoperazone metal complexes and their antimicrobial investigations. <i>Journal of the Turkish Chemical Society, Section A: Chemistry</i> , 0, , 375-390.	0.4	1
6998	Theoretical Studies of Rare-Earth-Catalyzed [3 + 2] Annulation of Aromatic Aldimine with Styrene: Mechanism and Origin of Diastereoselectivity. <i>Journal of Organic Chemistry</i> , 2021, 86, 4236-4244.	1.7	16
6999	Assembly of [Ni(Schiff)] Films on an Inert Surface: A Multiscale Computational Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2926-2937.	1.5	4
7000	HMNTA Complexes of Tetravalent Metal Ions: On the Roles of Carbonyl Oxygen and Amine Nitrogen in the Stabilization of Gas-Phase M(HMNTA) ₂ ⁴⁺ Complexes. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 700-706.	1.2	2
7001	Serotonin and Melatonin Show Different Modes of Action on α -2 Protofibril Destabilization. <i>ACS Chemical Neuroscience</i> , 2021, 12, 799-809.	1.7	24
7002	Theoretical Framework for Encapsulation of Inorganic B ₁₂ N ₁₂ Nanoclusters with Alkaline Earth Metals for Efficient Hydrogen Adsorption: A Step Forward toward Hydrogen Storage Materials. <i>Inorganic Chemistry</i> , 2021, 60, 2816-2828.	1.9	43
7003	Bifurcated Halogen Bonding Involving Two Rhodium(I) Centers as an Integrated π -Hole Acceptor. <i>Jacs Au</i> , 2021, 1, 354-361.	3.6	39
7004	C3N Non-metallic Catalyst for Propane Dehydrogenation: A Density Functional Theory Study. <i>Catalysis Letters</i> , 2021, 151, 3154-3164.	1.4	0
7005	Efficient fixation of CO ₂ into carbonates by tertiary N-functionalized poly(ionic liquids): Experimental-theoretical investigation. <i>Journal of CO₂ Utilization</i> , 2021, 44, 101427.	3.3	30
7006	Effective Separation of Condensed Arenes from High-Temperature Coal Tar and Insight into Related Intermolecular Interactions. <i>Energy & Fuels</i> , 2021, 35, 4267-4272.	2.5	6
7007	The Adsorption Mechanism of Montmorillonite for Different Tetracycline Species at Different pH Conditions: the Novel Visual Analysis of Intermolecular Interactions. <i>Water, Air, and Soil Pollution</i> , 2021, 232, 1.	1.1	14
7008	Comparison of Ferroptosis-Inhibitory Mechanisms between Ferrostatin-1 and Dietary Stilbenes (Piceatannol and Astringin). <i>Molecules</i> , 2021, 26, 1092.	1.7	7
7009	Accelerated liquefaction of vulcanized natural rubber by thermo-oxidative degradation. <i>Polymer Bulletin</i> , 2022, 79, 1767-1786.	1.7	11
7010	Electronic Properties of Triangle Molybdenum Disulfide (MoS ₂) Clusters with Different Sizes and Edges. <i>Molecules</i> , 2021, 26, 1157.	1.7	8
7011	Novel donor-acceptor non-fullerene metal-organic solar cells based on open edge Sc@BN: a DFT and TD-DFT study. <i>Journal of the Iranian Chemical Society</i> , 2021, 18, 2271-2282.	1.2	4
7012	Biomass-Derived Ionic Liquids Based on a 5-HMF Platform Chemical: Synthesis, Characterization, Biological Activity, and Tunable Interactions at the Molecular Level. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 3552-3570.	3.2	27
7013	Density Functional Theory and Information-Theoretic Approach Study on the Origin of Homochirality in Helical Structures. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1269-1278.	1.1	17

#	ARTICLE	IF	CITATIONS
7014	Boosting Room Temperature Phosphorescence Performance by Alkyl Modification for Intravital Orthotopic Lung Tumor Imaging. <i>Small</i> , 2021, 17, e2005449.	5.2	41
7015	Facile Synthesis of Nitrogen-Doped [(6,6)-m ⁸ n]Cyclacene Carbon Nanobelts by a One-Pot Self-Condensation Reaction. <i>Journal of the American Chemical Society</i> , 2021, 143, 2716-2721.	6.6	38
7016	Responsive Zwitterionic Polymers with Humidity and Voltage Dual-Switching for Multilevel Data Encryption and Anticounterfeiting. <i>Chemistry of Materials</i> , 2021, 33, 1477-1488.	3.2	10
7017	Electron-Donating C-NH ₂ Link Backbone for Highly Alkaline and Mechanical Stable Anion Exchange Membranes. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 10490-10499.	4.0	22
7018	Study on UV Spectrum and Antioxidant Properties of 3-tert-Butyl-4-hydroxyanisole Molecule. <i>Russian Journal of Physical Chemistry A</i> , 2021, 95, 343-348.	0.1	2
7019	Experimental and DFT studies on Hexacoordinated acyl(alkyl)and Pentacoordinated Hydroxyalkyl(phosphinite)rhodium(III). <i>Catalytic Hydrolysis of Ammonia Borane. European Journal of Inorganic Chemistry</i> , 2021, 2021, 879-891.	1.0	4
7020	A novel aggregation induced emission (AIE) fluorescence probe by combining tetraphenylethylene and 2- ϵ ,3- ϵ -O-isopropylideneadenosine for localizing Golgi apparatus. <i>Sensors and Actuators B: Chemical</i> , 2021, 329, 129245.	4.0	28
7021	Quantum chemical study in exploring the role of donor-acceptor interactions in 1,3-bis carbene-stabilized guanidinium cations. <i>Journal of Molecular Modeling</i> , 2021, 27, 87.	0.8	2
7022	Hydrogen bonded complexes of rhodanine with H ₂ X/CH ₃ XH (X=O, S, Se). <i>Computational and Theoretical Chemistry</i> , 2021, 1196, 113134.	1.1	5
7023	Probing the dynamical behavior in glass transition of PVPh-PEO blend. <i>Journal of Non-Crystalline Solids</i> , 2021, 554, 120561.	1.5	0
7024	Theoretical investigation on the degradation of methyl vinyl ketone initiated by \cdot OH and \cdot Cl in the atmosphere and aqueous particles: Mechanism, kinetics, and environmental impact analysis. <i>Atmospheric Environment</i> , 2021, 246, 118107.	1.9	7
7025	The Interaction Energy between Solvent Molecules and Graphene as an Effective Descriptor for Graphene Dispersion in Solvents. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5167-5171.	1.5	3
7026	Enhanced Two-Photon Absorption in Two Triphenylamine-Based All-Organic Compounds. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1870-1879.	1.1	4
7027	Intermolecular Interactions between Thiocyanato Ligands in Metal Complexes. <i>Crystal Growth and Design</i> , 2021, 21, 1636-1644.	1.4	4
7028	One-Dimensional Silver-Thiolate Cluster-Assembly: Effect of Argentophilic Interactions on Excited-State Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2154-2159.	2.1	10
7029	Design, docking, and DFT investigations of 2,6-bis(3,4-dihydroxyphenyl)-3-phenethylpiperidin-4-one. <i>Heliyon</i> , 2021, 7, e06127.	1.4	18
7030	Theoretical study of the mixed π -conjugated bridge effect on the nonlinear optical properties of corannulene derivative. <i>Journal of Molecular Modeling</i> , 2021, 27, 66.	0.8	5
7031	Insights into the Chiral Phosphoric Acid-Catalyzed Dynamic Kinetic Asymmetric Hydroamination of Racemic Allenes: An Allyl Carbocation/Phosphate Pair Mechanism. <i>Journal of Organic Chemistry</i> , 2021, 86, 4121-4130.	1.7	8

#	ARTICLE	IF	CITATIONS
7032	Comparison of Anion–Anion Halogen Bonds with Neutral–Anion Halogen Bonds in the Gas Phase and Polar Solvents. <i>ChemPlusChem</i> , 2021, 86, 232-240.	1.3	15
7033	Dual-ionic imidazolium salts to promote synthesis of cyclic carbonates at atmospheric pressure. <i>Green Energy and Environment</i> , 2022, 7, 1327-1339.	4.7	32
7034	A Theoretical Study on the Degenerate Cope Rearrangement of Hypostrophene Using the RRKM Theory and Topological Approaches. <i>ChemistrySelect</i> , 2021, 6, 1607-1615.	0.7	1
7035	Quantum Chemical Simulation of the Qy Absorption Spectrum of Zn Chlorin Aggregates for Artificial Photosynthesis. <i>Molecules</i> , 2021, 26, 1086.	1.7	1
7036	Molecular engineering of triphenylamine–based metal–free organic dyes for dye–sensitized solar cells. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26620.	1.0	7
7038	Impact of \hat{P}^{ST} on Delayed Fluorescence Rate, Lifetime, and Intensity Ratio of Tetrahedral Cu(I) Complexes: Theoretical Simulation in Solution and Solid Phases. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2232-2244.	2.1	6
7039	Ultralong and Color-Tunable Room-Temperature Phosphorescence Based on Commercial Melamine for Anticounterfeiting and Information Recognition. <i>Analytical Chemistry</i> , 2021, 93, 4075-4083.	3.2	31
7040	ZSM-5(8T)@ γ -Al ₂ O ₃ supported AlCl ₃ core-shell catalyst: Mechanism research on disproportionation reaction of methylchlorosilanes. <i>Inorganica Chimica Acta</i> , 2021, 516, 120148.	1.2	4
7041	Control of quantum interference in single-molecule junctions via Jahn-Teller distortion. <i>Cell Reports Physical Science</i> , 2021, 2, 100329.	2.8	12
7042	Novel naphthalimide derived fluorescent probe based on aggregation-induced emission for turn-on detection of hydrogen sulfide. <i>Tetrahedron</i> , 2021, 81, 131923.	1.0	17
7043	Mechanistic insights into the C(sp ³)-H heteroarylation of amides and Fukui function analysis of regioselectivity. <i>Molecular Catalysis</i> , 2021, 502, 111394.	1.0	8
7044	Structure and Reactivity of IrO _x Nanoparticles for the Oxygen Evolution Reaction in Electrocatalysis: An Electronic Structure Theory Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4379-4390.	1.5	15
7045	Broadening the Horizon of the Bell–Evans–Polanyi Principle towards Optically Triggered Structure Planarization. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 7205-7212.	7.2	18
7046	Quantum chemical investigation of the antiradical property of avenanthramides, oat phenolics. <i>Heliyon</i> , 2021, 7, e06125.	1.4	9
7047	Aromaticity indices, electronic structural properties, and fuzzy atomic space investigations of naphthalene and its aza-derivatives. <i>Heliyon</i> , 2021, 7, e06138.	1.4	37
7048	Do Secondary Electrostatic Interactions Influence Multiple Dihydrogen Bonds? A π - π Array on an Amine–Borane Aza–Coronand: Theoretical Studies and Synthesis. <i>ChemPhysChem</i> , 2021, 22, 593-605.	1.0	9
7049	Synthesis, Cytotoxic Activity, Crystal Structure, DFT Studies and Molecular Docking of 3-Amino-1-(2,5-dichlorophenyl)-8-methoxy-1H-benzo[f]chromene-2-carbonitrile. <i>Crystals</i> , 2021, 11, 184.	1.0	27
7050	When Electrons Step in: Polarizing Effects Explored with Triisobutylaluminum. <i>Inorganic Chemistry</i> , 2021, 60, 2872-2877.	1.9	1

#	ARTICLE	IF	CITATIONS
7051	A tris-spiro metalla-aromatic system featuring Craig-MÃ¶bius aromaticity. Nature Communications, 2021, 12, 1319.	5.8	35
7052	Degradation mechanisms, kinetics and eco-toxicity assessment of 2,4-Dinitrophenol by oxygen-containing free radicals in aqueous solution. Molecular Physics, 2021, 119, e1886365.	0.8	6
7053	Steric and Electronic Effects on the Structure and Photophysical Properties of Hg(II) Complexes. Inorganic Chemistry, 2021, 60, 3851-3870.	1.9	7
7054	A New Brominated Norsesquiterpene Glycoside From the Rhizomes of <i>Acorus tatarinowii</i> Schott. Natural Product Communications, 2021, 16, 1934578X2199226.	0.2	0
7055	Theoretical Calculation and Structural Analysis of the Cocrystals of Three Flavonols with Praziquantel. Crystal Growth and Design, 2021, 21, 2292-2300.	1.4	27
7056	Ozonation Treatment Increases Chlorophenylacetonitrile Formation in Downstream Chlorination or Chloramination. Environmental Science & Technology, 2021, 55, 3747-3755.	4.6	19
7057	Hydrogen bonding interactions in the 1,1,1,3,3,3-hexafluoro-2-propanolâ€”1,4-dioxane complex: Rotational spectroscopy and density functional theory calculations. Journal of Molecular Spectroscopy, 2021, 376, 111408.	0.4	2
7060	Effective suppression of conductance in multichannel molecular wires. Cell Reports Physical Science, 2021, 2, 100342.	2.8	8
7061	Theoretical Study of the Structure and Property of Ionic Liquids as Corrosion Inhibitor. , 0, , .		3
7062	3,4-Methylenedioxypropylvalerone (MDPV) Sensing Based on Electropolymerized Molecularly Imprinted Polymers on Silver Nanoparticles and Carboxylated Multi-Walled Carbon Nanotubes. Nanomaterials, 2021, 11, 353.	1.9	10
7063	On the Proton-Bound Noble Gas Dimers (Ng-H-Ng) ⁺ and (Ng-H-Ngâ€”) ⁺ (Ng, Ngâ€” = He-Xe): Relationships between Structure, Stability, and Bonding Character. Molecules, 2021, 26, 1305.	1.7	8
7064	Mechanistic Understanding of Baseâ€”Catalyzed Aldimine/Ketoamine Condensations: An Old Story and A New Model. Asian Journal of Organic Chemistry, 2021, 10, 634-641.	1.3	7
7065	The sequential activation of H ₂ and N ₂ mediated by the gas-phase Sc ₃ N ⁺ clusters: Formation of amido unit. Journal of Chemical Physics, 2021, 154, 054307.	1.2	11
7066	Comprehensive Bonding Analysis of Tetravalent f-Element Complexes of the Type [M(salen) ₂]. Inorganic Chemistry, 2021, 60, 2514-2525.	1.9	23
7067	Highâ€”capacity hydrogen storage on Liâ€”decorated B ₁₆ N ₁₆ . Environmental Progress and Sustainable Energy, 2021, 40, e13623.	1.3	3
7068	Theoretical investigations on the density, detonation performance and stability of fluorinated hexanitroadamantanes. Structural Chemistry, 2021, 32, 1651-1657.	1.0	0
7069	Insights for diastereoselectivity in synthesis of 2,3-dihydropyrroles by photochemical ring contraction of 1,4-dihydropyridines. Tetrahedron Letters, 2021, 65, 152797.	0.7	3
7070	Mesoionic tetrazolium-5-aminides: Synthesis, molecular and crystal structures, UVâ€”vis spectra, and DFT calculations. Beilstein Journal of Organic Chemistry, 2021, 17, 385-395.	1.3	3

#	ARTICLE	IF	CITATIONS
7071	A density matrix renormalization group investigation on the electronic states of $\langle \text{MnGe} \rangle_n$ ($n = 1-3$) clusters. International Journal of Quantum Chemistry, 2021, 121, e26619.	1.0	10
7072	Quantum Simulations of Hydrogen Bonding Effects in Glycerol Carbonate Electrolyte Solutions. Journal of Physical Chemistry B, 2021, 125, 2157-2166.	1.2	7
7073	Intramolecular Electric Field Construction in Metal Phthalocyanine as Dopant-Free Hole Transporting Material for Stable Perovskite Solar Cells with $>21\%$ Efficiency. Angewandte Chemie, 2021, 133, 6364-6369.	1.6	11
7074	Intramolecular Electric Field Construction in Metal Phthalocyanine as Dopant-Free Hole Transporting Material for Stable Perovskite Solar Cells with $>21\%$ Efficiency. Angewandte Chemie - International Edition, 2021, 60, 6294-6299.	7.2	101
7075	Morphological engineering of carbon-based materials: in the quest of efficient catalysts for overall water splitting. International Journal of Hydrogen Energy, 2021, 46, 7284-7296.	3.8	12
7076	Excited-state electronic properties, structural studies, noncovalent interactions, and inhibition of the novel severe acute respiratory syndrome coronavirus 2 proteins in Ripretinib by first-principle simulations. Journal of Molecular Liquids, 2021, 324, 115134.	2.3	23
7077	15.3% Efficiency All-Small-Molecule Organic Solar Cells Achieved by a Locally Asymmetric F, Cl Disubstitution Strategy. Advanced Science, 2021, 8, 2004262.	5.6	76
7078	Electron configurations at 3d orbital of metal ion determining charge transition process in memory devices. Science China Materials, 2021, 64, 1713-1722.	3.5	7
7079	Molecular docking, spectroscopic, and quantum chemical studies on aromatic heterocycle tetrakis(4-pyridyl)cyclobutane regioisomers: potential membrane-permeable inhibitors. Journal of Molecular Modeling, 2021, 27, 94.	0.8	4
7080	The Role of Benzylpenicilloyl Epimers in Specific IgE Recognition. Frontiers in Pharmacology, 2021, 12, 585890.	1.6	3
7081	Large-Scale Analysis of Bioactive Ligand Conformational Strain Energy by <i>Ab Initio</i> Calculation. Journal of Chemical Information and Modeling, 2021, 61, 1180-1192.	2.5	16
7082	Computational analysis the relationships of energy and mechanical properties with sensitivity for FOX-7 based PBXs via MD simulation. Royal Society Open Science, 2021, 8, 200345.	1.1	12
7083	Intramolecular-Locked High Efficiency Ultrapure Violet-Blue (CIE $y < 0.046$) Thermally Activated Delayed Fluorescence Emitters Exhibiting Amplified Spontaneous Emission. Advanced Functional Materials, 2021, 31, 2009488.	7.8	88
7084	Metal-Organic Layers with an Enhanced Two-Photon Absorption Cross-Section and Up-Converted Emission. Chemistry of Materials, 2021, 33, 1618-1624.	3.2	8
7085	Effect of Water Microsolvation on the Excited-State Proton Transfer of 3-Hydroxyflavone Enclosed in β -Cyclodextrin. Molecules, 2021, 26, 843.	1.7	8
7086	A Nitroxide Containing Organic Molecule in a Deep Eutectic Solvent for Flow Battery Applications. Journal of the Electrochemical Society, 2021, 168, 020527.	1.3	29
7087	Full insights into the roles of pH on hydroxylation of aromatic acids/bases and toxicity evaluation. Water Research, 2021, 190, 116689.	5.3	22
7088	Synthesis, structural and computational studies of new tetrazole derivatives. Journal of Molecular Structure, 2021, 1226, 129341.	1.8	8

#	ARTICLE	IF	CITATIONS
7089	Guanidine- <i>Amide</i> -Catalyzed Aza-Henry Reaction of Isatin-Derived Ketimines: Origin of Selectivity and New Catalyst Design. <i>Molecules</i> , 2021, 26, 1965.	1.7	1
7090	Adaptive Aromaticity in Metallasilapentalynes. <i>Organometallics</i> , 2021, 40, 899-906.	1.1	16
7091	Aromaticity of <i>ortho</i> and <i>meta</i> π -Cycloparaphenylene and Their Dications: Induced Magnetic Field Analysis with Localized and Delocalized Orbitals in Strained Nano hoops. <i>ChemPhysChem</i> , 2021, 22, 741-751.	1.0	6
7092	Van der Waals interactions of the disulfide bond revealed: A microwave spectroscopic study of the diethyl disulfide-argon complex. <i>Journal of Chemical Physics</i> , 2021, 154, 124306.	1.2	0
7093	Probing the geometric and electronic structures of the lanthanide oxide HoO_n ($n=1/0$ ($n=1-3$) clusters. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 248, 119287.	2.0	2
7094	Density functional theory study on optical and electronic properties of co-doped graphene quantum dots based on different nitrogen doping patterns. <i>Diamond and Related Materials</i> , 2021, 113, 108264.	1.8	35
7095	Effects of the number of imidazoline ring and the length of alkyl group chain of imidazoline derivatives on corrosion inhibition of carbon steel in HCl solution: Molecular simulation and experimental validation. <i>Petroleum</i> , 2022, 8, 447-457.	1.3	6
7096	Quantum chemical studies on molecular structure, AIM, ELF, RDG and antiviral activities of hybrid hydroxychloroquine in the treatment of COVID-19: Molecular docking and DFT calculations. <i>Journal of King Saud University - Science</i> , 2021, 33, 101334.	1.6	86
7097	Relative Strengths of a Pnictogen and a Tetrel Bond and Their Mutual Effects upon One Another. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2631-2641.	1.1	13
7099	Photooxidation of Isoprene by Titanium Oxide Cluster Anions with Dimensions up to a Nanosize. <i>Journal of the American Chemical Society</i> , 2021, 143, 3951-3958.	6.6	15
7100	Chiral Spiro-Axis Induced Blue Thermally Activated Delayed Fluorescence Material for Efficient Circularly Polarized OLEDs with Low Efficiency Roll-Off. <i>Angewandte Chemie</i> , 2021, 133, 8516-8521.	1.6	29
7101	Phenyl Trifluoromethane sulfonate as a novel electrolyte additive for enhancing performance of $\text{LiNiO}_2\text{-6CoO}_2\text{-2MnO}_2\text{-2O}_2$ /Graphite cells working in wide temperature ranges. <i>Journal of Power Sources</i> , 2021, 487, 229416.	4.0	13
7102	Light-Induced Change of Arginine Conformation Modulates the Rate of Adenosine Triphosphate to Cyclic Adenosine Monophosphate Conversion in the Optogenetic System Containing Photoactivated Adenylyl Cyclase. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1215-1225.	2.5	13
7103	Highly Efficient Simple-Structure Sky-Blue Organic Light-Emitting Diode Using a Bicarbazole/Cyanopyridine Bipolar Host. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 13459-13469.	4.0	36
7104	New evidence on non-covalent interactions in crystalline halo-substituted boron difluoride acetylacetonates from vibrational spectra, model calculations and visualization program tools. <i>Journal of Molecular Structure</i> , 2021, 1227, 129532.	1.8	2
7105	Copper-carbon clusters Cu_nC_m ($n, m=1-6$): Segregation, bonding and Raman spectra. <i>Materials Today Communications</i> , 2021, 26, 102035.	0.9	3
7106	Multiple Functional Organocatalyst-Promoted Inert C-C Activation: Mechanism and Origin of Selectivities. <i>ACS Catalysis</i> , 2021, 11, 3443-3454.	5.5	38
7107	Nitrene-mediated intermolecular N-N coupling for efficient synthesis of hydrazides. <i>Nature Chemistry</i> , 2021, 13, 378-385.	6.6	65

#	ARTICLE	IF	CITATIONS
7108	Spatial donor/acceptor architecture for intramolecular charge-transfer emitter. Chinese Chemical Letters, 2021, 32, 1245-1248.	4.8	17
7109	Using Bases as Initiators to Isomerize Allylic Alcohols: Insights from Density Functional Theory Studies. Journal of Physical Chemistry A, 2021, 125, 2316-2323.	1.1	1
7110	Franck-Condon Tuning of Optical Cycling Centers by Organic Functionalization. Physical Review Letters, 2021, 126, 123002.	2.9	26
7111	Condensed-phase relative Gibbs free energy and E/Z descriptors for 2-acetylthiophene and 2-acetylthiophene-N1-phenyl thiosemicarbazones. Journal of Molecular Modeling, 2021, 27, 101.	0.8	1
7112	Computational Exploration of Ambiphilic Reactivity of Azides and Sustmann's Paradigmatic Parabola. Journal of Organic Chemistry, 2021, 86, 5792-5804.	1.7	11
7113	Reactivity of Cobalt Clusters Co_6^{+0} with Dinitrogen: Superatom Co_6^{+0} and Superatomic Complex $\text{Co}_5\text{N}_6^{+0}$. Journal of Physical Chemistry A, 2021, 125, 2130-2138.	1.1	8
7114	Strong Interaction between Cyclo[18]Carbon and Graphene. Advanced Theory and Simulations, 2021, 4, 2100022.	1.3	16
7115	$[\text{Sn}_8]^{6+}$ Bridged Mixed Valence Zn I / Zn II in $\{[\text{K}_2\text{ZnSn}_8(\text{ZnMes})_2]^{4+}\}^{-}$ Inverse Sandwich-Type Cluster Supported by a Zn I \sim Zn I Bond. Angewandte Chemie, 2021, 133, 10078-10083.	1.6	0
7116	The explicit role of electron exchange in the hydrogen bonded molecular complexes. Journal of Computational Chemistry, 2021, 42, 870-882.	1.5	11
7117	Magnetism, chemical bonding of Co_5M clusters ($\text{M} = \text{Ag}$). European Physical Journal Plus, 2021, 136, 112		2
7118	Intermolecular interactions between the heavy alkenes $\text{H}_2\text{Si} = \text{TH}_2$ ($\text{T} = \text{C}, \text{Si}, \text{Ge}, \text{Sn}, \text{Pb}$) and acetylene. Journal of Molecular Modeling, 2021, 27, 110.	0.8	5
7119	Theoretical prediction of the host of Helium: $(\text{HSiO}_3/2)_n$ ($n = 4, 6, 8$) POSS material. Materials Today Communications, 2021, 26, 101972.	0.9	0
7120	Experimental and theoretical study on the hydrogen bond interactions between ascorbic acid and glycine. Zeitschrift Fur Physikalische Chemie, 2021, 235, 1777-1790.	1.4	2
7121	Synthesizing Hindered Structure Poly (p-Phenylenediamine) by Enzymatic Catalysis and Evaluating Its Antioxidation Mechanism in Biodegradable Castor Oils. JAOCS, Journal of the American Oil Chemists' Society, 2021, 98, 673-682.	0.8	2
7122	Pagoda[5]arene with Large and Rigid Cavity for the Formation of 1^+2^- Host-Guest Complexes and Acid/Base-Responsive Crystalline Vapochromic Properties. CCS Chemistry, 2022, 4, 318-330.	4.6	53
7123	Thermochemical Properties and Growth Mechanism of the Ag-Doped Germanium Clusters, AgGe_n with $n = 13$ and $n = 1, 0$, and $+1$. ACS Omega, 2021, 6, 9813-9827.	1.6	6
7124	Effect of thermal annealing on gas separation performance and aggregation structures of block polyimide membranes. Polymer, 2021, 219, 123538.	1.8	22
7125	Reversible Addition of Carbon Dioxide to Main Group Metal Complexes at Temperatures about 0°C . Chemistry - A European Journal, 2021, 27, 5745-5753.	1.7	22

#	ARTICLE	IF	CITATIONS
7126	Physical and chemical aspects of the interaction of chitosan and cellulose acetate with ions Ca ²⁺ and K ⁺ using DFT methods. <i>Journal of Molecular Modeling</i> , 2021, 27, 103.	0.8	6
7127	Synergistic Dinuclear Rhodium Induced Rhodium-Walking Enabling Alkene Terminal Arylation: A Theoretical Study. <i>ACS Catalysis</i> , 2021, 11, 3975-3987.	5.5	11
7128	New Salts and Cocrystals of Pymetrozine with Improvements on Solubility and Humidity Stability: Experimental and Theoretical Study. <i>Crystal Growth and Design</i> , 2021, 21, 2371-2388.	1.4	33
7129	Adsorption and Activation of CO ₂ on Small-Sized Cu-Zr Bimetallic Clusters. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2558-2572.	1.1	25
7130	Sterically Locked Donor-Acceptor Conjugated Polymers Showing Efficient Thermally Activated Delayed Fluorescence. <i>Angewandte Chemie</i> , 2021, 133, 9721-9727.	1.6	14
7132	Decrypting the Structural, Electronic and Spectroscopic Properties of GeMg _n (n = 12) Clusters: A DFT Study. <i>Journal of Cluster Science</i> , 2022, 33, 1093-1101.	1.7	6
7133	Theoretical Study of closo-Borate Anions [B _n H _n] ²⁻ (n = 5-12): Bonding, Atomic Charges, and Reactivity Analysis. <i>Symmetry</i> , 2021, 13, 464.	1.1	21
7134	Electrochemical Properties of the closo-Decaborate Anion [B ₁₀ H ₁₀] ²⁻ and a New Method for Preparation of the [B ₂₀ H ₁₈] ²⁻ Anion. <i>Russian Journal of Inorganic Chemistry</i> , 2021, 66, 295-304.	0.3	10
7135	Chromium(III) complexes based on phenoxy-imine ligands with pendant N- and O-donor groups as precatalysts for ethylene oligomerization: synthesis, characterization, and DFT studies. <i>Journal of Organometallic Chemistry</i> , 2021, 936, 121710.	0.8	1
7136	Theoretical study on the electronic structure of NaS including spin-orbit coupling. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021, 262, 107520.	1.1	0
7137	Theoretical research about nonmetallic energetic salts with pentazolate anion. <i>Journal of Molecular Modeling</i> , 2021, 27, 100.	0.8	1
7138	Computational Insights into Different Mechanisms for Ag, Cu, and Pd-Catalyzed Cyclopropanation of Alkenes and Sulfonyl Hydrazones. <i>Chemistry - A European Journal</i> , 2021, 27, 5999-6006.	1.7	17
7139	Theoretical insights into chiral PMAADs coordinated with Am(III)/Eu(III) and separation selectivity enhanced by chiral-at Am(III)/Eu(III) complexes. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2021, 328, 205-216.	0.7	8
7140	Synergistically improving myricetin ESIPT and antioxidant activity via dexterously trimming atomic electronegativity. <i>Journal of Molecular Liquids</i> , 2021, 325, 115272.	2.3	26
7141	Comparison Between Electride Characteristics of Li ₃ @B ₄₀ and Li ₃ @C ₆₀ . <i>Frontiers in Chemistry</i> , 2021, 9, 638581.	1.8	11
7142	Thermally Activated Delayed Fluorescence Properties of Trioxoazatriangulene Derivatives Modified with Electron Donating Groups. <i>Advanced Optical Materials</i> , 2021, 9, 2002174.	3.6	35
7143	Insights into the Regioselective Hydrocarboxylation of Styrenes with CO ₂ Controlled by the Ligand of Nickel Catalysts. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 4091-4101.	3.2	9
7144	Theoretical insights of solvent effect on excited-state proton transfers of 2-aryl-3-hydroxyquinolone. <i>Journal of Molecular Liquids</i> , 2021, 325, 115035.	2.3	5

#	ARTICLE	IF	CITATIONS
7145	Investigation of the crystal structures and magnetic features of two bis(dithiolato)nickelate salts with flexible organic cations. <i>Transition Metal Chemistry</i> , 2021, 46, 353-362.	0.7	0
7146	A Comparative Study on the Photophysical Properties of Anthocyanins and Pyranoanthocyanins. <i>Chemistry - A European Journal</i> , 2021, 27, 5956-5971.	1.7	9
7147	Organocatalytic Amination of Pyrazolones with Azodicarboxylates: Scope and Limitations. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 2362-2366.	1.2	7
7148	Designing Organic Electron Transport Materials for Stable and Efficient Performance of Perovskite Solar Cells: A Theoretical Study. <i>ACS Omega</i> , 2021, 6, 7086-7093.	1.6	12
7149	Theoretical Model for N-Heterocyclic Carbene-Catalyzed Desymmetrizing [4 + 1] and [4 + 2] Annulations of an Enal and Aryldialdehyde with 1,3-Cyclopentenedione. <i>Organic Letters</i> , 2021, 23, 2421-2425.	2.4	26
7150	Engineering Oxaliplatin Prodrug Nanoparticles for Second Near-Infrared Fluorescence Imaging-Guided Immunotherapy of Colorectal Cancer. <i>Small</i> , 2021, 17, e2007882.	5.2	44
7151	Photochemical C-H Activation Enables Nickel-Catalyzed Olefin Dicarbofunctionalization. <i>Journal of the American Chemical Society</i> , 2021, 143, 3901-3910.	6.6	106
7152	Unraveling photo-excited behaviors and proton transfer mechanisms for coexisting 5-methoxy-salicylaldehyde azine isomers. <i>Journal of Molecular Liquids</i> , 2021, 326, 115309.	2.3	44
7153	The interaction and mechanism between threonine-montmorillonite composite and Pb ²⁺ or Cu ²⁺ : Experimental study and theory calculation. <i>Journal of Molecular Liquids</i> , 2021, 326, 115243.	2.3	17
7154	Deciphering Benzene-Heterocycle Stacking Interaction Impact on the Electronic Structures and Photophysical Properties of Tetraphenylethene-Cored Foldamers. <i>CCS Chemistry</i> , 2022, 4, 286-303.	4.6	4
7155	Multinuclear Ag Clusters Sandwiched by Pt Complex Units: Fluxional Behavior and Chiral Cluster Photoluminescence. <i>Angewandte Chemie</i> , 2021, 133, 10749-10755.	1.6	6
7156	Multinuclear Ag Clusters Sandwiched by Pt Complex Units: Fluxional Behavior and Chiral Cluster Photoluminescence. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 10654-10660.	7.2	35
7157	Self-Assembled Copper Nanoclusters for Electrocatalytic Glucose Oxidation. <i>ACS Applied Nano Materials</i> , 2021, 4, 4129-4139.	2.4	8
7158	Effect of Molecular Substitution and Isomerization on Charge-Transport Parameters in Molecular Organic Semiconductors. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2660-2667.	2.1	5
7159	Atomic Evolution of Metal-Organic Frameworks into Co ₃ Coupling Vacancies by Cooperative Cascade Protection Strategy for Promoting Triiodide Reduction. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6147-6156.	1.5	13
7160	Fluorescence quenching mechanism of 9-hydroxyphenal-1-one carbon quantum dots by Cu ²⁺ ions: An experimental and computational investigation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 408, 113103.	2.0	4
7161	The cooperativity and diminutive effects between the cation-π and aerogen bond in some complexes of heterocyclic rings. <i>Molecular Physics</i> , 2021, 119, e1897172.	0.8	1
7162	Theoretical investigation of fluorescence changes caused by methanol bridge based on ESIPT reaction. <i>Chinese Physics B</i> , 0, , .	0.7	1

#	ARTICLE	IF	CITATIONS
7163	In silico search for planar hexacoordinate silicon atom: A kinetically viable species. International Journal of Quantum Chemistry, 2021, 121, e2664.	1.0	1
7164	Synthesis and exploring the excited-state PES of photochromic hydrogen bond-assembled [2]rotaxane based on 1,3-Diazabicyclo-[3.1.0]hex-3-enes. Research on Chemical Intermediates, 2021, 47, 2557-2572.	1.3	3
7165	Synthesis of All Thiophene-Based [7]Helicenes and Trithienothiepinines with Isomeric Location of Sulfur Atoms Based on Intramolecular Selectivity of Deprotonation. Journal of Organic Chemistry, 2021, 86, 4413-4422.	1.7	12
7166	Reactivity of Cu(I) Nacnac Complexes Toward Polypnictogen Compounds. Inorganic Chemistry, 2021, 60, 5840-5850.	1.9	7
7167	Metal-Free Aminoiodination of Alkynes Under Visible Light Irradiation for the Construction of a Nitrogen-Containing Eight-Membered Ring System. Advanced Synthesis and Catalysis, 2021, 363, 2746-2751.	2.1	5
7168	Electronic Spin Moment As a Catalytic Descriptor for Fe Single-Atom Catalysts Supported on C ₂ N. Journal of the American Chemical Society, 2021, 143, 4405-4413.	6.6	138
7169	Tunable Triplet-Mediated Multicolor Lasing from Nondoped Organic TADF Microcrystals. Nano Letters, 2021, 21, 3287-3294.	4.5	28
7170	Influences of BuNENA and BDNPA/F Plasticizers on the Properties of Binder for High-Energy NEPE Propellants. Propellants, Explosives, Pyrotechnics, 2021, 46, 950-961.	1.0	2
7171	Nature of the chemical interactions in the multifunctional ionic liquid tris(2-aminothiazolium) hydrogen sulfate sulfate monohydrate. Journal of Molecular Liquids, 2021, 326, 115366.	2.3	6
7172	Decoding the terahertz spectrum of allantoin crystal using DFT simulations and energy decomposition analysis. Chemical Physics Letters, 2021, 767, 138350.	1.2	8
7173	Integrating redox-response in crown ethers by disulfide incorporation: a computational approach. Structural Chemistry, 2021, 32, 1833-1842.	1.0	1
7174	Au(I)-Catalyzed Domino Cyclization of 1,6-Diynes Incorporated with Indole. Organic Letters, 2021, 23, 2279-2284.	2.4	11
7175	Fully Active Nitrogen Energetic Chains Mg ₂ (N ₅) ₂ N ₂ [Mg ₂ (N ₅) ₂ N ₂] _n under Ambient Conditions. Advanced Theory and Simulations, 2021, 4, 2000283.	1.3	2
7176	Chiral Spiro-Axis Induced Blue Thermally Activated Delayed Fluorescence Material for Efficient Circularly Polarized OLEDs with Low Efficiency Roll-Off. Angewandte Chemie - International Edition, 2021, 60, 8435-8440.	7.2	107
7177	Development of Pseudo-C ₂ -symmetric Chiral Binaphthyl Monocarboxylic Acids for Enantioselective C(sp ³)-H Functionalization Reactions under Rh(III) Catalysis. ACS Catalysis, 2021, 11, 4271-4277.	5.5	52
7178	IDENTIFICATION OF SUPRAMOLECULAR DIMERS IN THE CRYSTAL STRUCTURE OF (Z)-1-(((5-FLUOROPYRIDIN-2-YL)AMINO)METHYLENE)NAPHTHALEN-2(1H)-ONE via C(sp ²)-H...F HYDROGEN BONDING: A COMBINED EXPERIMENTAL AND THEORETICAL STUDY. Journal of Structural Chemistry, 2021, 62, 460-466.	0.3	5
7179	Electrolyte Interphase Built from Anionic Covalent Organic Frameworks for Lithium Dendrite Suppression. Advanced Functional Materials, 2021, 31, 2009718.	7.8	43
7180	Packing Effect on Light Emission of Naphthyridine-Based Luminophor: Insights from Quantum Mechanics and Quantum Mechanics/Molecular Mechanics Calculations. Journal of Physical Chemistry B, 2021, 125, 3005-3013.	1.2	2

#	ARTICLE	IF	CITATIONS
7181	Stabilization mechanisms of three novel full-nitrogen molecules. Monatshefte für Chemie, 2021, 152, 421-430.	0.9	3
7182	Computational investigation of the reaction of nickel-bis(dithiolene) and nickel-bis(diselenolene) complexes with OH. Canadian Journal of Chemistry, 2021, 99, 346-353.	0.6	0
7183	Electron-vibrational coupling on the absorption spectrum of dithienyl-diketopyrrolopyrrole dye. Dyes and Pigments, 2021, 187, 109140.	2.0	2
7184	Visible-Light-Driven and Self-Hydrogen-Donated Nanofibers Enable Rapid-Deployable Antimicrobial Bioprotection. Small, 2021, 17, e2100139.	5.2	18
7185	Improving the Solubility of Aripiprazole by Multicomponent Crystallization. Crystals, 2021, 11, 343.	1.0	6
7186	Assessment of New Expanded Porpholactones as UV/Vis/NIR Chromophores for Dye-Sensitized Solar Cell Applications. Journal of Physical Chemistry A, 2021, 125, 2267-2275.	1.1	4
7187	Do We Still Need a Laboratory to Study Advanced Oxidation Processes? A Review of the Modelling of Radical Reactions used for Water Treatment. Ecological Chemistry and Engineering S, 2021, 28, 11-28.	0.3	16
7188	Exploring the adsorption properties of doped phosphorene for the uptake of DNA nucleobases. Journal of Molecular Liquids, 2021, 325, 115183.	2.3	6
7189	Photovoltaic investigation of CPDT based small molecule for BHJ OSC devices. , 2021, , .		0
7190	Covalent Organic Frameworks Enabling Site Isolation of Viologen-Derived Electron-Transfer Mediators for Stable Photocatalytic Hydrogen Evolution. Angewandte Chemie, 2021, 133, 9728-9735.	1.6	16
7191	Single-Component Organic Solar Cells Based on Intramolecular Charge Transfer Photoabsorption. Materials, 2021, 14, 1200.	1.3	10
7192	Unravelling the Role of Alkyl Cocatalyst for the VO _x /SiO ₂ Ethylene Polymerization Catalyst: Diethylaluminum Chloride Vs. Triethylaluminum. ChemCatChem, 2021, 13, 2278-2292.	1.8	8
7193	Proposing a new complexing agent for cyanide-free silver electroplating through a comprehensive computational study of dimethyl hydantoin. Molecular Simulation, 0, , 1-9.	0.9	1
7194	Rational Molecular Design of Multifunctional Blue-Emitting Materials Based on Phenanthroimidazole Derivatives.. Chemistry - A European Journal, 2021, 27, 7275-7282.	1.7	23
7195	Hypseudohenrins: three new polycyclic polyprenylated acylphloroglucinol derivatives from Hypericum pseudohenryi. Journal of Asian Natural Products Research, 2021, 23, 536-544.	0.7	1
7196	Insight into the structure of the heulandite-type zeolite containing aromatic compounds using periodic density functional theory. Materials Today Communications, 2021, 26, 102028.	0.9	4
7197	A phenylalanine dynamic switch controls the interfacial activation of Rhizopus chinensis lipase. International Journal of Biological Macromolecules, 2021, 173, 1-12.	3.6	27
7198	Structure-Property Relationship in Selected Naphtho- and Anthra-Quinone Derivatives on the Basis of Density Functional Theory and Car-Parrinello Molecular Dynamics. Symmetry, 2021, 13, 564.	1.1	5

#	ARTICLE	IF	CITATIONS
7199	Hybrid Structure of Ionic Liquid and TiO ₂ Nanoclusters for Efficient Hydrogen Evolution Reaction. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2653-2665.	1.1	26
7200	Extended Push-Pull Type Bicyclic Fluorophores Based on Quinoline and Naphthyridine Frameworks with an Iminophosphorane Fragment. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 1123-1130.	1.3	2
7201	Highly Emissive Borafluorene Derivatives: Synthesis, Photophysical Properties and Device Fabrication. <i>Chemistry - A European Journal</i> , 2021, 27, 6274-6282.	1.7	13
7202	Intermolecular driving forces on the adsorption of DNA/RNA nucleobases to graphene and phosphorene: An atomistic perspective from DFT calculations. <i>Journal of Molecular Liquids</i> , 2021, 325, 115229.	2.3	17
7203	Homogenous Liquid-Liquid Extraction of Au(III) from Acidic Medium by Ionic Liquid Thermomorphic Systems. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 4894-4902.	3.2	13
7204	Thermochromic aggregation-induced dual phosphorescence via temperature-dependent sp ³ -linked donor-acceptor electronic coupling. <i>Nature Communications</i> , 2021, 12, 1364.	5.8	89
7205	Rational Design of Dual-Emission Lanthanide Metal-Organic Framework for Visual Alkaline Phosphatase Activity Assay. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 11646-11656.	4.0	66
7207	Synthesis and detailed characterization of a newly synthesized chalcone, 3-(2,5-dimethoxyphenyl)-1-(naphthalen-2-yl)prop-2-en-1-one. <i>European Journal of Chemistry</i> , 2021, 12, 69-76.	0.3	2
7208	Theoretical perspective on the interaction of CO ₂ and H ₂ O molecules with functionalized magnesium and scandium phthalocyanines. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	2
7209	Solution and Solid-State Photophysical Properties of Positional Isomeric Acrylonitrile Derivatives with Core Pyridine and Phenyl Moieties: Experimental and DFT Studies. <i>Molecules</i> , 2021, 26, 1500.	1.7	5
7210	Elucidating the therapeutic activity of selective curcumin analogues: DFT-based reactivity analysis. <i>Structural Chemistry</i> , 2021, 32, 1701-1715.	1.0	6
7211	Direct coherent switching with decay of mixing for intersystem crossing dynamics of thioformaldehyde: The effect of decoherence. <i>Journal of Chemical Physics</i> , 2021, 154, 094310.	1.2	15
7212	DFT investigation of the triphenylphosphine-assisted electrochemical dehydroxylative transformations. <i>Molecular Catalysis</i> , 2021, 504, 111470.	1.0	8
7213	A theoretical and experimental study of phosphate ester inhibitors for AISI 1018 in carbon dioxide-saturated 3.5%wt% NaCl solution. <i>Materials and Corrosion - Werkstoffe Und Korrosion</i> , 2021, 72, 1417-1432.	0.8	2
7214	Effects of CO ₂ /NO/SO ₂ in flue gas on selenium adsorption on carbonaceous surface. <i>Canadian Journal of Chemical Engineering</i> , 2021, 99, 2691-2701.	0.9	1
7215	Designing and Screening High-Performance Non-Fullerene Acceptors: A Theoretical Exploration of Modified Y6. <i>Solar Rrl</i> , 2021, 5, 2100023.	3.1	29
7216	Raman spectroscopy and quantum theory calculations on complexes in the KF-AlF ₃ -Al ₂ O ₃ system. <i>Journal of Molecular Liquids</i> , 2021, 326, 115267.	2.3	10
7217	Structures and spectroscopic properties of low-energy candidate structures for toluene-(H ₂ O) _n (n=1-10) clusters. <i>Journal of Molecular Liquids</i> , 2021, 326, 115213.	2.3	0

#	ARTICLE	IF	CITATIONS
7218	Ni/Cu-catalyzed silylation of allylic alcohol: Theoretical studies on the mechanisms, regioselectivity, and role of ligand. <i>Molecular Catalysis</i> , 2021, 504, 111456.	1.0	1
7219	The key role of adsorbate-catalyst interactions into catalytic activity of [CTA ⁺]-Si-MCM-41 from electron density analysis. <i>Molecular Catalysis</i> , 2021, 504, 111472.	1.0	1
7220	Mechanistic Insights into the Nickel-Catalyzed Regioselective Carboxylation of Allylic Alcohols. <i>Organometallics</i> , 2021, 40, 869-879.	1.1	15
7221	[Sn ₈] 6 ⁺ Bridged Mixed Valence Zn I / Zn II in {[K ₂ ZnSn ₈ (ZnMes)] ₂ } 4 ⁺ Inverse Sandwich Type Cluster Supported by a Zn I ⁺ Zn I Bond. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 9990-9995.	7.2	9
7222	Transition metal-doped Bn (n = 7-10) clusters: confirmation of a circular disk Jellium model. <i>European Physical Journal Plus</i> , 2021, 136, 1.	1.2	5
7223	Ultralong Room Temperature Phosphorescence from Boric Acid. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 9500-9506.	7.2	82
7224	Judicious design functionalized $3D$ COF to enhance CO_2 adsorption and separation. <i>Journal of Computational Chemistry</i> , 2021, 42, 888-896.	1.5	14
7225	2,5-Dibromothiophenes: Halogen Bond Involving Packing Patterns and Their Relevance to Solid-State Polymerization. <i>Crystal Growth and Design</i> , 2021, 21, 2526-2540.	1.4	9
7226	Access to Chiral Diamine Derivatives through Stereoselective Cu-Catalyzed Reductive Coupling of Imines and Allenamides. <i>Journal of Organic Chemistry</i> , 2021, 86, 5026-5046.	1.7	15
7227	Performable enhancement of C220-based dyes via inserting auxiliary electron acceptors for dye-sensitized solar cells: a theoretical investigation. <i>Journal of Computational Electronics</i> , 2021, 20, 1277-1288.	1.3	2
7228	Attractive fluorine-fluorine interactions between perfluorinated alkyl chains: a case of perfluorinated Cu(II) diiminate $Cu[C_2F_5C(NH)CF=C(NH)CF_3]_2$. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2021, 236, 117-122.	0.4	11
7229	Lithium Bond-Enhanced Capacity of Dipyridyl Polysulfides for LSBs. <i>ACS Applied Energy Materials</i> , 2021, 4, 3495-3501.	2.5	4
7230	Graphical Transition Moment Decomposition and Conceptual Density Functional Theory Approaches to Study the Fundamental and Lower-Level Overtone Absorption Intensities of Some OH Stretching Vibrations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2101-2113.	1.1	5
7231	Bi-functional hydrogen and coordination bonding surfactant: A novel and promising collector for improving the separation of calcium minerals. <i>Journal of Colloid and Interface Science</i> , 2021, 585, 787-799.	5.0	23
7232	Theoretical investigations on forward-backward ESIPT processes of three fluorophores deriving from 2-(2-hydroxyphenyl)thiazole. <i>Photochemical and Photobiological Sciences</i> , 2021, 20, 533-546.	1.6	4
7233	Conformational torsion, intramolecular hydrogen bonding and solvent effects in intersystem crossing of singlet-triplet excited states for heavy-atom-free organic long persistent luminescence. <i>Journal of Molecular Liquids</i> , 2021, 326, 115291.	2.3	5
7234	Experimental and Theoretical Insights into the Electronic Properties of Anionic N-Heterocyclic Dicarbenes through the Rational Synthesis of Their Transition Metal Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 4015-4025.	1.9	11
7235	Benchmarking density functional theory methods for modelling cationic metal-argon complexes. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	7

#	ARTICLE	IF	CITATIONS
7236	Covalent Organic Frameworks Enabling Site Isolation of Viologen-Derived Electron-Transfer Mediators for Stable Photocatalytic Hydrogen Evolution. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 9642-9649.	7.2	161
7237	Coexistence of Parallel and Rotary Stackings in the Lamellar Crystals of a Perylene Bisimide Dyad for Temperature-Sensitive Bicomponent Emission. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3373-3378.	2.1	5
7238	Mechanistic Insights into Formation of All-Carbon Quaternary Centers via Scandium-Catalyzed C-H Alkylation of Imidazoles with 1,1-Disubstituted Alkenes. <i>Journal of Organic Chemistry</i> , 2021, 86, 4598-4606.	1.7	7
7239	Ultralong Room-Temperature Phosphorescence from Boric Acid. <i>Angewandte Chemie</i> , 2021, 133, 9586-9592.	1.6	29
7240	Aggregation-Enhanced Thermally Activated Delayed Fluorescence Efficiency for Two-Coordinate Carbene-Metal-Amide Complexes: A QM/MM Study. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2944-2953.	2.1	44
7241	Electronic Structure Modification of Rectangular Phosphorene Quantum Dots Via Edge Passivation. <i>Journal of Physical Chemistry C</i> , 2021, 125, 5029-5036.	1.5	4
7242	Quantum chemical calculations, spectroscopic properties and molecular docking studies of a novel piperazine derivative. <i>Journal of King Saud University - Science</i> , 2021, 33, 101283.	1.6	53
7243	DFT Study on the Electrocatalytic Reduction of CO ₂ to CO by a Molecular Chromium Complex. <i>Inorganic Chemistry</i> , 2021, 60, 3635-3650.	1.9	18
7244	Advanced Tri-Layer Carbon Matrices with π - π Stacking Interaction for Binder-Free Lithium-Ion Storage. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 16516-16527.	4.0	18
7245	Sequential C-F bond functionalizations of trifluoroacetamides and acetates via spin-center shifts. <i>Science</i> , 2021, 371, 1232-1240.	6.0	166
7246	Sterically-Locked Donor-Acceptor Conjugated Polymers Showing Efficient Thermally Activated Delayed Fluorescence. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 9635-9641.	7.2	61
7247	Theoretical predict structure and property of the novel CL-20/2,4-DNI cocrystal by systematic search approach. <i>Defence Technology</i> , 2022, 18, 907-917.	2.1	6
7248	Rearrangement Strategy for the Preparation of Polymers With π -Conjugated Structures. <i>Frontiers in Chemistry</i> , 2021, 9, 665877.	1.8	2
7249	Z,E-Isomerism in a Series of Substituted Iminophosphonates: Quantum Chemical Research. <i>Organics</i> , 2021, 2, 84-97.	0.6	2
7250	The second-order nonlinear optical property of hydrazones-based photochromic complexes: A DFT study. <i>Journal of Molecular Liquids</i> , 2021, 327, 114882.	2.3	13
7251	Cyano-Isocyanide Iridium(III) Complexes with Pure Blue Phosphorescence. <i>Inorganic Chemistry</i> , 2021, 60, 6391-6402.	1.9	15
7252	Evaluating and understanding the affinity of metal ions to water and ammonia using density functional theory calculation. <i>Chemical Physics Letters</i> , 2021, 768, 138398.	1.2	1
7253	Sandwich complexes of ruthenium, and osmium with group 13 analogues of N-heterocyclic carbene ligands: Efficient future complexes to reduce carbon monoxide poisoning. <i>Computational and Theoretical Chemistry</i> , 2021, 1198, 113179.	1.1	0

#	ARTICLE	IF	CITATIONS
7254	The role of SO ₂ in arsenic removal by carbon-based sorbents: A DFT study. <i>Chemical Engineering Journal</i> , 2021, 410, 128439.	6.6	29
7255	Experimental and theoretical study on spectral features, reactivity, solvation, topoisomerase I inhibition and in vitro cytotoxicity in human HepG2 cells of guadiscine and guadiscidine aporphine alkaloids. <i>Journal of Molecular Structure</i> , 2021, 1229, 129844.	1.8	16
7256	Cetylpyridinium picrate: Spectroscopy, conductivity and DFT investigation of the structure of a new ionic liquid. <i>Journal of Molecular Structure</i> , 2021, 1229, 129803.	1.8	5
7257	Discovery of novel IDO1 inhibitors via structure-based virtual screening and biological assays. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 679-694.	1.3	2
7258	Competition between Inter and Intramolecular Tetrel Bonds: Theoretical Studies Complemented by CSD Survey. <i>ChemPhysChem</i> , 2021, 22, 924-934.	1.0	7
7259	Electronic and optical properties of tuning of phenoxazine-based D-A ₂ -A ₁ organic dyes for dye-sensitized solar cells. DFT/TDDFT investigations. <i>Heliyon</i> , 2021, 7, e06827.	1.4	24
7260	Proton Transfer in Nitromethane-Ammonia Clusters under VUV Single-Photon Ionization Explored by Infrared Spectroscopy and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3279-3287.	1.1	2
7261	Ionization Energies and Dyson Orbitals of the Iso-electronic SO ₂ , O ₃ , and S ₃ Molecules from Electron Propagator Calculations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3664-3680.	1.1	3
7262	Fluorination-Guided Li-Anchoring Behaviors on Phthalocyanines. <i>Journal of Physical Chemistry C</i> , 2021, 125, 8236-8243.	1.5	3
7263	Synergistic Recognition-Triggered Charge Transfer Enables Rapid Visual Colorimetric Detection of Fentanyl. <i>Analytical Chemistry</i> , 2021, 93, 6544-6550.	3.2	17
7264	Investigating the Influence of Electronic Effects of Functional Groups on the Fluorescence Mechanism of Probes in Water Samples. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2866-2875.	1.1	6
7265	Molecular dynamics simulations reveal the destabilization mechanism of Alzheimer's disease-related tau R3-R4 Protofilament by norepinephrine. <i>Biophysical Chemistry</i> , 2021, 271, 106541.	1.5	13
7266	Screening Ionic Liquids Based on Ionic Volume and Electrostatic Potential Analyses. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3653-3664.	1.2	20
7267	Probing the structural, electronic and spectral properties of a Nb ₂₀ ⁺ cluster. <i>Molecular Physics</i> , 2021, 119, e1910744.	0.8	3
7268	Polymorphs of 2-[2-[(2,6-dichlorophenyl)amino]phenyl]acetic acid (Diclofenac): Differences from crystallography, Hirshfeld surface, QTAIM and NCIPlots. <i>Chemical Physics</i> , 2021, 544, 111119.	0.9	4
7269	Isolated boron in zeolite for oxidative dehydrogenation of propane. <i>Science</i> , 2021, 372, 76-80.	6.0	155
7270	Confinement-Driven Flexible Acidity Properties of Porous Zeolite Catalysts with Varied Probe-Assisted Solid-State NMR Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2021, 125, 11580-11590.	1.5	8
7271	Enantioselective Access to Spirolactams via Nitrenoid Transfer Enabled by Enhanced Noncovalent Interactions. <i>Journal of the American Chemical Society</i> , 2021, 143, 6363-6369.	6.6	43

#	ARTICLE	IF	CITATIONS
7272	Chlorine π -Equatorial Belt Activation of CF_3Cl by CO_2 : The C \cdots Cl Tetrel Bond Dominance in $\text{CF}_3\text{Cl}\cdots\text{CO}_2$. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3907-3913.	2.1	17
7273	Bridged Azobenzene Enables Dynamic Control of Through-Space Charge Transfer for Photochemical Conversion. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3868-3874.	2.1	3
7274	Achieving Desirable Initial Coulombic Efficiencies and Full Capacity Utilization of Li -ion Batteries by Chemical Prelithiation of Graphite Anode. <i>Advanced Functional Materials</i> , 2021, 31, 2101181.	7.8	115
7275	Intrinsic hydroquinone-functionalized aggregation-induced emission core shows redox and pH sensitivity. <i>Communications Chemistry</i> , 2021, 4, .	2.0	6
7276	Exciton-Trion Conversion Dynamics in a Single Molecule. <i>ACS Nano</i> , 2021, 15, 7694-7699.	7.3	20
7277	Interfacial Carrier-Transfer Channel Optimization Based on Hydrogen Bonds for High-Performance Organic Solar Cells. <i>ACS Applied Energy Materials</i> , 2021, 4, 3881-3890.	2.5	5
7278	Hydrogen Bonding Versus π -Stacking in Charge-Transfer Co-crystals. <i>Crystal Growth and Design</i> , 2021, 21, 2609-2613.	1.4	13
7279	Nonmetallic Pentazole Salts Based on Furazan or 4-Nitropyrazole for Enhancing Density and Stability. <i>Crystal Growth and Design</i> , 2021, 21, 2690-2698.	1.4	11
7280	Designing Molecular Electrides from Defective Unit Cells of Cubic Alkaline Earth Oxides. <i>Journal of Physical Chemistry C</i> , 2021, 125, 9564-9570.	1.5	4
7281	Phosphorescent Metal Rotaxane-like Bimetallic Ag/Au Clusters. <i>Journal of Physical Chemistry C</i> , 2021, 125, 9400-9410.	1.5	11
7282	Spectroscopic, electron localization function, chemical reactivity and antihypertensive activity study on hordenine alkaloid by density functional theory approach. <i>Journal of Molecular Structure</i> , 2021, 1229, 129823.	1.8	0
7283	A protonated salt constructed by tetrafluoroterephthalic acid and 5, 6-dimethyl benzimidazole: Design, synthesis, proton transfer and luminescent property. <i>Journal of Molecular Structure</i> , 2021, 1229, 129781.	1.8	2
7284	Adsorption behaviors of carbon monoxide (CO) over aromatic magnesium nanoclusters: a DFT study. <i>Structural Chemistry</i> , 2021, 32, 1949-1960.	1.0	2
7285	Synthesis of molecularly imprinted polymers based on boronate affinity for diol-containing macrolide antibiotics with hydrophobicity-balanced and pH-responsive cavities. <i>Journal of Chromatography A</i> , 2021, 1642, 461969.	1.8	19
7286	Theoretical study of the interplay between double chalcogen-bonding interactions and halogen bonds in ditopic molecular module systems. <i>Computational and Theoretical Chemistry</i> , 2021, 1198, 113182.	1.1	3
7287	Ion-Pair Facilitated Non-Enzymatic Electrochemical Sensing of Cadaverine and Putrescine. <i>Journal of the Electrochemical Society</i> , 2021, 168, 047505.	1.3	7
7288	Selective Catalytic Isomerization of β -Pinene Oxide to Perillyl Alcohol Enhanced by Protic Tetraimidazolium Nitrate. <i>ChemistryOpen</i> , 2021, 10, 477-485.	0.9	2
7289	Unveiling the self-association and desolvation in crystal nucleation. <i>IUCr</i> , 2021, 8, 468-479.	1.0	14

#	ARTICLE	IF	CITATIONS
7290	Stretchable chiral pockets for palladium-catalyzed highly chemo- and enantioselective allenylation. <i>Nature Communications</i> , 2021, 12, 2416.	5.8	14
7291	High-Energy-Density Quinone-Based Electrodes with $[Al(OTf)]^{2+}$ Storage Mechanism for Rechargeable Aqueous Aluminum Batteries. <i>Advanced Functional Materials</i> , 2021, 31, 2102063.	7.8	61
7292	A New Method for Detecting Trace Methanol in Insulating Oil Based on Terahertz Spectroscopy. , 2021, ,.		0
7293	Perfect Spherical Tetrahedral Metallo-Borospherene Ta_4B_{18} as a Superatom Following the 18-Electron Rule. <i>ACS Omega</i> , 2021, 6, 10991-10996.	1.6	13
7294	A TD-DFT molecular screening for fluorescence probe based on excited-state intramolecular proton transfer of 2-hydroxychalcone derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 410, 113165.	2.0	12
7295	The adsorption and mechanism of benzothiazole and 2-hydroxybenzothiazole onto a novel ampholytic surfactant modified montmorillonite: Experimental and theoretical study. <i>Advanced Powder Technology</i> , 2021, 32, 1219-1232.	2.0	6
7296	Direct Tracking Excited-State Intramolecular Charge Redistribution of Acceptor-Donor-Acceptor Molecule by Means of Femtosecond Stimulated Raman Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4456-4464.	1.2	15
7297	Unveiling the theoretical mechanism of purely organic room temperature phosphorescence emission and heteroatomic effects on singlet-triplet intersystem crossing for isopropylthioxanthone derivatives. <i>Journal of Luminescence</i> , 2021, 232, 117864.	1.5	14
7298	Protonation of quinoline yellow WS in aqueous solutions: Spectroscopic and DFT theoretical studies. <i>Journal of Molecular Liquids</i> , 2021, 327, 114881.	2.3	7
7299	Metal-CO Bonding in Mononuclear Transition Metal Carbonyl Complexes. <i>Jacs Au</i> , 2021, 1, 623-645.	3.6	57
7300	Theoretical insight into the hybridization effect of donor and acceptor atoms on the cooperativity of C-H...N hydrogen bonds. <i>Journal of Molecular Modeling</i> , 2021, 27, 119.	0.8	0
7301	An Effective Strategy to Design a Large Bandgap Conjugated Polymer by Tuning the Molecular Backbone Curvature. <i>Macromolecular Rapid Communications</i> , 2021, 42, 2000757.	2.0	7
7302	2,3,4,5-Tetraiodopyrrole as a building block for halogen bonding: Formation of supramolecular hybrids with organic iodide salts in solid state. <i>Journal of Molecular Structure</i> , 2021, 1230, 129931.	1.8	4
7303	Theoretical insights into the direct radical scavenging activities of 8-hydroxyquinoline: Mechanistic, thermodynamic and kinetic studies. <i>Computational and Theoretical Chemistry</i> , 2021, 1198, 113174.	1.1	4
7304	Tuning optical properties of triphenylamine-pyrrole by alkyl-substituted thiobarbituric acid for dye-sensitized solar cell. <i>International Journal of Energy Research</i> , 2021, 45, 14804-14812.	2.2	10
7305	Computational evaluation on molecular structure (Monomer, Dimer), RDG, ELF, electronic (HOMO-LUMO, MEP) properties, and spectroscopic profiling of 8-Quinolinesulfonamide with molecular docking studies. <i>Computational and Theoretical Chemistry</i> , 2021, 1198, 113169.	1.1	42
7306	Facile synthesis of Fe ₃ O ₄ @MIL-100(Fe) towards enhancing photo-Fenton like degradation of levofloxacin via a synergistic effect between Fe ₃ O ₄ and MIL-100(Fe). <i>Chemical Engineering Journal</i> , 2021, 409, 128274.	6.6	130
7307	The cage-like structure enhanced magnetic moment in ScK _n (n = 2-12) clusters: A first-principles jointed particle swarm optimization investigation. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26654.	1.0	2

#	ARTICLE	IF	CITATIONS
7308	DFT Calculations and Molecular Docking Studies on a Chromene Derivative. <i>Journal of Chemistry</i> , 2021, 2021, 1-17.	0.9	13
7309	Comparative opto-electronic properties of perylene diimides derivatives with cyclization and high polarizability cores. <i>Journal of Physics: Conference Series</i> , 2021, 1865, 022073.	0.3	0
7310	A Molecular Transformer: A π -Conjugated Macrocyclic Host. <i>Angewandte Chemie</i> , 2021, 133, 11920-11924.	1.6	7
7311	Theoretical Studies on the Electronic Structure of Nano-graphenes for Applications in Nonlinear Optics. <i>Chemical Research in Chinese Universities</i> , 2022, 38, 579-587.	1.3	6
7313	Rational design of π bridge to forecast photoelectric performance of dye. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2021, 29, 045007.	0.8	1
7314	Enantioseparations of polyhalogenated 4,4'-bipyridines on polysaccharide-based chiral stationary phases and molecular dynamics simulations of selector-selectand interactions. <i>Electrophoresis</i> , 2021, 42, 1853-1863.	1.3	9
7315	Propeptide in <i>Rhizopus chinensis</i> Lipase: New Insights into Its Mechanism of Activity and Substrate Selectivity by Computational Design. <i>Journal of Agricultural and Food Chemistry</i> , 2021, 69, 4263-4275.	2.4	17
7316	Understanding solvent polarity dependent excited state behavior and ESIPT mechanism for 2-benzo[b]thiophen-3-yl-3-hydroxy-6-methoxy-chroman-4-one compound. <i>Chemical Physics Letters</i> , 2021, 769, 138409.	1.2	33
7317	Theoretical investigation of X12O12 (X=Be, Mg, and Ca) in sensing CH ₂ N ₂ : A DFT study. <i>Computational and Theoretical Chemistry</i> , 2021, 1198, 113168.	1.1	35
7318	Decorating electron redundant Si _n Al ₁₂ nanocages with superalkalis M ₃ O (M=Li, Na, K): excess electron frameworks and nonlinear optical properties. <i>Molecular Physics</i> , 2021, 119, e1909161.		2
7319	Microscopic adsorption mechanism of montmorillonite for common ciprofloxacin emerging contaminant: Molecular dynamics simulation and Multiwave function analysis. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 614, 126186.	2.3	27
7320	How the Donor/Acceptor Spin States Affect the Electronic Couplings in Molecular Charge-Transfer Processes?. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2917-2927.	2.3	2
7321	A computational investigation of the selectivity and mechanism of the Lewis acid catalyzed oxa-Diels-Alder cycloaddition of substituted diene with benzaldehyde. <i>Journal of Computational Chemistry</i> , 2021, 42, 1296-1311.	1.5	10
7322	Thermally activated delayed fluorescence: A critical assessment of environmental effects on the singlet-triplet energy gap. <i>Journal of Chemical Physics</i> , 2021, 154, 134112.	1.2	16
7323	Influence of atmospheric conditions on the role of trifluoroacetic acid in atmospheric sulfuric acid-dimethylamine nucleation. <i>Atmospheric Chemistry and Physics</i> , 2021, 21, 6221-6230.	1.9	11
7324	Insight into the Formation of Cocrystals of Flavonoids and 4,4'-Vinylendipyridine: Heteromolecular Hydrogen Bonds, Molar Ratio, and Structural Analysis. <i>Crystal Growth and Design</i> , 2021, 21, 2720-2733.	1.4	12
7325	Vibrationally Resolved Absorption Spectra and Exciton Dynamics in Zinc Phthalocyanine Aggregates: Effects of Aggregation Lengths and Remote Exciton Transfer. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2932-2943.	1.1	11
7326	Unraveling the Mechanism of Near-Infrared Thermally Activated Delayed Fluorescence of TPA-Based Molecules: Effect of Hydrogen Bond Steric Hindrance. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2905-2912.	1.1	9

#	ARTICLE	IF	CITATIONS
7327	Optical Cycling Functionalization of Arenes. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3989-3995.	2.1	20
7328	Theoretical Investigation of the Na ⁺ Transport Mechanism and the Performance of Ionic Liquid-Based Electrolytes in Sodium-Ion Batteries. <i>ACS Applied Energy Materials</i> , 2021, 4, 4444-4458.	2.5	27
7329	Boronic Acids as Prospective Inhibitors of Metallo- β -Lactamases: Efficient Chemical Reaction in the Enzymatic Active Site Revealed by Molecular Modeling. <i>Molecules</i> , 2021, 26, 2026.	1.7	11
7330	New insights into DPP3Th and C70 based planar solar cells: A study combining DFT and experimental approach. <i>Materials Chemistry and Physics</i> , 2021, 262, 124271.	2.0	4
7331	Methane C-H Activation by [Cu ₂ O] ²⁺ and [Cu ₃ O ₃] ²⁺ in Copper-Exchanged Zeolites: Computational Analysis of Redox Chemistry and X-ray Absorption Spectroscopy. <i>Inorganic Chemistry</i> , 2021, 60, 6218-6227.	1.9	5
7332	A Versatile Competitive Coordination Strategy for Tailoring Bioactive Zeolitic Imidazolate Framework Composites. <i>Small</i> , 2021, 17, e2007586.	5.2	17
7333	Facile mitochondria localized fluorescent probe for viscosity detection in living cells. <i>Talanta</i> , 2021, 225, 121996.	2.9	30
7334	Impact of Polypyrrole Functionalization on the Anodic Performance of Boron Nitride Nanosheets: Insights From First-Principles Calculations. <i>Frontiers in Chemistry</i> , 2021, 9, 670833.	1.8	6
7335	Riboflavin sensitized photodegradation of Furaneol in a β -cyclodextrin complex. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 411, 113188.	2.0	3
7336	A time-dependent density function theory study on the substituent effect on excited-state intramolecular proton transfer of 4-methoxy- β -hydroxyl flavone. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4216.	0.9	5
7337	Role of Hydrogen Bonds in Formation of Co-amorphous Valsartan/Nicotinamide Compositions of High Solubility and Durability with Anti-hypertension and Anti-COVID-19 Potential. <i>Molecular Pharmaceutics</i> , 2021, 18, 1970-1984.	2.3	23
7338	Theoretical Study of the Resveratrol Adsorption on B ₁₂ N ₁₂ and Mg-decoration B ₁₂ N ₁₂ Fullerenes. <i>Bulletin of the Korean Chemical Society</i> , 2021, 42, 878-888.	1.0	11
7339	Nitrate Additives Coordinated with Crown Ether Stabilize Lithium Metal Anodes in Carbonate Electrolyte. <i>Advanced Functional Materials</i> , 2021, 31, 2102128.	7.8	56
7340	Optical-electronic performance and mechanism investigation of dihydroindolocarbazole-based organic dyes for DSSCs. <i>Results in Physics</i> , 2021, 23, 103939.	2.0	8
7341	Evaluation of Electrochemical Stability of Substituted Sulfolanes Based on Bond Orders. <i>Russian Journal of Physical Chemistry A</i> , 2021, 95, 730-735.	0.1	3
7342	Mechanistic insight into the hydrogenation of acetylene on the Pd ₂ /g-C ₃ N ₄ catalyst: effect of Pd clustering on the barrier energy and selectivity. <i>Structural Chemistry</i> , 2021, 32, 2087-2097.	1.0	1
7343	Adsorption and desorption behaviors of hydroxyurea drug on delivery systems of B ₁₂ N ₁₂ fullerene and its Al-, Si- and P-dopings from theoretical perspective. <i>Molecular Physics</i> , 2021, 119, e1921296.	0.8	14
7344	Structure-property study of pristine and dehydrofluorinated poly(vinylidene fluoride) using density functional theory. <i>Monatshefte für Chemie</i> , 2021, 152, 559-567.	0.9	4

#	ARTICLE	IF	CITATIONS
7345	Mechanistic Study of the <i>N</i> -Quaternized Pyridoxal-Catalyzed Biomimetic Asymmetric Mannich Reaction: Insights into the Origins of Enantioselectivity and Diastereoselectivity. <i>Journal of Organic Chemistry</i> , 2021, 86, 6592-6599.	1.7	3
7346	Computational insight into newly anomalous delayed fluorescence emitters based on D-A-A structures. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 250, 119392.	2.0	0
7347	Swelling-controlled positioning of nanofillers through a polyamide layer in thin-film nanocomposite membranes for CO ₂ separation. <i>Journal of Membrane Science</i> , 2021, 624, 119095.	4.1	22
7348	Responsive mechanism of 2-fluoro-5-nitrobenzoate based two-photon fluorescent probes for H ₂ S detection: A theoretical perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 250, 119244.	2.0	2
7349	Sequence-dependent nanomolar binding of tripeptides containing N-terminal phenylalanine by Cucurbit[7]uril: A theoretical study. <i>Journal of Molecular Liquids</i> , 2021, 328, 115479.	2.3	12
7350	Iodine-Substituted Lithium/Sodium <i>closo</i> -Decaborates: Syntheses, Characterization, and Solid-State Ionic Conductivity. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 17554-17564.	4.0	26
7351	Exploring influence of fluorine substitution on the strength and nature of halogen bond between iodobenzene and hydrogen cyanide. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4213.	0.9	3
7352	Spirofluorene based small molecules as an alternative to traditional non-fullerene acceptors for organic solar cells. <i>Optical and Quantum Electronics</i> , 2021, 53, 1.	1.5	19
7353	Syntheses and Properties of Triruthenium Polyhydrido Complexes Composed of 1,2,4-tri- <i>tert</i> -butylcyclopentadienyl and <i>p</i> -Cymene Ruthenium Units. <i>Organometallics</i> , 2021, 40, 1303-1313.	1.1	1
7354	(6-Diphenylphosphinoacenaphth-5-yl)indium and -nickel Compounds: Synthesis, Structure, Transmetalation, and Cross-Coupling Reactions. <i>Organometallics</i> , 2021, 40, 1284-1295.	1.1	5
7355	Quantifications and Applications of Relative Fisher Information in Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3802-3811.	1.1	27
7356	Cyclo[<i>n</i>]carbons Form Strong N ⁺ C Dative/Covalent Bonds with Piperidine. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2923-2931.	1.1	13
7357	Planar Tetracoordinate Carbons in Allene-Type Structures. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3009-3014.	1.1	12
7358	Bright Frenkel Excitons in Molecular Crystals: A Survey. <i>Chemistry of Materials</i> , 2021, 33, 3368-3378.	3.2	22
7359	CAI ₄ MgO: Global Minima with a Planar Tetracoordinate Carbon Atom. <i>Atoms</i> , 2021, 9, 24.	0.7	18
7360	Anion-Anion Interactions in Aerogen-Bonded Complexes. Influence of Solvent Environment. <i>Molecules</i> , 2021, 26, 2116.	1.7	13
7361	Effective adsorption of A-series chemical warfare agents on graphdiyne nanoflake: a DFT study. <i>Journal of Molecular Modeling</i> , 2021, 27, 117.	0.8	26
7362	Theoretical study of putrescine and X ₁₂ Y ₁₂ (X=Al, B and Y=N, P) nanocage interactions. <i>Journal of Nanoparticle Research</i> , 2021, 23, 1.	0.8	10

#	ARTICLE	IF	CITATIONS
7363	The Structures of ZnCl ₂ -Ethanol Mixtures, a Spectroscopic and Quantum Chemical Calculation Study. <i>Molecules</i> , 2021, 26, 2498.	1.7	12
7364	Spin accommodation and reactivity of nickel clusters with oxygen: Aromatic and magnetic metalloxocube Ni ₁₃ O ₈ . <i>Nano Research</i> , 2021, 14, 4822-4827.	5.8	7
7365	Hydrogen evolution from water molecule reactions with Ge ₇ and Ge ₆ Al clusters. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 12693-12700.	3.8	10
7366	Negative Charge Management to Make Fragile Bonds Less Fragile toward Electrons for Robust Organic Optoelectronic Materials. <i>CCS Chemistry</i> , 2022, 4, 331-343.	4.6	10
7367	Highly stable electron-withdrawing C O link-free backbone with branched cationic side chain as anion exchange membrane. <i>Journal of Membrane Science</i> , 2021, 624, 119052.	4.1	25
7368	Introducing a Surface-Enhanced-Raman-Scattering Enhancer for Experimental Estimation of the Debye Screening Length in Organic Field-Effect Transistors. <i>ACS Applied Electronic Materials</i> , 2021, 3, 1920-1930.	2.0	3
7369	A Computational Mechanistic Analysis of Iridium-Catalyzed C(sp ³)-H Borylation Reveals a One-Stone-Two-Birds Strategy to Enhance Catalytic Activity. <i>ACS Catalysis</i> , 2021, 11, 4833-4847.	5.5	14
7370	Spiro Rhodamine-Perylene Compact Electron Donor-Acceptor Dyads: Conformation Restriction, Charge Separation, and Spin-Orbit Charge Transfer Intersystem Crossing. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4187-4203.	1.2	21
7371	On-off-on fluorescence switch of graphene quantum dots: A cationic control strategy. <i>Applied Surface Science</i> , 2021, 546, 149110.	3.1	13
7372	A pH-Universal Hollow Mn ₃ O ₄ /MWCNT/Nafion [®] Modified Glassy Carbon Electrode for Electrochemical Oxygen Reduction. <i>ChemElectroChem</i> , 2021, 8, 1775-1783.	1.7	3
7373	Characterizing the electronic structure of ionic liquid/benzene catalysts for the isobutane alkylation. <i>Journal of Molecular Liquids</i> , 2021, 328, 115411.	2.3	7
7374	Application of the Molecular Invariom Model for the Study of Interactions Involving Fluorine Atoms in the $\{Yb\}_2\{III\}_3(\frac{1}{2}-OCH(CF_3)_2)_3(\frac{1}{4}-OCH(CF_3)_2)_2YbIII(OCH(CF_3)_2)_2(THF)(Et_2O)\}$ Complex. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2021, 47, 235-243.	0.3	3
7375	Enhancing the understanding of the redox properties of lithium-inserted anthraquinone derivatives by regulating molecular structure. <i>Journal of Electroanalytical Chemistry</i> , 2021, 887, 115172.	1.9	6
7376	Electrostatic Balance Parameter Mediated Energy Functions Toward the Stability and Performance of Explosives. <i>Propellants, Explosives, Pyrotechnics</i> , 2021, 46, 1313-1323.	1.0	2
7377	Li ₈ Si ₈ , Li ₁₀ Si ₉ , and Li ₁₂ Si ₁₀ : Assemblies of Lithium-Silicon Aromatic Units. <i>ChemPhysChem</i> , 2021, 22, 906-910.	1.0	4
7378	Azabuckybowl-based molecular pincers of fullerenes: A noncovalent intermolecular D-A-D system. <i>Diamond and Related Materials</i> , 2021, 114, 108293.	1.8	1
7379	Identification of a copper ion recognition peptide sequence in the subunit II of cytochrome c oxidase: a combined theoretical and experimental study. <i>Journal of Biological Inorganic Chemistry</i> , 2021, 26, 411-425.	1.1	4
7380	f-Hole and f-lump interactions between gold clusters Au _n (n = 2-8) and benzene. <i>Journal of Molecular Modeling</i> , 2021, 27, 132.	0.8	0

#	ARTICLE	IF	CITATIONS
7381	Nanotechnology-based approaches for targeting and delivery of drugs via Hexakis (m-PE) macrocycles. <i>Scientific Reports</i> , 2021, 11, 8256.	1.6	11
7382	2-Amino-6-methylpyridine based co-crystal salt formation using succinic acid: Single-crystal analysis and computational exploration. <i>Journal of Molecular Structure</i> , 2021, 1230, 129893.	1.8	29
7383	Solubility Behavior of CO ₂ in Ionic Liquids Based on Ionic Polarity Index Analyses. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3665-3676.	1.2	17
7384	Comparative study of the hydrogen bonding properties between bis(fluorosulfonyl)imide/bis(trifluoromethyl)sulfonylimide-based ether-functionalized ionic liquids and methanol. <i>Journal of Molecular Liquids</i> , 2021, 328, 115333.	2.3	18
7385	Empirical and computational studies on newly synthesis cyclohexylammonium perchlorate. <i>Journal of Molecular Structure</i> , 2021, 1230, 129820.	1.8	34
7386	Complexation of Mono-anionic Bidentate Ligand Dithiocarbamate with <i>f</i> -Aromatic M ³⁺ Clusters: A DFT Study. <i>Journal of Chemical Sciences</i> , 2021, 133, 1.	0.7	5
7387	Multiscale Computational Screening of Metal-Organic Frameworks for Kr/Xe Adsorption Separation: A Structure-Property Relationship-Based Screening Strategy. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 17998-18009.	4.0	15
7388	Electride characteristics of M ₂ (<i>f</i> -E ₅) ₂ (M = Be, Mg; E = Sb ⁵⁻). <i>Structural Chemistry</i> , 2021, 32, 2107-2114.	1.0	5
7389	Comparison of the Microsolvation of CaX ₂ (X = F, Cl, Br, I) in Water: Size-Selected Anion Photoelectron Spectroscopy and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3288-3306.	1.1	5
7390	In-depth insight into the inhibition mechanism of pyrimidine derivatives on the corrosion of carbon steel in CO ₂ -containing environment based on experiments and theoretical calculations. <i>Corrosion Science</i> , 2021, 181, 109236.	3.0	40
7391	Side-chain manipulation of poly (phenylene oxide) based anion exchange membrane: Alkoxy extender integrated with flexible spacer. <i>Journal of Membrane Science</i> , 2021, 624, 119088.	4.1	47
7392	A theoretical exploration of the effect and mechanism of CO on NO ₂ heterogeneous reduction over carbonaceous surfaces. <i>Fuel</i> , 2021, 290, 120102.	3.4	11
7393	Studies on hydrogen bonding of adrenaline/acetone and adrenaline/methanol complexes: computational and experimental approach. <i>Structural Chemistry</i> , 2021, 32, 2115-2138.	1.0	10
7394	Discovery of Non-Isolated-Pentagon-Rule Fullerenes from Computational Characterization of U ₂ O@C ₇₂ . <i>Inorganic Chemistry</i> , 2021, 60, 6492-6502.	1.9	6
7395	Using Room Temperature Phosphorescence of Gold(I) Complexes for PAHs Sensing. <i>Molecules</i> , 2021, 26, 2444.	1.7	7
7396	Natural Gas Dehydration with Ionic-Liquid-Based Mixed Solvents. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 6033-6047.	3.2	32
7397	DFT insight into mechanism of the Ni(II)-catalyzed enantioselective Michael addition: A combined computational and experimental study. <i>Molecular Catalysis</i> , 2021, 505, 111463.	1.0	7
7398	From LAr to L-ArBeO (L = He, Ne, Ar, HF): Switching on <i>f</i> -hole effects in non-covalent interactions. <i>Chemical Physics Letters</i> , 2021, 768, 138402.	1.2	8

#	ARTICLE	IF	CITATIONS
7399	An oxalate-bridged oxidovanadium(IV) binuclear complex that improves the in vitro cell uptake of a fluorescent glucose analog. <i>Polyhedron</i> , 2021, 198, 115071.	1.0	5
7400	Investigation of strength and nature of the weak intermolecular bond in NH ₂ radical-noble gas atom adducts and evaluation of their basic spectroscopic features. <i>Chemical Physics Letters</i> , 2021, 769, 138386.	1.2	3
7401	Dual-redox enhanced supercapacitors with sodium anthraquinone-2-sulfonate and potassium bromide. <i>Electrochimica Acta</i> , 2021, 374, 137889.	2.6	14
7402	Adsorption and sensor applications of C ₂ N surface for G-series and mustard series chemical warfare agents. <i>Microporous and Mesoporous Materials</i> , 2021, 317, 110984.	2.2	19
7403	Relativistic DFT Probe for Reaction Energies and Electronic/Bonding Properties of Polypyrrrolic Hetero-Bimetallic Actinide Complexes: Effects of Uranyl-Oxo Functionalization. <i>Inorganic Chemistry</i> , 2021, 60, 5747-5756.	1.9	5
7404	Nonlinear optical response of first-row transition metal doped Al ₁₂ P ₁₂ nanoclusters; a first-principles study. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 151, 109914.	1.9	18
7405	Effects of edge substitution of subazaphthalenephthalocyanine with electron withdrawing and/or donating groups on electronic and optical properties: A DFT/TDDFT study. <i>Materials Chemistry and Physics</i> , 2021, 263, 124420.	2.0	4
7406	Ruthenium (II) η^2 -diketimine as hydroamination catalyst, crystal structure and DFT computations. <i>Transition Metal Chemistry</i> , 2021, 46, 403-413.	0.7	1
7407	Dual-enhancement on electrochemical performance with thioacetamide as an electrolyte additive for lithium-sulfur batteries. <i>Electrochimica Acta</i> , 2021, 376, 138041.	2.6	21
7408	Mechanism of secondary organic aerosol formation from the reaction of isoprene with sulfoxy radicals. <i>Environmental Science and Pollution Research</i> , 2021, 28, 42562-42569.	2.7	2
7409	A New Strategy of bi-Alkali Metal Doping to Design Boron Phosphide Nanocages of High Nonlinear Optical Response with Better Thermodynamic Stability. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2021, 31, 3062-3076.	1.9	25
7410	A comparative study on the reactivity of cationic niobium clusters with nitrogen and oxygen. <i>Chinese Chemical Letters</i> , 2021, , .	4.8	3
7411	A Molecular Transformer: A π -Conjugated Macrocyclic Host as an Adaptable Host. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 11814-11818.	7.2	19
7412	Catalyst-free activation of permanganate under visible light irradiation for sulfamethazine degradation: Experiments and theoretical calculation. <i>Water Research</i> , 2021, 194, 116915.	5.3	124
7413	Solvent polarity dependent excited state hydrogen bond effects and intramolecular double proton transfer mechanism for 2-hydroxyphenyl-substituted benzo[1,2-d:4,5-d']bisimidazole system. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 250, 119394.	2.0	34
7414	Cajanusoids A-D, Unusual Atropisomeric Stilbene Dimers with PTP1B Inhibitory Activities from the Leaves of <i>Cajanus cajan</i> . <i>Journal of Organic Chemistry</i> , 2021, 86, 5870-5882.	1.7	7
7415	Effect of H ₂ O Molecules on the CO ₂ Replacement in CH ₄ Hydrate Behavior by Molecular Simulation. <i>Energy & Fuels</i> , 2021, 35, 8126-8140.	2.5	8
7416	Pillar[5]arene-Derived π -Functionalized Molecular Tube for Mimicking Protein-Ligand Interactions. <i>Journal of Organic Chemistry</i> , 2021, 86, 6467-6477.	1.7	7

#	ARTICLE	IF	CITATIONS
7417	DFT study of the radical scavenging activity of isoxanthohumol, humulones (β -acids), and iso- β -acids from beer. <i>Structural Chemistry</i> , 2021, 32, 2051-2059.	1.0	5
7418	First principles details into the grafting of aryl radicals onto the free-standing and borophene/Ag(111) surface. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4323-4333.	0.9	21
7419	Transition-Metal-Modified Vanadoborate Clusters as Stable and Efficient Photocatalysts for CO ₂ Reduction. <i>Inorganic Chemistry</i> , 2021, 60, 7364-7371.	1.9	12
7420	Selective adsorption of ofloxacin and ciprofloxacin from a binary system using lignin-based adsorbents: Quantitative analysis, adsorption mechanisms, and structure-activity relationship. <i>Science of the Total Environment</i> , 2021, 765, 144427.	3.9	46
7421	Modulation of trithiophene-based chalcone positional isomers by twist angle variation: Ultrafast nonlinear optical properties and excited-state dynamics. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 411, 113210.	2.0	6
7422	Substituent effect on ESIPT mechanisms and photophysical properties of HBT derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 250, 119375.	2.0	45
7423	Structural Uniqueness of the [Nb(As ₅) ₂] ⁵⁺ Cluster in the Zintl Phase Cs ₅ NbAs ₁₀ . <i>Journal of Physical Chemistry A</i> , 2021, 125, 4323-4333.	1.1	2
7424	Effect of electron donor and acceptor on the photovoltaic properties of organic dyes for efficient dye-sensitized solar cells. <i>Physica B: Condensed Matter</i> , 2021, 609, 412815.	1.3	6
7425	A regioselectivity descriptor based on atomic Weizsäcker kinetic energy. <i>Chemical Physics Letters</i> , 2021, 770, 138455.	1.2	1
7426	Tuning the antioxidant property of potential calixdrug calix[4]tyrosol: role of aza and thia linkages. <i>Structural Chemistry</i> , 2021, 32, 2223-2234.	1.0	3
7427	A joint experimental and theoretical study on structural, electronic, and magnetic properties of MnGen ⁿ⁺ (n = 3-14) clusters. <i>Journal of Chemical Physics</i> , 2021, 154, 204302.	1.2	24
7428	Theoretical Simulations of Thermochromic and Aggregation-Induced Emission Behaviors of a Series of Red-Light Anthracene-carborane Derivatives. <i>Chemistry - A European Journal</i> , 2021, 27, 9571-9579.	1.7	5
7429	Reaction Mechanisms of the Degradation of Fluoroethylene Carbonate, an Additive of Lithium-Ion Batteries, Unraveled by Radiation Chemistry. <i>Chemistry - A European Journal</i> , 2021, 27, 8185-8194.	1.7	9
7430	Theoretical prediction on photoelectric and supramolecular properties of benzoquinone-tetrathiafulvalene macrocyclic molecules. <i>Journal of Molecular Modeling</i> , 2021, 27, 157.	0.8	1
7431	Molecular dynamics simulation of small gas molecule permeation through CAU-1 membrane. <i>Chinese Journal of Chemical Engineering</i> , 2021, 33, 104-111.	1.7	9
7432	Understanding the Electronic Structure and Stability of B ₂ X ₂ O ₂ (X = N, O) (n = 4, 6; X ₂ = N ₂ , O ₂). <i>Journal of Physical Chemistry A</i> , 2021, 125, 4323-4333.	0.9	21
7433	Theoretical Study of Actinide(III)-DOTA Complexes. <i>ACS Omega</i> , 2021, 6, 13321-13330.	1.6	13
7434	A highly-sensitive α -probe based on coumarin β -diketone for hydrazine detection in PBS and living cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 252, 119510.	2.0	27

#	ARTICLE	IF	CITATIONS
7435	Regulating Interfacial Coupling and Electron Transport for Efficient Electron-Transporting Materials. <i>Journal of Physical Chemistry C</i> , 2021, 125, 10140-10150.	1.5	1
7436	High regioselectivity in the amination reaction of isoquinolinequinone derivatives using conceptual DFT and NCI analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 104, 107828.	1.3	5
7437	The Adsorption of 1-Chloro-1,2,2,2-Tetrafluoroethane Onto the Pristine, Al-, and Ga-Doped Boron Nitride Nanosheet. <i>Iranian Journal of Science and Technology, Transaction A: Science</i> , 2021, 45, 1287-1300.	0.7	29
7438	Triangular Interchalcogen Interactions: A Joint Crystallographic Data Analysis and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4173-4183.	1.1	7
7439	Quantum chemical study on sensing of NH ₃ , NF ₃ , NCl ₃ and NBr ₃ by using cyclic tetrapyrrole. <i>Computational and Theoretical Chemistry</i> , 2021, 1199, 113221.	1.1	18
7440	Atomically dispersed antimony on carbon nitride for the artificial photosynthesis of hydrogen peroxide. <i>Nature Catalysis</i> , 2021, 4, 374-384.	16.1	474
7441	Are There Only Fold Catastrophes in the Diels-Alder Reaction Between Ethylene and 1,3-Butadiene?. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5152-5165.	1.1	19
7442	Mechanism of Deep Eutectic Solvent Delignification: Insights from Molecular Dynamics Simulations. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 7101-7111.	3.2	38
7443	Tetrahedral Pt ₁₀ Cluster with Unique Beta Aromaticity and Superatomic Feature in Mimicking Methane. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5115-5122.	2.1	20
7444	A Water-Soluble Schiff Base Turn-on Fluorescent Chemosensor for the Detection of Al ³⁺ and Zn ²⁺ Ions at the Nanomolar Level: Application in Live-Cell Imaging. <i>Journal of Fluorescence</i> , 2021, 31, 1277-1290.	1.3	14
7445	Theoretical study on the two novel planar-type all-nitrogen N ₄ ⁻ anions: Structures, stability, reaction rate and their stable mechanisms via protonation. <i>Chemical Physics Letters</i> , 2021, 771, 138519.	1.2	1
7446	Multifunctional Mg/Al layered double hydroxides intercalated by sorbate anion via low-cost co-precipitation. <i>Colloids and Interface Science Communications</i> , 2021, 42, 100396.	2.0	1
7447	Neuroprotective schinortriterpenoids from <i>Schisandra neglecta</i> collected in Medog County, Tibet, China. <i>Bioorganic Chemistry</i> , 2021, 110, 104785.	2.0	10
7448	Arylazopyrazole-Based Dendrimer Solar Thermal Fuels: Stable Visible Light Storage and Controllable Heat Release. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 22655-22663.	4.0	33
7449	Ensemble machine learning to evaluate the in vivo acute oral toxicity and in vitro human acetylcholinesterase inhibitory activity of organophosphates. <i>Archives of Toxicology</i> , 2021, 95, 2443-2457.	1.9	13
7450	On-The-Fly Non-Adiabatic Dynamics Simulations on Photoinduced Ring-Closing Reaction of a Nucleoside-Based Diarylethene Photoswitch. <i>Molecules</i> , 2021, 26, 2724.	1.7	4
7451	Tetranitro-diazinodiazines as high energy materials: computational investigation of structural aspects of fused heterocyclic backbone and isomerism. <i>Structural Chemistry</i> , 2021, 32, 2175-2181.	1.0	4
7452	A new metal-organic framework of 3,9-diazatetraasterane-1,5,7,11-tetracarboxylic acid-3,6,9,12-tetraphenyl with sodium ion: Synthesis, characterization and DFT calculations. <i>Chemical Physics Letters</i> , 2021, 771, 138469.	1.2	4

#	ARTICLE	IF	CITATIONS
7453	A comparative study of PffBT4T-2OD/EH-IDTBR and PffBT4T-2OD/PC71BM organic photovoltaic heterojunctions. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 412, 113225.	2.0	9
7454	Metal Oxo-Fluoride Molecules OnMF ₂ (M = Mn and Fe; n = 1–4) and O ₂ MnF: Matrix Infrared Spectra and Quantum Chemistry. <i>Inorganic Chemistry</i> , 2021, 60, 7687-7696.	1.9	3
7455	Mechanism and kinetics of ClO ⁻ -mediated degradation of aromatic compounds in aqueous solution: DFT and QSAR studies. <i>Chemical Engineering Journal</i> , 2021, 412, 128728.	6.6	25
7456	The theoretical investigation on properties of paeonol and its isomers. <i>Molecular Physics</i> , 2021, 119, e1925363.	0.8	5
7457	An acid induction strategy to construct an ultralight and durable amino-functionalized graphene oxide aerogel for enhanced quinoline pollutants extraction from coking wastewater. <i>Chemical Engineering Journal</i> , 2021, 412, 128686.	6.6	27
7458	Nanosopic characterization of type II porous liquid and its use for CO ₂ absorption from molecular simulation. <i>Journal of Molecular Liquids</i> , 2021, 330, 115660.	2.3	15
7459	Interface Engineering of a Sandwich Flexible Electrode PAn@CoHCF Rooted in Carbon Cloth for Enhanced Sodium-Ion Storage. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 23794-23802.	4.0	6
7460	Towards the Highly Efficient Synthesis and Selective Methylation of C(sp ³)-Bridged [6]Cycloparaphenylenes from Fluoren[3]arenes. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 13021-13028.	7.2	34
7461	The mechanisms of a bifunctional fluorescent probe for detecting fluoride and sulfite based on excited-state intramolecular proton transfer and intramolecular charge transfer. <i>Structural Dynamics</i> , 2021, 8, 034103.	0.9	8
7462	Computational Insights Into the Influence of Substitution Groups on the Inclusion Complexation of β -Cyclodextrin. <i>Frontiers in Chemistry</i> , 2021, 9, 668400.	1.8	5
7463	A low sensitivity energetic cocrystal of ammonium pentazolate. <i>Journal of Energetic Materials</i> , 2023, 41, 99-116.	1.0	6
7464	Contribution of the Molecular Fluorophore IPCA to Excitation-Independent Photoluminescence of Carbon Dots. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12140-12148.	1.5	22
7465	Ni ₂ P Nanosheets: A High Catalytic Activity Platform for Electrochemical Detection of Acetaminophen. <i>Chinese Journal of Chemistry</i> , 2021, 39, 1849-1854.	2.6	18
7466	A Multiscale Simulation Study of Influence of Morphology on Ion Transport in Block Copolymeric Ionic Liquids. <i>Macromolecules</i> , 2021, 54, 4997-5010.	2.2	16
7467	Experimental and computational study of hydrolysis and photolysis of antibiotic ceftriaxone: Degradation kinetics, pathways, and toxicity. <i>Science of the Total Environment</i> , 2021, 768, 144991.	3.9	23
7468	Understanding intermolecular interactions of large systems in ground state and excited state by using density functional based tight binding methods. <i>Journal of Chemical Physics</i> , 2021, 154, 194106.	1.2	9
7469	High-rate aqueous zinc-organic battery achieved by lowering HOMO/LUMO of organic cathode. <i>Energy Storage Materials</i> , 2021, 37, 378-386.	9.5	162
7470	Theoretical investigation on the reactive and interaction properties of sorafenib – DFT, AIM, spectroscopic and Hirshfeld analysis, docking and dynamics simulation. <i>Journal of Molecular Liquids</i> , 2021, 330, 115652.	2.3	34

#	ARTICLE	IF	CITATIONS
7471	Theoretical Study of Excited State Charge Transfer Characteristics based on Aa€“Dâ€“A and Aa€“DAâ€“2Dâ€“A Type Nonfullerene Acceptors. <i>Journal of Physical Chemistry C</i> , 2021, 125, 10250-10259.	1.5	40
7472	Efficient and remarkable SO ₂ capture: A discovery of imidazole-based ternary deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2021, 330, 115595.	2.3	18
7473	Unexpected favourable noncovalent interaction between chlorine oxyanions (ClO ⁻ ; x = 1-4) and benzene: Benchmarking DFT and SAPT methods with respect to CCSD(T). <i>Computational and Theoretical Chemistry</i> , 2021, 1199, 113214.	1.1	6
7474	Rational Design and Experimental Research on the Self-Assembled System of Thermosensitive Molecularly Imprinted Polymers Formed by Lipoic Acid and N-Vinyl Caprolactam. <i>International Journal of Polymer Science</i> , 2021, 2021, 1-11.	1.2	0
7475	Neither too Classic nor too Exotic: Oneâ€“Electron Naâ€“...B Bond in NaBH ₃ ⁺ Cluster. <i>Angewandte Chemie</i> , 2021, 133, 12857-12863.	1.6	4
7476	The O to S substitution in urea brings inhibition activity against thiocyanate dehydrogenase. <i>Mendeleev Communications</i> , 2021, 31, 373-375.	0.6	1
7477	Structural exploration and properties of (BN) ₆ cluster via ab initio in combination with particle swarm optimization method. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	4
7478	Investigation of tetrabutylammonium bromide-glycerol-based deep eutectic solvents and their mixtures with water by spectroscopic techniques. <i>Journal of Molecular Liquids</i> , 2021, 330, 115617.	2.3	27
7479	Molecular chirality of Macrolide antibiotics. <i>Chemical Physics</i> , 2021, 545, 111120.	0.9	0
7480	Vibrational spectroscopy and DFT analysis of 4-cyanophenylhydrazine: A potential SERS probe. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 253, 119574.	2.0	1
7481	An unexpected Cu(II) complex of oxidized 1,4-dihydropyridine derivative: Synthesis, characterization and DFT calculations. <i>Journal of Molecular Structure</i> , 2021, 1232, 130057.	1.8	0
7482	Key structural features that determine the selectivity of UV/acetylacetone for the degradation of aromatic pollutants when compared to UV/H ₂ O ₂ . <i>Water Research</i> , 2021, 196, 117046.	5.3	33
7483	Design of High-Contrast Mechanochromic Materials Based on Aggregation-Induced Emissive Pyran Derivatives Guided by Polymorph Predictions. <i>CCS Chemistry</i> , 2022, 4, 899-909.	4.6	18
7484	Unveiling the Reaction Mechanism of the Das/Chechik/Marek Synthesis of Stereodefined Quaternary Carbon Centers. <i>Applied Sciences (Switzerland)</i> , 2021, 11, 5002.	1.3	0
7485	A computational study on the complexation of bisbenzimidazolyl derivatives with cucurbituril and cyclohexylcucurbituril. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2021, 100, 217.	0.9	4
7486	Pyrido[3,4-d]pyrimidine as an Acceptor of Thermally Activated Delayed Fluorescent Emitters: Timeâ€“dependent Density Functional Theory Study. <i>Bulletin of the Korean Chemical Society</i> , 2021, 42, 977-982.	1.0	2
7487	Speculative assessment, molecular composition, PDOS, topology exploration (ELF, LOL, RDG), ligand-protein interactions, on 5-bromo-3-nitropyridine-2-carbonitrile. <i>Heliyon</i> , 2021, 7, e07061.	1.4	44
7488	K-means clustering analysis, ADME/pharmacokinetic prediction, MEP, and molecular docking studies of potential cytotoxic agents. <i>Structural Chemistry</i> , 2021, 32, 2235-2249.	1.0	10

#	ARTICLE	IF	CITATIONS
7489	Vinyl Groups Containing Tetraphenylethylene Derivatives as Fluorescent Probes Specific for Palladium and the Quenching Mechanism. <i>Chinese Journal of Chemistry</i> , 2021, 39, 1599-1605.	2.6	12
7490	Modeling Adsorption and Optical Properties for the Design of CO ₂ Photocatalytic Metal-Organic Frameworks. <i>Molecules</i> , 2021, 26, 3060.	1.7	4
7491	Modeling the structural and reactivity properties of hydrazono methyl-4H-chromen-4-one derivatives: wavefunction-dependent properties, molecular docking, and dynamics simulation studies. <i>Journal of Molecular Modeling</i> , 2021, 27, 186.	0.8	9
7492	Cocrystals of Oxymatrine: Reducing Hygroscopicity and Affecting the Dissolution Rate. <i>Crystal Growth and Design</i> , 2021, 21, 3874-3888.	1.4	12
7493	Combined MD and QM/MM Investigations of Hydride Reduction of 5 α -Dihydrotestosterone Catalyzed by Human 3 α -Hydroxysteroid Dehydrogenase Type 3: Importance of Noncovalent Interactions. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4998-5008.	1.2	4
7494	Insights into the Structures and Bonding of Medium-Sized Cerium-Doped Boron Clusters. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4126-4132.	1.1	9
7495	Pyrene Derived aggregation-induced emission sensor for highly selective detection of explosive CL-20. <i>Journal of Luminescence</i> , 2021, 233, 117871.	1.5	8
7496	Relativistic Hirshfeld atom refinement of an organo-gold(I) compound. <i>IUCr</i> , 2021, 8, 608-620.	1.0	9
7497	Computational insights into promoting effects of alkali metals, Re, and Cl for silver catalysts of ethylene epoxidation. <i>Molecular Catalysis</i> , 2021, 507, 111574.	1.0	1
7498	Unexpected Role of Achiral Glycine in Determining the Suprastructural Handedness of Peptide Nanofibrils. <i>ACS Nano</i> , 2021, 15, 10328-10341.	7.3	28
7499	London Dispersion Helps Refine Steric A-Values: The Halogens. <i>Journal of Organic Chemistry</i> , 2021, 86, 7701-7713.	1.7	14
7500	Aggregation-induced emission or aggregation-caused quenching? Impact of covalent bridge between tetraphenylethylene and naphthalimide. <i>Chinese Chemical Letters</i> , 2021, 32, 1790-1794.	4.8	54
7501	Chitosan and chitosan/PEG nanoparticles loaded with indole-3-carbinol: Characterization, computational study and potential effect on human bladder cancer cells. <i>Materials Science and Engineering C</i> , 2021, 124, 112089.	3.8	10
7502	Red-light excited efficient metal-free near-infrared room-temperature phosphorescent films. <i>National Science Review</i> , 2022, 9, nwab085.	4.6	63
7503	Theoretical studies on the catalytic hydrogenation of carbon dioxide by 3d transition metals single-atom catalyst supported on covalent triazine frameworks. <i>Molecular Catalysis</i> , 2021, 508, 111581.	1.0	10
7504	Transition-metal complexes of N,N'-di(4-bromophenyl)-4-hydroxycoumarin-3-carboximidamide: synthesis, characterization, biological activities, ADMET and drug-likeness analysis. <i>Inorganic Chemistry Communication</i> , 2021, 127, 108509.	1.8	10
7505	Highly Efficient Near-Infrared Photosensitizers with Aggregation-Induced Emission Characteristics: Rational Molecular Design and Photodynamic Cancer Cell Ablation. <i>ACS Applied Bio Materials</i> , 2021, 4, 5231-5239.	2.3	14
7506	Effects of Comonomers on the Performance of Stable Phosphonate-Based Gel Terpolymer Electrolytes for Sodium-Ion Batteries with Ultralong Cycling Stability. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 25024-25035.	4.0	11

#	ARTICLE	IF	CITATIONS
7507	Inhibition of cyclooxygenase by blocking the reducing cosubstrate at the peroxidase site: Discovery of galangin as a novel cyclooxygenase inhibitor. <i>European Journal of Pharmacology</i> , 2021, 899, 174036.	1.7	7
7508	Quantitative analysis of the relationship of derivatization reagents and detection sensitivity of electrospray ionization-triple quadrupole tandem mass spectrometry: Hydrazines as prototypes. <i>Analytica Chimica Acta</i> , 2021, 1158, 338402.	2.6	3
7509	Interpreting the nature of interactions in the inclusion complex of danofloxacin, a third-generation fluoroquinolone with Cucurbit[7]uril: A computational study. <i>Computational and Theoretical Chemistry</i> , 2021, 1199, 113210.	1.1	1
7510	Theoretical insights into the cineole-based deep eutectic solvents. <i>Journal of Chemical Physics</i> , 2021, 154, 184504.	1.2	14
7511	Effect of an electric field on the molecular properties of tributyrin, tricaproin and tricaprylin: a theoretical study. <i>Journal of the Korean Physical Society</i> , 2021, 79, 369-379.	0.3	1
7512	Exploring Li4N and Li4O superalkalis as efficient dopants for the Al12N12 nanocage to design high performance nonlinear optical materials with high thermodynamic stability. <i>Polyhedron</i> , 2021, 200, 115145.	1.0	12
7513	Predicting the Adsorption of Amoxicillin and Ibuprofen on Chitosan and Graphene Oxide Materials: A Density Functional Theory Study. <i>Polymers</i> , 2021, 13, 1620.	2.0	8
7514	Combined Use of Structure Analysis, Studies of Molecular Association in Solution, and Molecular Modelling to Understand the Different Propensities of Dihydroxybenzoic Acids to Form Solid Phases. <i>Pharmaceutics</i> , 2021, 13, 734.	2.0	3
7515	Adsorption of melphalan anticancer drug on C24, B12N12, B12C6N6, B6C12N12 and B6C6N12 nanocages: A comparative DFT study. <i>Journal of Molecular Liquids</i> , 2021, 329, 115528.	2.3	34
7516	Insights into the selective sensing mechanism of a luminescent Cd(II)-based MOF chemosensor toward NACs: roles of the host-guest interactions and PET processes. <i>Journal of Materials Science</i> , 2021, 56, 13684-13704.	1.7	14
7517	Characterization of orthogonal hydrogen and halogen bonds in thiobarbituric acid complexes with halogen molecules (X = I 2 , Br 2 , and Cl 2): Structural and spectroscopic study. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 1630.	0.8	0
7519	Understanding the Fe-CO bond through the electronic structure of Fem+(CO)6-nLn, m = 2, 3, n = 0, 1, 2, 3, 0.8. <i>Journal of Molecular Modeling</i> , 2021, 27, 148.	0.8	0
7520	A revisited study of the low-lying electronic states of HF molecule. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021, 271, 107737.	1.1	6
7521	How Do Defects in Carbon Nanostructures Regulate the Photoinduced Electron Transfer Processes? The Case of Phenine Nanotubes. <i>ChemPhysChem</i> , 2021, 22, 1178-1186.	1.0	7
7522	Low-bandgap conjugated polymers based on benzodipyrrolidone with reliable unipolar electron mobility exceeding 1 cm ² V ⁻¹ s ⁻¹ . <i>Science China Chemistry</i> , 2021, 64, 1219-1227.	4.2	19
7523	Redox-active NIR Iridium(III) Emitters: Synthesis, Photophysical and Computational Study, the Effects of Cyclometalating and β -diketonate Ligands. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 2163-2170.	1.0	11
7524	Molecular insights of metal-metal interactions in transition metal complexes using computational methods. <i>Pure and Applied Chemistry</i> , 2021, 93, 579-589.	0.9	1
7525	Ion Dipole Chemistry Drives Rapid Evolution of Li Ions Solvation Sheath in Low-Temperature Li Batteries. <i>Advanced Energy Materials</i> , 2021, 11, 2100935.	10.2	95

#	ARTICLE	IF	CITATIONS
7526	Study on the Mechanism of Ionic Liquids Improving the Extraction Efficiency of Essential Oil Based on Experimental Optimization and Density Functional Theory: The Fennel (<i>Foeniculi fructus</i>) Essential Oil Case. <i>Molecules</i> , 2021, 26, 3169.	1.7	4
7527	Identification of NSAIDs as lipoxygenase inhibitors through highly sensitive chemiluminescence method, expression analysis in mononuclear cells and computational studies. <i>Bioorganic Chemistry</i> , 2021, 110, 104818.	2.0	20
7528	Evaluating mutual influences of cation- π interactions and H-bonding: Cases of indole and BN-indole. <i>Polyhedron</i> , 2021, 200, 115131.	1.0	4
7529	Real-time monitoring of aristolochic acid I reduction process using surface-enhanced Raman Spectroscopy with DFT simulation. <i>Biosensors and Bioelectronics</i> , 2021, 179, 113061.	5.3	8
7530	Co (II) and Cd (II) complexes with imidazole- α - β -carboxaldehyde groups: spectroscopic, antibacterial, Hirshfeld surfaces analyses, and TD/DFT calculations. <i>Applied Organometallic Chemistry</i> , 2021, 35, e6279.	1.7	15
7531	Heterohelicenes through 1,3-Dipolar Cycloaddition of Sydnone with Arynes: Synthesis, Origins of Selectivity, and Application to pH-Triggered Chiroptical Switch with CPL Sign Reversal. <i>Jacs Au</i> , 2021, 1, 807-818.	3.6	29
7532	Structural characterization of hydrogen bonding for antipyrine derivatives: Single-crystal X-ray diffraction and theoretical studies. <i>Fine Chemical Technologies</i> , 2021, 16, 113-137.	0.1	4
7533	Synergistic effect of polystyrene nanoplastics and contaminants on the promotion of insulin fibrillation. <i>Ecotoxicology and Environmental Safety</i> , 2021, 214, 112115.	2.9	20
7534	A theoretical study of the photophysical properties of coumarin-carbohydrazone and coumarin-thiocarbohydrazone. <i>Computational and Theoretical Chemistry</i> , 2021, 1199, 113213.	1.1	3
7535	Triazine COF-supported single-atom catalyst (Pd1/trzn-COF) for CO oxidation. <i>Science China Materials</i> , 2021, 64, 1939-1951.	3.5	28
7536	Electron Transfer Facilitated by π - π Stacking during the Nitrobenzene Recognition Process of an MOF Sensor. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12433-12440.	1.5	21
7537	Theoretical prediction of an NXeH ₄ ⁺ ion with N-Xe triple bond. <i>Computational and Theoretical Chemistry</i> , 2021, 1199, 113193.	1.1	2
7538	Neither too Classic nor too Exotic: One-Electron Na \cdots B Bond in NaBH ₃ ⁺ Cluster. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 12747-12753.	7.2	13
7539	Enantioselective, Catalytic Multicomponent Synthesis of Homoallylic Amines Enabled by Hydrogen-Bonding and Dispersive Interactions. <i>Journal of the American Chemical Society</i> , 2021, 143, 7272-7278.	6.6	15
7540	Research of weak interaction between water and different monolayer graphene systems. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 104, 107835.	1.3	1
7541	Excited state electronic structures and photochemistry of different oxidation states of 2,2'-azino-bis-(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 253, 119503.	2.0	0
7542	Effect of static external electric field on bulk and interfaces in organic solar cell systems: A density-functional-theory-based study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 253, 119565.	2.0	9
7543	Insights into the mechanism of fatty acid photodecarboxylase: A theoretical investigation. <i>Chemical Physics Letters</i> , 2021, 771, 138550.	1.2	2

#	ARTICLE	IF	CITATIONS
7544	Towards the Highly Efficient Synthesis and Selective Methylation of C(sp ³)-Bridged [6]Cycloparaphenylenes from Fluoren[3]arenes. <i>Angewandte Chemie</i> , 2021, 133, 13131-13138.	1.6	11
7545	Photocatalytic degradation of naproxen by Bi ₂ MoO ₆ /g-C ₃ N ₄ heterojunction photocatalyst under visible light: Mechanisms, degradation pathway, and DFT calculation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 412, 113235.	2.0	43
7546	The roles of HO•, ClO• and BrO• radicals in caffeine degradation: A theoretical study. <i>Science of the Total Environment</i> , 2021, 768, 144733.	3.9	31
7547	Conformational Analysis, Spectroscopic Insights, Chemical Descriptors, ELF, LOL and Molecular Docking Studies of Potential Pyrimidine Derivative with Biological Activities. <i>Polycyclic Aromatic Compounds</i> , 2022, 42, 5160-5170.	1.4	5
7548	Cation-Anion Interactions, Stability, and IR Spectra of Dicationic Amino Acid-Based Ionic Liquids Probed Using Density Functional Theory. <i>Journal of Molecular Modeling</i> , 2021, 27, 180.	0.8	4
7549	Pyrolysis and carbonization of polyvinyl chloride under electric field: A computational study. <i>Chemical Physics Letters</i> , 2021, 770, 138450.	1.2	4
7550	Theoretical research of covalent and controllable molecular brake based on 9-triptycene. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	0
7551	DFT study of effect of substituents on second-order NLO response of novel BODIPY dyes. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	1
7552	Theoretical study on cubane molecule and its reduced states (C ₈ H ₈ n; n=0 and 1 to 4); a first principle DFT study. <i>Journal of the Iranian Chemical Society</i> , 2021, 18, 3303.	1.2	1
7553	Role of Dynamical Electron Correlation in the Differences in Bonding between CaAlH ₃ and MgAlH ₃ . <i>Journal of Physical Chemistry A</i> , 2021, 125, 3912-3919.	1.1	0
7554	Molecular design of long intra-annular nitrogen chains: 3H-tetrazolo[1,5-d]tetrazole-based high-energy-density materials. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26743.	1.0	3
7555	Computational investigation and screening of high-energy-density materials: Based on nitrogen-rich 1,2,4,5-tetrazine energetic derivatives. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26742.	1.0	3
7556	Multifunctional Materials Serving as Efficient Non-Doped Violet-Blue Emitters and Host Materials for Phosphorescence. <i>Chemistry - A European Journal</i> , 2021, 27, 9102-9111.	1.7	12
7557	Theoretical Insights into the Actinide-Silicon Bonding Nature and Stability of a Series of Actinide Complexes with Different Oxidation States. <i>Organometallics</i> , 2021, 40, 1719-1727.	1.1	5
7558	Molecular Properties and Aggregation Behavior of Small-Molecule Acceptors Calculated by Molecular Simulation. <i>ACS Omega</i> , 2021, 6, 14467-14475.	1.6	5
7559	2-Mercaptobenzothiazole modified carbon paste electrode as a novel copper sensor: An electrochemical and computational study. <i>Journal of Electroanalytical Chemistry</i> , 2021, 888, 115208.	1.9	13
7560	Hydrogen-bond donor and acceptor cooperative catalysis strategy for cyclic dehydration of diols to access O-heterocycles. <i>Science Advances</i> , 2021, 7, .	4.7	19
7561	C ₄ N ₈ O ₆ : A Promising Ternary CNO Compound With Good Detonation Performance And Low Sensitivity. <i>Propellants, Explosives, Pyrotechnics</i> , 2021, 46, 1286-1291.	1.0	2

#	ARTICLE	IF	CITATIONS
7562	Adsorption of two \hat{I}^2 -blocker pollutants on modified montmorillonite with environment-friendly cationic surfactant containing amide group: Batch adsorption experiments and Multiwave function analysis. <i>Journal of Colloid and Interface Science</i> , 2021, 590, 601-613.	5.0	25
7563	DFT study of the catalytic effect of Fe on the gasification of char-CO ₂ . <i>Fuel</i> , 2021, 292, 120203.	3.4	15
7565	C ₃₆ and C ₃₅ E (E=N and B) Fullerenes as Potential Nanovehicles for Neuroprotective Drugs: A Comparative DFT Study. <i>ChemistrySelect</i> , 2021, 6, 4844-4858.	0.7	5
7566	In silico modeling: electronic properties of phosphorene monoflakes and biflakes substituted with Al, Si, and S heteroatoms. <i>Journal of Molecular Modeling</i> , 2021, 27, 171.	0.8	3
7567	Study on novel PtNP@sorafenib and its interaction with VEGFR2. <i>Journal of Biochemistry</i> , 2021, 170, 411-417.	0.9	2
7568	Aqueous L-alanine molecular interaction from Gibbs' free energy: CPCM and SMD in DFT and ultrasonic studies. <i>Journal of Physics: Conference Series</i> , 2021, 1913, 012007.	0.3	0
7569	Unveiling the influence of solvent polarity on structural, electronic properties, and ³¹ P NMR parameters of rhenabenzynes complex. <i>Inorganic Chemistry Communication</i> , 2021, 127, 108497.	1.8	6
7570	A new diastereomeric type of N-morpholino-spiro derivative. Structural, spectroscopic and computational studies. <i>Journal of Molecular Structure</i> , 2021, 1232, 130018.	1.8	0
7571	New insights into structural, electronic, reactivity, spectroscopic and pharmacological properties of Bergenin: Experimental, DFT calculations, MD and docking simulations. <i>Journal of Molecular Liquids</i> , 2021, 330, 115625.	2.3	12
7572	The suppression of intramolecular charge transfer emission by tautomerism in 2-(4-amino-2-hydroxyphenyl)-1H-imidazo-[4,5-c]pyridine: Intramolecular proton transfer versus intermolecular proton transfer. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 413, 113199.	2.0	3
7573	Assessing the potential of para-donor and para-acceptor substituted 5-benzylidenebarbituric acid derivatives as push-pull electronic systems: Experimental and quantum chemical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 253, 119576.	2.0	1
7574	Mechanism of Ir-Mediated Selective Pyridine C-H Activation: The Role of Lewis Acidic Boryl Group. <i>ACS Catalysis</i> , 2021, 11, 6186-6192.	5.5	7
7575	An aromatic Ca ₂ B ₈ complex for reversible hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 19023-19030.	3.8	18
7576	A Combined Experimental and Computational Study of Halogen and Hydrogen Bonding in Molecular Salts of 5-Bromocytosine. <i>Molecules</i> , 2021, 26, 3111.	1.7	1
7577	Comparative Structural Study of Three Tetrahalophthalic Anhydrides: Recognition of X $\cdot\cdot$ O(anhydride) Halogen Bond and $\hat{I}\hat{H}\cdot\cdot\hat{O}$ (anhydride) Interaction. <i>Molecules</i> , 2021, 26, 3119.	1.7	1
7578	Relationship Between Matrix Metalloproteinase-2 Inhibition Constants With APP-IP Oligopeptide and Its Mutant Forms and Electronic Binding Descriptors. <i>Russian Journal of Physical Chemistry B</i> , 2021, 15, 394-398.	0.2	1
7579	Revisiting stacking interactions in tetrathiafulvalene and selected derivatives using tight-binding quantum chemical calculations and local coupled-cluster method. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 311-320.	0.5	6
7580	Effects of Multiple OH/SH Substitution on the $\hat{H}\hat{B}$ onding/Stability versus Aromaticity of Benzene Rings: From Computational Insights. <i>ChemistrySelect</i> , 2021, 6, 5120-5139.	0.7	6

#	ARTICLE	IF	CITATIONS
7581	Removal of oxytetracycline by graphene oxide and Boron-doped reduced graphene oxide: A combined density function Theory, molecular dynamics simulation and experimental study. FlatChem, 2021, 27, 100238.	2.8	28
7582	Molecular-Scale Mechanism of Sequential Reaction of Oxalic Acid with SO ₃ : Potential Participator in Atmospheric Aerosol Nucleation. Journal of Physical Chemistry A, 2021, 125, 4200-4208.	1.1	8
7583	Directional Exciton Migration in Benzoimidazole-Based Metal-Organic Frameworks. Journal of Physical Chemistry Letters, 2021, 12, 4917-4927.	2.1	10
7584	Anion Specific Effects Drive the Formation of Li-Salt Based Aqueous Biphasic Systems. Journal of Physical Chemistry B, 2021, 125, 5365-5372.	1.2	9
7585	Interaction between carboplatin with B12P12 and Al12P12 nano-clusters: A computational investigation. Phosphorus, Sulfur and Silicon and the Related Elements, 2021, 196, 751-759.	0.8	10
7586	Theoretical Investigation of Hydrogen-Bond-Assisted Tetradentate N4 Copper(I) Chloride and trans- λ_1, λ_2 -Peroxodicopper Complexes. European Journal of Inorganic Chemistry, 2021, 2021, 2194-2200.	1.0	1
7587	The O to S substitution in urea brings inhibition activity against thiocyanate dehydrogenase. Mendeleev Communications, 2021, 31, 373-375.	0.6	0
7588	The Electrophilicities of XCF ₃ and XCl (X=H, Cl, Br, I) and the Propensity of These Molecules To Form Hydrogen and Halogen Bonds with Lewis Bases: An Ab Initio Study. ChemPlusChem, 2021, 86, 778-784.	1.3	6
7589	Analysis of Intermolecular Weak Interactions and Vibrational Characteristics for Vanillin and Ortho-Vanillin by Terahertz Spectroscopy and Density Functional Theory. IEEE Transactions on Terahertz Science and Technology, 2021, 11, 318-329.	2.0	15
7590	Synthesis and Structure of an <i>oxo</i> -Carboranyl-Substituted Three-Coordinate Borane Radical Anion. Chemistry - A European Journal, 2021, 27, 8159-8167.	1.7	23
7591	Corrosion inhibition performance of a structurally well-defined 1,2,3-triazole derivative on mild steel-hydrochloric acid interface. Journal of Molecular Structure, 2021, 1231, 129895.	1.8	33
7593	Interaction Region Indicator: A Simple Real Space Function Clearly Revealing Both Chemical Bonds and Weak Interactions**. Chemistry Methods, 2021, 1, 231-239.	1.8	516
7594	Salting-out effect promoting highly efficient ambient ammonia synthesis. Nature Communications, 2021, 12, 3198.	5.8	105
7596	Treatment of phenol wastewater using nitrogen-doped magnetic mesoporous hollow carbon. Chemosphere, 2021, 271, 129595.	4.2	14
7597	Charge Transfer as the Key Parameter Affecting the Color Purity of Thermally Activated Delayed Fluorescence Emitters. ACS Applied Materials & Interfaces, 2021, 13, 28529-28537.	4.0	43
7598	Asymmetric Nucleophilic Allylation of $\hat{1}\pm$ -Chloro Glycinate via Squaramide Anion-Abstraction Catalysis: S _N 1 or S _N 2 Mechanism, or Both?. Journal of Organic Chemistry, 2021, 86, 8414-8424.	1.7	5
7599	Mechanisms of Molecular Ferroelectrics Made Simple. Journal of Physical Chemistry C, 2021, 125, 12461-12467.	1.5	3
7600	A computational study of N ₂ adsorption on aromatic metal Mg ₁₆ M;(M=Be, Mg, and Ca) nanoclusters. Journal of Molecular Graphics and Modelling, 2021, 105, 107862.	1.3	3

#	ARTICLE	IF	CITATIONS
7601	Zn(II) cation-induced solution emission of 4-(4-(1,2,2-triphenylvinyl)phenyl)benzoic acid: Intuitionistic evidence of RIM mechanism. <i>Journal of Molecular Structure</i> , 2021, 1234, 130128.	1.8	0
7602	Using Quantum Density Functional Theory Methods to Study the Adsorption of Fluorouracil Drug on Pristine and Al, Ga, P and As Doped Boron Nitride Nanosheets. <i>ChemistrySelect</i> , 2021, 6, 6119-6131.	0.7	7
7603	Zn(II) Heteroleptic Halide Complexes with 2-Halopyridines: Features of Halogen Bonding in Solid State. <i>Molecules</i> , 2021, 26, 3393.	1.7	6
7604	Effect of cobalt doping on H ₂ generation mechanism of Mo-edge from density functional theory. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	2
7605	Simulation and surface topology of activity of pyrazoloquinoline derivatives as corrosion inhibitor on the copper surfaces. <i>Scientific Reports</i> , 2021, 11, 12223.	1.6	2
7606	Theoretical study on charge distribution in cetylpyridinium cationic surfactant. <i>Journal of Molecular Modeling</i> , 2021, 27, 203.	0.8	6
7607	Non-noble metal single atom catalysts with S, N co-doped defective graphene support: A theoretical study of highly efficient acetylene hydration. <i>Materials Today Communications</i> , 2021, 27, 102216.	0.9	2
7608	Intramolecular H-Bond Dynamics of Catechol Investigated by THz High-Resolution Spectroscopy of Its Low-Frequency Modes. <i>Molecules</i> , 2021, 26, 3645.	1.7	9
7609	Mononuclear Zn(II) 3,5-Diiodosalicylate Complex with 3-Chloropyridine: Synthesis and Features of Non-Covalent Interactions in the Solid State. <i>Russian Journal of Inorganic Chemistry</i> , 2021, 66, 814-819.	0.3	2
7610	Coordination from Heteroscorpionate Ligand Towards Pd(II) via Pd...H ⁺ C(sp ³) Interaction: Structural and Catalytic Studies. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 2661-2668.	1.0	3
7611	Diffusion-Controlled Z-Scheme-Steered Charge Separation across PDI/BiOI Heterointerface for Ultraviolet, Visible, and Infrared Light-Driven Photocatalysis. <i>Advanced Functional Materials</i> , 2021, 31, 2102315.	7.8	73
7612	Tchnetium Hydrides Revisited: Syntheses, Structures, and Reactions of [TcH ₃ (PPh ₃) ₃] and [TcH(CO) ₃ (PPh ₃) ₂]. <i>Organometallics</i> , 2021, 40, 3095-3112.	1.1	11
7613	Interaction of Cu _n , Ag _n and Au _n (n = 1-4) nanoparticles with ChCl:Urea deep eutectic solvent. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107866.	1.3	6
7614	Mechanisms of Diels-Alder reactions between pyridines and dienophiles: A DFT investigation. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4254.	0.9	1
7615	Facile Fabrication of Functionalized Separators for Lithium-Ion Batteries with Ionic Conduction Path Modifications via the ¹³⁷ Cs-Ray Co-irradiation Grafting Process. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 27663-27673.	4.0	12
7616	Density Prediction of Ionic Liquids at Different Temperatures Using the Average Free Volume Model. <i>ACS Omega</i> , 2021, 6, 14869-14874.	1.6	7
7617	Theoretical Insight into the Effect of Fluorine-Functionalized Metal-Organic Framework Supported Palladium Single-Site Catalyst in the Ethylene Dimerization Reaction. <i>Chemistry - A European Journal</i> , 2021, 27, 10413-10421.	1.7	3
7618	Single-crystal structure of two-dimensional organic framework based on donor-acceptor interactions with charge-transfer effect. <i>Science China Chemistry</i> , 2021, 64, 1510-1514.	4.2	7

#	ARTICLE	IF	CITATIONS
7619	Uptake of microplastics by carrots in presence of As (III): Combined toxic effects. <i>Journal of Hazardous Materials</i> , 2021, 411, 125055.	6.5	165
7620	Insight into the formation of organosulfur compounds from the reaction of methyl vinyl ketone with sulfite radical in atmospheric aqueous phase. <i>Science of the Total Environment</i> , 2021, 774, 145817.	3.9	8
7621	Encapsulation of Pollutant Gaseous Molecules by Adsorption on Boron Nitride Nanotubes: A Quantum Chemistry Study. <i>ACS Omega</i> , 2021, 6, 14824-14837.	1.6	9
7622	Theoretical design of D-Ï€-A system new dyes candidate for DSSC application. <i>Heliyon</i> , 2021, 7, e07171.	1.4	23
7623	Detailed Structural Examination, Quantum Mechanical Studies of the Aromatic Compound Solarimfetol and Formation of Inclusion Compound with Cucurbituril. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-13.	1.4	4
7624	Magneto-Refractive Effect and Mechanism Analysis of Erbium-Ytterbium Co-Doped Silica Fiber. <i>IEEE Photonics Journal</i> , 2021, 13, 1-11.	1.0	5
7625	Combined experimental and theoretical study on photoionization cross sections of benzonitrile and <i>m</i> -cyanotoluene. <i>Journal of Chemical Physics</i> , 2021, 154, 244301.	1.2	5
7626	Insight into the effects of hydroxyl groups on the rates and pathways of tetracycline antibiotics degradation in the carbon black activated peroxydisulfate oxidation process. <i>Journal of Hazardous Materials</i> , 2021, 412, 125256.	6.5	70
7627	Role of Size and Composition on the Design of Superalkalis. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5886-5894.	1.1	5
7628	Controlling Ï€-Ï€ Interactions through Coordination Bond Formation: Assembly of 1-D Chains of acac-Based Coordination Compounds. <i>Crystal Growth and Design</i> , 2021, 21, 3756-3769.	1.4	4
7629	Gold(I)-Catalyzed Reactivity of Furan-ynes with <i>N</i> -Oxides: Synthesis of Substituted Dihydropyridinones and Pyranones. <i>Journal of Organic Chemistry</i> , 2021, 86, 8295-8307.	1.7	4
7630	Comprehensive Insight into the Probability of Cyclotriphosphazene Derivatives as the Functional Electrolyte Additives in Lithium-Ion Batteries: Which Is Better and Why?. <i>ACS Applied Energy Materials</i> , 2021, 4, 7101-7111.	2.5	23
7631	Process monitoring of the Au-S bond conversion in acetylene hydrochlorination. <i>Chinese Journal of Chemical Engineering</i> , 2022, 45, 32-40.	1.7	10
7632	The non-covalent interaction studies of <i>o</i> -nitrophenol and methyl acetate in benzene: By ultrasonics, FTIR and DFT methods. <i>Materials Today: Proceedings</i> , 2021, 47, 4527-4527.	0.9	0
7633	Acidic Stabilization of the Dual-Aromatic Heterocyclic Anions. <i>Catalysts</i> , 2021, 11, 766.	1.6	3
7634	On the bonding nature of noble gas compounds MRg ⁺ and MRgF (M=Co, Rh, Ir; Rg=Ar, Kr, Xe). <i>Chinese Journal of Chemical Physics</i> , 2021, 34, 297-308.	0.6	0
7635	Efficiency of water treatment with crushed shell of jatobã-do-cerrado (<i>Hymenaea stigonocarpa</i>) fruit to adsorb Cu(II) and Ni(II) ions: experimental and quantum chemical assessment of the complexation process. <i>Environmental Science and Pollution Research</i> , 2021, 28, 60041-60059.	2.7	3
7636	A molecular electron density theory study of the [3+2] cycloaddition reaction of nitronic ester with methyl acrylate. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	8

#	ARTICLE	IF	CITATIONS
7637	Synergetic influence between adsorption and photodegradation of Rhodamine B using synthesized fly ash based inorganic polymer. <i>Surfaces and Interfaces</i> , 2021, 24, 101136.	1.5	14
7638	Endowing water-based polyacrylics adhesives with enhanced water-resistant capability by integrating with tannic acid. <i>Reactive and Functional Polymers</i> , 2021, 163, 104890.	2.0	13
7639	DFT study on the sensitivity of silver-graphene quantum dots for vital and harmful analytes. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 153, 110028.	1.9	16
7640	Mechanism analysis of extractive distillation for separation of acetic acid and water based on quantum chemical calculation and molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , 2021, 332, 115866.	2.3	17
7641	Study on the dissolution of aluminium carbide formed on the graphite cathode in aluminium electrolysis. <i>Journal of Molecular Liquids</i> , 2021, 331, 115767.	2.3	2
7642	Interplay between invasive single atom Pt and native oxygen vacancy in rutile TiO ₂ (110) surface: A theoretical study. <i>Nano Research</i> , 2022, 15, 669-676.	5.8	15
7643	Regioselectivity of the Conjugate Addition of Amines to Dissymmetrical Pullan Alkenes. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 3278-3288.	1.2	4
7644	Asymmetric [2+2] cycloaddition of isatin with ketene catalyzed by N, N'-dioxide-Sc(III) complex: Mechanism and selectivity. <i>Molecular Catalysis</i> , 2021, 510, 111657.	1.0	0
7645	Electronic structure theory study of the reactivity and structural molecular properties of halo-substituted (F, Cl, Br) and heteroatom (N, O, S) doped cyclobutane. <i>ChemistrySelect</i> , 2023, 8, 715-739.	0.7	2
7646	Synthesis, spectroscopic, quantum computation, electronic, AIM, Wavefunction (ELF, LOL) and Molecular Docking investigation on (E)-1-(2,5-dichlorothiophen-3-yl)-3-(thiophen-2-yl)-2-propen-1-one. <i>Chemical Data Collections</i> , 2021, 33, 100701.	1.1	24
7647	Revealing the role of 1,2,4-triazolate fragment of blue-emitting bis-tridentate Ir(III) phosphors: photophysical properties, photo-stabilities, and applications. <i>Materials Today Energy</i> , 2021, 20, 100636.	2.5	10
7648	Tuning the optoelectronic properties of dibenzochrysene (DBC) based small molecules for organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2021, 127, 105689.	1.9	41
7649	Different Reactivities of (5-Ph) ₂ P-Ace-6-MeSiH toward the Rhodium(I) Chlorides [(C) ₂ H ₄] ₂ RhCl and [(CO) ₂ RhCl] ₂ . Hirshfeld Atom Refinement of a Rh-H \cdot Si Interaction. <i>Organometallics</i> , 2021, 40, 2027-2038.	1.1	6
7650	DFT study of therapeutic potential of graphitic carbon nitride (g-C ₃ N ₄) as a new drug delivery system for carboplatin to treat cancer. <i>Journal of Molecular Liquids</i> , 2021, 331, 115607.	2.3	51
7651	Tetraphenylethylene-vitamin E Conjugates as sensitive aggregation-induced emission probes for selective detection of explosive FOX-7. <i>Analytica Chimica Acta</i> , 2021, 1164, 338525.	2.6	6
7652	Pyridine Ring Modification of Indane-1,3-dione Dimers for Control of their Crystal Structure. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 2690-2696.	1.3	2
7653	Synthesis, characterization, DFT, and TD-DFT studies of (E)-5-((4,6-dichloro-1,3,5-triazin-2-yl)amino)-4-hydroxy-3-(phenyldiazenyl)naphthalene-2,7-diylbis(hydrogen) Tj ETQq0500rgB18Overlock	0.5	1
7654	Computational modeling in enhanced CO ₂ and C ₂ H ₂ capture on chalcogen atom (Se, Te)-decorated graphene: structural and mechanistic aspects. <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 447-461.	1.2	5

#	ARTICLE	IF	CITATIONS
7655	Experimental and theoretical spectroscopic (FT-IR, FT-Raman, UV-VIS) analysis, natural bonding orbitals and molecular docking studies on 2-bromo-6-methoxynaphthalene: A potential anti-cancer drug. Heliyon, 2021, 7, e07213.	1.4	11
7656	New deep eutectic solvent based superparamagnetic nanofluid for determination of perfluoroalkyl substances in edible oils. Talanta, 2021, 228, 122214.	2.9	19
7657	Boron-Doped Polycyclic π -Electron Systems with an Antiaromatic Borole Substructure That Forms Photoresponsive σ -P Lewis Adducts. Journal of the American Chemical Society, 2021, 143, 9944-9951.	6.6	70
7658	Heterobimetallic Silver(I) and Copper(I) pyrazolates supported with 1,1'-bis(diphenylphosphino)ferrocene. Journal of Organometallic Chemistry, 2021, 942, 121813.	0.8	6
7659	Tuning the reactivity of tri-s-triazine, trinitro-tri-s-triazine and ternary tri-s-triazine graphitic C ₃ N ₄ quantum dots through H-functionalized and B-doped complexes: A density functional study. Chemosphere, 2021, 272, 129901.	4.2	6
7660	Systematic Study of Aromatic π -Targeted Cycloadditions of 5-Hydroxymethylfurfural Platform Chemicals. ChemSusChem, 2021, 14, 3110-3123.	3.6	13
7661	C \equiv C Bond Formation between the π -Alkylidyne Ligands in a Diruthenium Bis(π -Alkylidyne) Complex; π -Aromaticity of the Ru ₂ C ₂ Core. European Journal of Inorganic Chemistry, 2021, 2021, 2505-2513.	1.0	0
7662	Theoretical Insights into Excited-State Intermolecular Proton Transfers of 2,7-Diazaindole in Water Using a Microsolvation Approach. Journal of Physical Chemistry A, 2021, 125, 5314-5325.	1.1	9
7663	In-situ pyrolysis of Taihu blue algae biomass as appealing porous carbon adsorbent for CO ₂ capture: Role of the intrinsic N. Science of the Total Environment, 2021, 771, 145424.	3.9	44
7664	Predicting microwave-induced relative volatility changes in binary mixtures using a novel dimensionless number. Chemical Engineering Science, 2021, 237, 116576.	1.9	13
7665	Azobispyrazole Family as Photoswitches Combining (Near ϵ) Quantitative Bidirectional Isomerization and Widely Tunable Thermal Half-Lives from Hours to Years**. Angewandte Chemie - International Edition, 2021, 60, 16539-16546.	7.2	42
7666	Photoluminescence quenching of thermally treated waste-derived carbon dots for selective metal ion sensing. Environmental Research, 2021, 197, 111008.	3.7	24
7667	Reaction pathways and cyclic chain model of free radicals during coal spontaneous combustion. Fuel, 2021, 293, 120436.	3.4	65
7668	Isomeric Dibenzothiazethrenes for Air-Stable Organic Field-Effect Transistors. Angewandte Chemie - International Edition, 2021, 60, 16230-16236.	7.2	42
7669	Theoretical studies of novel high energy density materials based on oxadiazoles. Journal of Molecular Modeling, 2021, 27, 204.	0.8	8
7670	Halogenation of the Side Chains in Donor-Acceptor Based Small Molecules for Photovoltaic Applications: Energetics and Charge-Transfer Properties from DFT/TDDFT Studies. ChemistrySelect, 2021, 6, 5254-5265.	0.7	3
7671	Capture of Fullerenes in Cages and Rings by Forming Metal- π Bond Arene Interactions. Materials, 2021, 14, 3424.	1.3	1
7672	Characterization of the binding affinity between some anti-Parkinson agents and Mn ²⁺ , Fe ³⁺ and Zn ²⁺ metal ions: A DFT insight. Inorganic Chemistry Communication, 2021, 128, 108582.	1.8	5

#	ARTICLE	IF	CITATIONS
7673	Competition of Intra- and Intermolecular Forces in Anthraquinone and Its Selected Derivatives. <i>Molecules</i> , 2021, 26, 3448.	1.7	6
7674	Molecular structure, vibrational spectroscopic, frontier molecular orbital and natural bond orbital analysis of anti-cancer drug 6-chloro-3- pyridine carbonitrile. <i>Spectroscopy Letters</i> , 2021, 54, 419-436.	0.5	8
7675	High selective gas-phase rearrangement reaction of TCDD induced by excess electron attachment: Theoretical insight on the decomposition mechanism of one of the most toxic chemical known to science. <i>Chemosphere</i> , 2021, 272, 129617.	4.2	2
7676	On the nature of inter- and intramolecular interactions involving benzo[h]quinoline and 10-hydroxybenzo[h]quinoline: Electronic ground state vs excited state study. <i>Journal of Molecular Structure</i> , 2021, 1234, 130126.	1.8	7
7677	Understanding the CO ₂ capture performance by MDEA-based deep eutectics solvents with excellent cyclic capacity. <i>Fuel</i> , 2021, 293, 120466.	3.4	39
7678	DFT and TD-DFT Investigation of a Charge Transfer Surface Resonance Raman Model of N3 Dye Bound to a Small TiO ₂ Nanoparticle. <i>Nanomaterials</i> , 2021, 11, 1491.	1.9	7
7679	Degradation of a fluorescent tracer-PTSA in circulating cooling water: Kinetics, pathways, and degradation efficiency of a polycyclic aromatic hydrocarbon derivative. <i>Journal of Water Process Engineering</i> , 2021, 41, 102036.	2.6	3
7680	Prediction of procarbazine adsorption on the hydroxyethyl cellulose: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2021, 1200, 113250.	1.1	1
7681	Concentric Inner $2f$ and Outer $10f$ Aromaticity Underlies the Dynamic Structural Fluxionality of Planar B ₁₉ Wankel Motor Cluster. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5022-5030.	1.1	3
7682	Catalytic Asymmetric Aza-Diels-Alder Reaction of Ketimines and Unactivated Dienes. <i>Angewandte Chemie</i> , 2021, 133, 17749-17755.	1.6	2
7683	A computational toolbox for molecular property prediction based on quantum mechanics and quantitative structure-property relationship. <i>Frontiers of Chemical Science and Engineering</i> , 0, , 1.	2.3	7
7684	Theoretical study of the [3+4] annulation reaction of 2-bromoenals with malonates catalyzed by N-heterocyclic carbene. <i>Molecular Catalysis</i> , 2021, 509, 111647.	1.0	2
7685	Distinct roles of Ag(I) and Cu(II) as cocatalysts in the intramolecular cyclization of N-methyl-N-phenylanthranilic acid: A theoretical investigation. <i>Molecular Catalysis</i> , 2021, 509, 111634.	1.0	0
7687	Comparative Investigation into the Complexation and Extraction Properties of Tridentate and Tetradentate Phosphine Oxide-Functionalized 1,10-Phenanthroline Ligands toward Lanthanides and Actinides. <i>Chemistry - A European Journal</i> , 2021, 27, 10717-10730.	1.7	27
7688	Spectroscopic (FT-IR, FT-Raman, UV-Vis) molecular structure, electronic, molecular docking, and thermodynamic investigations of indole-3-carboxylic acid by DFT method. <i>Journal of Molecular Structure</i> , 2021, 1234, 130182.	1.8	21
7689	A novel acetylcholinesterase biosensor with dual-recognized strategy based on molecularly imprinted polymer. <i>Sensors and Actuators B: Chemical</i> , 2021, 337, 129760.	4.0	15
7690	Binding Between Cyclohexanohemicucurbit[n]urils and Polar Organic Guests. <i>Frontiers in Chemistry</i> , 2021, 9, 701028.	1.8	2
7691	Nanocellulose as template to prepare rough-hydroxy rich hollow silicon mesoporous nanospheres (R-nCHMSNs) for drug delivery. <i>International Journal of Biological Macromolecules</i> , 2021, 180, 432-438.	3.6	5

#	ARTICLE	IF	CITATIONS
7692	Hydrogen-Bonded and Halogen-Bonded: Orthogonal Interactions for the Chloride Anion of a Pyrazolium Salt. <i>Molecules</i> , 2021, 26, 3982.	1.7	8
7693	Density functional study on Am(III)/Eu(III) selectivity using crown ether type ligands. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2021, 329, 77-84.	0.7	1
7694	Use of 1-octyl-3-methylimidazole hexafluorophosphate modified magnetic hyperbranched polyamideamine as sorbent for the extraction of pyrethroid insecticides from tea infusion. <i>Journal of Separation Science</i> , 2021, 44, 2957-2964.	1.3	0
7695	Role of Graphite Felt Electrode and Electron Delocalization of Cinnamate Ester in Electrochemical Hydrogenation Reaction. <i>Journal of Physical Chemistry C</i> , 2021, 125, 13871-13879.	1.5	3
7696	Photophysical Properties of Simple Palladium(0) Complexes Bearing Triphenylphosphine Derivatives. <i>Inorganic Chemistry</i> , 2021, 60, 9516-9528.	1.9	7
7697	Synthesis, spectroscopic characterization, and SC-XRD study of one privileged heteronuclear Ni(II)/Hg(II)-Salen complex: An exclusive DFT outlook. <i>Inorganic Chemistry Communication</i> , 2021, 128, 108609.	1.8	17
7698	Azobispyrazole Family as Photoswitches Combining (Near) Quantitative Bidirectional Isomerization and Widely Tunable Thermal Half-Lives from Hours to Years**. <i>Angewandte Chemie</i> , 2021, 133, 16675-16682.	1.6	11
7699	Predicting Dinitrogen Coupling with a Series of Small Molecules Catalyzed by a Pincer Complex. <i>Chemistry - an Asian Journal</i> , 2021, 16, 2063-2067.	1.7	13
7700	Di-ortho-C H arylation of phenylalanine: A bimetallic interaction between Pd(IV)-Ag(I). <i>Tetrahedron Letters</i> , 2021, 74, 153158.	0.7	8
7701	Persulfate enhanced visible light photocatalytic degradation of iohexol by surface-loaded perylene diimide/acidified biochar. <i>Chemical Engineering Journal</i> , 2021, 414, 128793.	6.6	32
7702	Sensing mechanism of fluorescent sensor to Cu ²⁺ based on inhibiting ultra-fast intramolecular proton transfer process. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 254, 119685.	2.0	6
7703	Kirkendall Effect Boosts Phosphorylated nZVI for Efficient Heavy Metal Wastewater Treatment. <i>Angewandte Chemie</i> , 2021, 133, 17252-17259.	1.6	44
7704	Kirkendall Effect Boosts Phosphorylated nZVI for Efficient Heavy Metal Wastewater Treatment. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 17115-17122.	7.2	95
7705	A critical review on bismuth oxyhalide based photocatalysis for pharmaceutical active compounds degradation: Modifications, reactive sites, and challenges. <i>Journal of Hazardous Materials</i> , 2021, 412, 125186.	6.5	100
7706	Achieve panchromatic absorption for all-small-molecule organic solar cells based on mono-porphyrin molecules by π -bridge modification. <i>Materials Today Energy</i> , 2021, 20, 100658.	2.5	11
7708	The effect of the central metal ion on photovoltaic properties of bacteriochlorin derivatives. <i>Materials Today Communications</i> , 2021, 27, 102367.	0.9	1
7709	Spectroscopic and Computational Studies on a Dansyl Based Luminescent Probe: Detection of Water Contaminant in Hygroscopic Deuterated Solvents. <i>Letters in Organic Chemistry</i> , 2022, 19, 71-82.	0.2	2
7710	Mo Fischer Carbene Complexes: A DFT Study on the Prediction of Redox Potentials. <i>Journal of the Electrochemical Society</i> , 2021, 168, 066523.	1.3	6

#	ARTICLE	IF	CITATIONS
7711	Adsorption properties and mechanism of montmorillonite modified by two Gemini surfactants with different chain lengths for three benzotriazole emerging contaminants: Experimental and theoretical study. <i>Applied Clay Science</i> , 2021, 207, 106086.	2.6	19
7712	Detonation properties and impact sensitivities of trinitromethane derivatives of three-membered heterocyclic ring compounds. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107863.	1.3	4
7713	A deep insight into polybenzoxazole formation in the heterocycle-containing polybenzoxazine: An enlightening thought for smarter precursor design. <i>Polymer</i> , 2021, 226, 123789.	1.8	5
7714	Molecular Design of Dispersed Nickel Phthalocyanine@Nanocarbon Hybrid Catalyst for Active and Stable Electroreduction of CO ₂ . <i>Journal of Physical Chemistry C</i> , 2021, 125, 13836-13849.	1.5	16
7715	Insights into the interfacial interaction mechanisms of p-arsanilic acid adsorption on ionic liquid modified porous cellulose. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 105225.	3.3	26
7716	Enhanced ammonia sensing properties of rGO/WS ₂ heterojunction based chemiresistive sensor by marginal sulfonate decoration. <i>Sensors and Actuators B: Chemical</i> , 2021, 337, 129776.	4.0	31
7717	Analysis and comparison of metal-doped on Graphene-Genistein using QM/MM calculations. <i>Revista Facultad De Ingenier�a</i> , 0, , .	0.5	1
7718	The application of graphyne and its boron nitride analogue in Li-ion batteries. <i>Computational and Theoretical Chemistry</i> , 2021, 1200, 113243.	1.1	4
7719	Quantum chemical insight on the uranyl benzoates association with cetylpyridinium. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2021, 329, 661-670.	0.7	2
7720	Electron and Proton Donating Ability of the Pyrrolyl and Diazolyl Derivatives of Cycloalkanones. <i>Russian Journal of General Chemistry</i> , 2021, 91, 991-1008.	0.3	0
7721	Through Bridge Spin Coupling in Homo- and Heterobimetallic Porphyrin Dimers upon Stepwise Oxidations: A Spectroscopic and Theoretical Investigation. <i>Chemistry - A European Journal</i> , 2021, 27, 11428-11441.	1.7	4
7722	Facilitating effect of heavy metals on di(2-ethylhexyl) phthalate adsorption in soil: New evidence from adsorption experiment data and quantum chemical simulation. <i>Science of the Total Environment</i> , 2021, 772, 144980.	3.9	14
7723	Chlorine dioxide radicals triggered by chlorite under visible-light irradiation for enhanced degradation and detoxification of norfloxacin antibiotic: Radical mechanism and toxicity evaluation. <i>Chemical Engineering Journal</i> , 2021, 414, 128768.	6.6	55
7724	Highly active electrocatalytic CO ₂ reduction with manganese N-heterocyclic carbene pincer by para electronic tuning. <i>Chinese Chemical Letters</i> , 2022, 33, 262-265.	4.8	15
7725	A comprehensive investigation of structural features, electron delocalization, optoelectronic and anti-corrosion characteristics in furan oligomers by DFT/TDDFT method. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	1
7726	Facile Charge Transfer between Barbituric Acid and Chloranilic Acid over g-C ₃ N ₄ : Synthesis, Characterization and DFT Study. <i>Crystals</i> , 2021, 11, 636.	1.0	3
7727	Catalytic Asymmetric Aza-Diels-Alder Reaction of Ketimines and Unactivated Dienes. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 17608-17614.	7.2	25
7728	Theoretical exploration of third-order nonlinear optical properties of black phosphorus quantum dots doped with alkali and alkaline-earth metal atoms. <i>Journal of Molecular Liquids</i> , 2021, 331, 115720.	2.3	8

#	ARTICLE	IF	CITATIONS
7729	Room-Temperature Amination of Chloroheteroarenes in Water by a Recyclable Copper(II)-Phosphaadamantanum Sulfonate System. <i>Journal of Organic Chemistry</i> , 2021, 86, 8900-8925.	1.7	14
7730	Femtosecond dynamics of diphenylpropynylidene in ethanol and dichloromethane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 254, 119606.	2.0	0
7731	Structure property relationships of N-acylsulfonamides and related bioisosteres. <i>European Journal of Medicinal Chemistry</i> , 2021, 218, 113399.	2.6	20
7732	Enhanced Li ⁺ ion adsorption on pristine and defected graphene via organic radical interaction – A DFT study. <i>Physica B: Condensed Matter</i> , 2021, 611, 412700.	1.3	1
7733	Experimental and density functional theory investigations on the antioxidant mechanism of carbon nanotubes. <i>Carbon</i> , 2021, 177, 189-198.	5.4	14
7734	Which triel bond is stronger? TrHX ⁺ H ₂ Y versus TrH ₂ X ⁺ H ₂ Y (Tr = Ga, In; X = F, Cl, Br, I; Y = O, S). <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	4
7735	A first principle study of heme molecule as an active adsorbent for halogenated hydrocarbons. <i>Journal of Molecular Modeling</i> , 2021, 27, 209.	0.8	3
7736	Density functional theory-based investigation of CaO/char catalyzing the transformation of NH ₃ to N ₂ . <i>Journal of Analytical and Applied Pyrolysis</i> , 2021, 156, 105124.	2.6	11
7737	Electrostatic Switching of Stereoselectivity in Aldol Reactions. <i>Journal of Organic Chemistry</i> , 2021, 86, 9076-9083.	1.7	6
7738	Cocrystallization Enabling Photoinduced Rotation of an Azopyridine Crystal. <i>Crystal Growth and Design</i> , 2021, 21, 3936-3946.	1.4	6
7739	Acetylation of Malvidin-3-O-glucoside Impedes Intermolecular Copigmentation: Experimental and Theoretical Investigations. <i>Journal of Agricultural and Food Chemistry</i> , 2021, 69, 7733-7741.	2.4	10
7740	Insights into Intermolecular Interactions of Spironolactone Solvates. <i>Crystal Growth and Design</i> , 2021, 21, 3677-3688.	1.4	14
7741	Theoretical Study of Effects of Solvents, Ligands, and Anions on Separation of Trivalent Lanthanides and Actinides. <i>Inorganic Chemistry</i> , 2021, 60, 9552-9562.	1.9	14
7742	Bandgap Modulation in Zr-Based Metal-Organic Frameworks by Mixed-Linker Approach. <i>Inorganic Chemistry</i> , 2021, 60, 8908-8916.	1.9	24
7743	Density Functional Theory Guide for an Allyl Monomer Polymerization Mechanism: Photoinduced Radical-Mediated [3 + 2] Cyclization. <i>ACS Omega</i> , 2021, 6, 15608-15616.	1.6	7
7744	Theoretical insight into different energetic groups on the performance of energetic materials featuring RDX ring. <i>Fuel</i> , 2021, 294, 120497.	3.4	21
7745	A theoretical design of bipolar host materials for blue phosphorescent OLED. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107845.	1.3	3
7746	A DFT study of graphene-FeNx (x = 4, 3, 2, 1) catalysts for acetylene hydrochlorination. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 618, 126495.	2.3	10

#	ARTICLE	IF	CITATIONS
7747	Theoretical study of the formation process of HLCT state in multiple donor-acceptor molecular systems. <i>Computational and Theoretical Chemistry</i> , 2021, 1200, 113247.	1.1	3
7748	Photocatalytic performance and mechanism of AgI/Ag/ZnO composites as catalysts for the visible-light-driven degradation of naproxen. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 414, 113283.	2.0	14
7749	Micro-Aqueous Organic System: A Neglected Model in Computational Lipase Design?. <i>Biomolecules</i> , 2021, 11, 848.	1.8	2
7750	Dual-Responsive Thermally Activated Delayed Fluorescence of Spiropyran Derivatives. <i>CCS Chemistry</i> , 2022, 4, 2080-2089.	4.6	19
7751	Perspective of Zn3O3 ring cluster via density functional theory. <i>Materials Today Communications</i> , 2021, 27, 102343.	0.9	3
7752	Epigenetically modified nucleobases (5hmC, 5fC, and 5caC) interaction with boron and nitrogen doped porous graphene (B/N-pGr) as promising materials for biosensing application: A density functional theory calculations. <i>Environmental Research</i> , 2021, 197, 111133.	3.7	4
7753	A novel method for selective recovery of indium from end-of-life liquid crystal displays by 15-crown-5 ether and its derivatives. <i>Hydrometallurgy</i> , 2021, 202, 105601.	1.8	10
7754	Zwitterions for impedance spectroscopy: The new buffers in town. <i>Analytica Chimica Acta</i> , 2021, 1166, 338547.	2.6	3
7755	Doping Platinum with Germanium: An Effective Way to Mitigate the CO Poisoning. <i>ChemPhysChem</i> , 2021, 22, 1603-1610.	1.0	5
7756	A novel BODIPY-based fluorescent probe for sensitive and selective detection of nerve agent simulants through base-assisted photo-induced electron transfer process. <i>Sensors and Actuators B: Chemical</i> , 2021, 337, 129804.	4.0	17
7757	Integration of oxygen vacancies into BiOI via a facile alkaline earth ion-doping strategy for the enhanced photocatalytic performance toward indometacin remediation. <i>Journal of Hazardous Materials</i> , 2021, 412, 125147.	6.5	40
7758	Highly efficient catalysts of phytic acid-derivative cobalt phosphide encapsulated in N, P-codoped carbon for activation of peroxydisulfate in norfloxacin degradation. <i>Separation and Purification Technology</i> , 2021, 264, 118367.	3.9	28
7759	A comparative study on surface/interface mechanism and antibacterial properties of different hybrid materials prepared with essential oils active ingredients and palygorskite. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 618, 126455.	2.3	16
7760	Insights into complexation and enantioselectivity of uranyl(2-hydroxy-3-methoxyphenyl)(2-hydroxyphenyl)thiopyrano[3,2-h]thiochromene-4,7-dione with R/S organophosphorus pesticides. <i>Applied Organometallic Chemistry</i> , 2021, 35, e6331.	4.7	16
7761	Enhancing the Solubility and Transdermal Delivery of Drugs Using Ionic Liquid-in-Oil Microemulsions. <i>Advanced Functional Materials</i> , 2021, 31, 2102794.	7.8	28
7762	Super selective ammonia separation through multiple-site interaction with ionic liquid-based hybrid membranes. <i>Journal of Membrane Science</i> , 2021, 628, 119264.	4.1	31
7763	Hydrogen adsorption on pillar[6]arene: A computational study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 130, 114719.	1.3	16
7764	Inexpensive activated coke electrocatalyst for high-efficiency hydrogen peroxide production: Coupling effects of amorphous carbon cluster and oxygen dopant. <i>Applied Catalysis B: Environmental</i> , 2021, 286, 119860.	10.8	55

#	ARTICLE	IF	CITATIONS
7765	Synthesis, Spectroscopic Characterization, Crystal Structure and Theoretical Studies on New Organic Single Crystal of 1-(3,5-Difluorophenyl)-3-(2-Nitrophenyl)Urea. Celal Bayar Universitesi Fen Bilimleri Dergisi, 0, , .	0.1	0
7766	Ultrafast Rechargeable Aqueous Zinc-Ion Batteries Based on Stable Radical Chemistry. Advanced Functional Materials, 2021, 31, 2102011.	7.8	56
7767	Proximity Effects of Substituents on Halogen Bond Strength. Journal of Physical Chemistry A, 2021, 125, 5069-5077.	1.1	17
7768	Grossly warped nanographene-phenothiazine nanocomposite as photoactive layer for solar cells: Insights from theoretical study. Chemical Physics Letters, 2021, 773, 138607.	1.2	1
7769	Nano-porous bimetallic CuCo-MOF-74 with coordinatively unsaturated metal sites for peroxymonosulfate activation to eliminate organic pollutants: Performance and mechanism. Chemosphere, 2021, 273, 129643.	4.2	68
7770	Insights on biodiesel blends with alkanol solvents. Journal of Molecular Liquids, 2021, 332, 115864.	2.3	8
7771	Investigation of the assembly mechanism of N1, N4-di (pyridin-4-yl) terephthalamide with pillar[5]arene: Experiment and quantum chemical study. Chemical Physics Letters, 2021, 772, 138533.	1.2	3
7772	Diboron Bonds Between BX ₃ (X=H, F, CH ₃) and BYZ ₂ (Y=H, F; Z=CO, N ₂ , CNH). ChemPhysChem, 2021, 22, 1461-1469.	1.0	4
7773	Facile Access to Uranium and Thorium Phosphaethynolate Complexes Supported by Tren: Experimental and Theoretical Study. Chinese Journal of Chemistry, 2021, 39, 2125-2131.	2.6	15
7774	Competition between (18, 18) and (18, 16) configurations in Ni ₂ (CO) ₅ : An isomerization energy decomposition analysis. Chinese Journal of Chemical Physics, 2021, 34, 287-296.	0.6	0
7775	A study of cation-dependent inverse hydrogen bonds and magnetic exchange-couplings in lanthanacarborane complexes. IScience, 2021, 24, 102760.	1.9	7
7776	Antibacterial efficacy and molecular docking analysis of Huang-Lian-Jie-Du Decoction against the phytopathogenic bacteria P. carotovorum PC1. Journal of Molecular Structure, 2021, 1234, 130141.	1.8	0
7777	Direct Current Electricity Generation from Dynamic Polarized Water-Semiconductor Interface. Journal of Physical Chemistry C, 2021, 125, 14180-14187.	1.5	20
7778	High Performance NIR OLEDs with Low Efficiency Roll-Off by Leveraging Os(II) Phosphors and Exciplex Co-Host. Advanced Functional Materials, 2021, 31, 2102787.	7.8	25
7779	Molecular interaction mechanism in the separation of a binary azeotropic system by extractive distillation with ionic liquid. Green Energy and Environment, 2021, 6, 329-338.	4.7	33
7780	CO ₂ and H ₂ adsorption on 3D nitrogen-doped porous graphene: Experimental and theoretical studies. Journal of CO ₂ Utilization, 2021, 48, 101517.	3.3	18
7781	Sensing capability and diameter-dependent electronic structure of boron nitride nanotubes. Materials Today Communications, 2021, 27, 102252.	0.9	8
7782	Structural, Electronic, and Nonlinear Optical Properties of C ₆₆ H ₄ and C ₇₀ Cl ₆ Encapsulating Li and F Atoms. ACS Omega, 2021, 6, 16234-16240.	1.6	4

#	ARTICLE	IF	CITATIONS
7783	Heterometallic Niâ€“Pt Chini-Type Carbonyl Clusters: An Example of Molecular Random Alloy Clusters. <i>Inorganic Chemistry</i> , 2021, 60, 8811-8825.	1.9	4
7784	Rotational Spectrum and Molecular Structures of the Binary Aggregates of 1,1,1,3,3,3-Hexafluoro-2-propanol with Ne and Ar. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5355-5364.	1.1	4
7785	Novel Green Three-Constituent Natural Deep Eutectic Solvent Enhances Biomass Extraction from <i>Acanthopanax senticosus</i> and the Extraction Mechanism. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 8835-8847.	3.2	9
7786	Small Amount Makes a Big Difference: Critical ($n \approx 1$)d Valence Orbitals of Heavy Alkaline Earth Metals inside Cage Clusters. <i>Inorganic Chemistry</i> , 2021, 60, 8621-8630.	1.9	2
7787	Extraction and multi-scale mechanism explorations for separating indole from coal tar via tetramethylguanidine-based ionic liquids. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 105255.	3.3	14
7788	Solventâ€“Antisolvent Competitive Interactions Mediate Imidacloprid Polymorphs in Antisolvent Crystallization. <i>Crystal Growth and Design</i> , 2021, 21, 4318-4328.	1.4	7
7789	Structural, spectroscopic and DFT theoretical studies of phosphorescent CuP ₂ S-containing cuprous complexes. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 331-339.	0.2	2
7790	Isomeric Dibenzooheptazethrenes for Airâ€“Stable Organic Fieldâ€“Effect Transistors. <i>Angewandte Chemie</i> , 2021, 133, 16366-16372.	1.6	14
7791	Stable Highâ€“Capacity Organic Aluminumâ€“Porphyrin Batteries. <i>Advanced Energy Materials</i> , 2021, 11, 2101446.	10.2	54
7792	Nonâ€“Dissociative Activation of Chemisorbed Dinitrogen on One or Two Vanadium Atoms Supported by a Mo ₆ S ₈ Cluster. <i>ChemPhysChem</i> , 2021, 22, 1645-1654.	1.0	13
7793	New insights into the detection mechanism of Î²-galactosidase in living cells with fluorescent probes. <i>Chemical Physics Letters</i> , 2021, 773, 138597.	1.2	5
7794	Combining Evolutionary Conservation and Quantum Topological Analyses To Determine Quantum Mechanics Subsystems for Biomolecular Quantum Mechanics/Molecular Mechanics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4524-4537.	2.3	6
7795	Efficient ethylene purification by a robust ethane-trapping porous organic cage. <i>Nature Communications</i> , 2021, 12, 3703.	5.8	70
7796	Probing the origin of ambiphilic reactivity in osmapentayne complexes: Interplay of ring strain, aromaticity, and phosphonium substituent. <i>Journal of Organometallic Chemistry</i> , 2021, 945, 121866.	0.8	1
7797	Ultrafast Hole Deformation Revealed by Molecular Attosecond Interferometry. <i>Ultrafast Science</i> , 2021, 2021, .	5.8	36
7798	Probing the effect of carbon doping on structures, properties, and stability of magnesium clusters. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	3
7799	A theoretical investigation on ESIPT process of a red-emitting ratiometric fluorescent probe and its fluorescent detection mechanism for cyanide anion. <i>Journal of Industrial and Engineering Chemistry</i> , 2021, 99, 126-133.	2.9	12
7800	Multifunctional Optical Polymeric Films with Photochromic, Fluorescent, and Ultraâ€“Long Room Temperature Phosphorescent Properties. <i>Advanced Optical Materials</i> , 2021, 9, 2101266.	3.6	26

#	ARTICLE	IF	CITATIONS
7801	Phenolate-bridged A ₂ B-type subporphyrin dimer. <i>Journal of Porphyrins and Phthalocyanines</i> , 2021, 25, 975-980.	0.4	2
7802	Hydrogen Evolution Prediction for Alternating Conjugated Copolymers Enabled by Machine Learning with Multidimension Fragmentation Descriptors. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 34033-34042.	4.0	12
7803	Self-powered flexible artificial synapse for near-infrared light detection. <i>Cell Reports Physical Science</i> , 2021, 2, 100507.	2.8	19
7804	Functional triterpenoids from medicinal fungi <i>Ganoderma applanatum</i> : A continuous search for antiadipogenic agents. <i>Bioorganic Chemistry</i> , 2021, 112, 104977.	2.0	9
7805	Direct Observation of Diastereomeric $\hat{\pm}$ -C-Bound Enolates during Enantioselective $\hat{\pm}$ -Arylations: Synthesis, Characterization, and Reactivity of Arylpalladium Fluorooxindole Complexes. <i>Journal of the American Chemical Society</i> , 2021, 143, 11741-11750.	6.6	15
7806	Experimental and molecular modeling study on the binary mixtures of [EMIM][BF ₄] and [EMIM][TFSI] ionic liquids. <i>Journal of Molecular Liquids</i> , 2021, 334, 116049.	2.3	14
7807	Tuning the optoelectronic properties of oligothieryl silane derivatives and their photovoltaic properties. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 106, 107918.	1.3	25
7808	Substituent Effects on Electride Characteristics of Mg ₂ (I ⁺) ₅ -C ₅ H ₅ ₂ : A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6207-6220.	1.1	10
7809	Design of low dielectric constant and high transparent polyarylate containing spiral ring. <i>Polymer</i> , 2021, 228, 123948.	1.8	17
7810	How Does Ti-Doping Affect Hydrogen Storage Properties of MgH ₂ at Nanosize?. <i>Russian Journal of Physical Chemistry A</i> , 2021, 95, 1424-1431.	0.1	2
7811	Carbon nitride of five-membered rings with low optical bandgap for photoelectrochemical biosensing. <i>CheM</i> , 2021, 7, 2708-2721.	5.8	64
7812	Comprehensive Evaluation of a Deep Eutectic Solvent Based CO ₂ Capture Process through Experiment and Simulation. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 10250-10265.	3.2	48
7813	The interaction between carboplatin anticancer drug and B12N12 nano-cluster: A computational investigation. <i>Main Group Chemistry</i> , 2021, 20, 345-354.	0.4	9
7814	The synthesis and characterization of a new diphosphine-protected gold hydride nanocluster. <i>Journal of Chemical Physics</i> , 2021, 155, 034307.	1.2	9
7815	Evaluation on Cocrystal Screening Methods and Synthesis of Multicomponent Crystals: A Case Study. <i>Crystal Growth and Design</i> , 2021, 21, 4531-4546.	1.4	29
7816	Theoretical Analysis of Properties of Ground and Excited States for Photodissociation of the C=O Bond in Polycarbonates. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6662-6673.	1.1	1
7817	Reactivity of Coinage Metal Hydrides for the Production of H ₂ Molecules. <i>ChemistryOpen</i> , 2021, 10, 724-730.	0.9	1
7818	A Universal Compensation Strategy to Anchor Polar Organic Molecules in Bilayered Hydrated Vanadates for Promoting Aqueous Zinc Ion Storage. <i>Advanced Materials</i> , 2021, 33, e2102701.	11.1	76

#	ARTICLE	IF	CITATIONS
7819	Can metal halides be electron donors in π -hole and σ -hole tetrel bonds? Cooperativity with an alkaline-earth bond. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26771.	1.0	1
7820	Understanding Gas Solubility of Pure Component and Binary Mixtures within Multivalent Ionic Liquids from Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8165-8174.	1.2	9
7821	Antimicrobial activities of cadmium (II) and nickel (II) complexes containing pyridine ring: Investigation of crystallographic, spectroscopic, Hirshfeld surface analysis, and TD/DFT calculations. <i>Applied Organometallic Chemistry</i> , 2021, 35, e6360.	1.7	13
7822	Molecular thermodynamic and dynamic insights into gas dehydration with imidazolium-based ionic liquids. <i>Chemical Engineering Journal</i> , 2021, 416, 129168.	6.6	27
7823	Phosphorus Deficiency Promoted Hydrolysis of Organophosphate Esters in Plants: Mechanisms and Transformation Pathways. <i>Environmental Science & Technology</i> , 2021, 55, 9895-9904.	4.6	25
7824	Theoretical studies on the products formed by cerium atom reacting with XF_3 ($\text{X}=\text{N}$, P and As). <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113253.	1.1	0
7825	Lepipyrrolins A-B, two new dimeric pyrrole 2-carbaldehyde alkaloids from the tubers of <i>Lepidium meyenii</i> . <i>Bioorganic Chemistry</i> , 2021, 112, 104834.	2.0	4
7826	A combined experimental and theoretical study on diglyme+1-alkanol liquid mixtures. <i>Journal of Molecular Liquids</i> , 2021, 334, 116048.	2.3	1
7828	Pyrimethamine-Based Novel Co-Crystal Salt: Synthesis, Single-Crystal Investigation, Hirshfeld surface analysis and DFT inspection of the 2,4-diamino-5-(4-chlorophenyl)-6-ethylpyrimidin-1-ium 2,4-dichlorobenzoate (1:1) (DECB). <i>Journal of Molecular Structure</i> , 2021, 1235, 130215.	1.8	35
7829	Understanding of Light Absorption Properties of the N-Doped Graphene Oxide Quantum Dot with TD-DFT. <i>Journal of Physical Chemistry C</i> , 2021, 125, 14979-14990.	1.5	20
7830	$[\text{Cu}_{36}\text{H}_{10}(\text{PET})_{24}(\text{PPh}_3)_6\text{Cl}_2]$ Reveals Surface Vacancy Defects in Ligand-Stabilized Metal Nanoclusters. <i>Journal of the American Chemical Society</i> , 2021, 143, 11026-11035.	6.6	46
7831	Physical Mechanism of Photoinduced Charge Transfer in One- and Two-Photon Absorption in D-D-A Systems. <i>Materials</i> , 2021, 14, 3925.	1.3	2
7832	Speciation of Substituted Benzoic Acids in Solution: Evaluation of Spectroscopic and Computational Methods for the Identification of Associates and Their Role in Crystallization. <i>Crystal Growth and Design</i> , 2021, 21, 4823-4836.	1.4	5
7833	Combined DFT calculation, Hirshfeld surface analysis, and Energy framework study of non-covalent interactions in the crystal structure of (Z)-5-ethylidene-2-thiohydantoin determined by powder X-ray diffraction. <i>Journal of Molecular Structure</i> , 2021, 1236, 130361.	1.8	2
7834	Unveiling $[\text{3}+\text{2}]$ cycloaddition reactions of benzonitrile oxide and diphenyl diazomethane to cyclopentene and norbornene: a molecular electron density theory perspective. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	8
7835	Pyramidal Dicationic Ge(II) Complexes with Homoleptic Neutral Pnictine Coordination: A Combined Experimental and Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2021, 60, 12100-12108.	1.9	6
7836	Non-additive electronic polarizabilities of ionic liquids: Charge delocalization effects. <i>Journal of Molecular Liquids</i> , 2022, 346, 117099.	2.3	9
7837	Theoretical study on the ESIPT processes and fluorescence properties of 2-(1H-Benzimidazol-2-yl)phenol-based derivatives. <i>Journal of Molecular Structure</i> , 2021, 1236, 130370.	1.8	13

#	ARTICLE	IF	CITATIONS
7838	Computational investigation of interaction between titanocene dichloride and nanoclusters (B12N12,) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.4	3
7839	Accelerated discovery of boron-dipyrromethene sensitizer for solar cells by integrating data mining and first principle. <i>Journal of Materiomics</i> , 2021, 7, 790-801.	2.8	7
7840	A two-photon fluorescent probe for imaging of mitochondrial cysteine in λ -carrageenan induced arthritis. <i>Sensors and Actuators B: Chemical</i> , 2021, 338, 129749.	4.0	12
7841	Quantum chemical calculation, performance of selective antimicrobial activity using molecular docking analysis, RDG and experimental (FT-IR, FT-Raman) investigation of thiazol-5(4H)-ylidene} methyl benzonitrile. <i>Helvion</i> , 2021, 7, e07634.	1.4	14
7842	Polycyclic polyprenylated acylphloroglucinol derivatives from <i>Hypericum pseudohenryi</i> . <i>Phytochemistry</i> , 2021, 187, 112761.	1.4	1
7843	Effects of photophysical properties of 1,4-cyclohexadiene derivatives on their [2 + 2] photocycloaddition reactivities: Experimental and theoretical studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 416, 113336.	2.0	3
7844	Molecular insertion regulates the donor-acceptor interactions in cocrystals for the design of piezochromic luminescent materials. <i>Nature Communications</i> , 2021, 12, 4084.	5.8	41
7845	Supramolecular Polymerization of C3-Symmetric, Triphenylene-Cored Aza-Polycyclic Aromatic Hydrocarbons with Excellent and Switchable Circularly Polarized Luminescence Performance. <i>Macromolecules</i> , 2021, 54, 7291-7297.	2.2	3
7846	Tetrabromoethane as σ -Hole Donor toward Bromide Ligands: Halogen Bonding between C ₂ H ₂ Br ₄ and Bromide Dialkylcyanamide Platinum(II) Complexes. <i>Crystals</i> , 2021, 11, 835.	1.0	3
7847	Visualizing Non-Covalent interactions between Propylamine and 2-Chlorobenzyl alcohol in Benzene: Theoretical and Dielectric relaxation studies. <i>Journal of Physics: Conference Series</i> , 2021, 1964, 032004.	0.3	1
7848	The influence of humic and fulvic acids on polytetrafluoroethylene-adsorbed arsenic: a mechanistic study. <i>Environmental Science and Pollution Research</i> , 2021, 28, 64503-64515.	2.7	8
7849	Search for Global Minimum Structures of P _{2n+1} + (n = 1-15) Using xTB-Based Basin-Hopping Algorithm. <i>Frontiers in Chemistry</i> , 2021, 9, 694156.	1.8	3
7850	Insight into the morphology and crystal growth of DL-methionine in aqueous solution with presence of cellulose polymers. <i>Journal of Molecular Liquids</i> , 2021, 343, 116967.	2.3	14
7851	Theoretical Insights into the Reduction Mechanism of Np(VI) with Phenylhydrazine. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6180-6188.	1.1	5
7852	Characterization of Structure-Property Relations and Second Harmonic Generation of 6-Methoxy-2-Naphthaldehyde. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-13.	1.4	0
7853	Pyrolysis of penicillin fermentation residue and sludge to produce biochar: Antibiotic resistance genes destruction and biochar application in the adsorption of penicillin in water. <i>Journal of Hazardous Materials</i> , 2021, 413, 125385.	6.5	43
7854	A novel carbazole-based highly sensitive and selective turn-on fluorescent probe for mercury (II) ions in aqueous THF. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 416, 113322.	2.0	14
7855	Two, Three, or Not to Be? Elucidating Multiple Bonding in d ⁶ Pseudotetrahedral Oxo and Imide Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 13854-13860.	1.9	4

#	ARTICLE	IF	CITATIONS
7856	Investigations of adsorption behavior and anti-cancer activity of curcumin on pure and platinum-functionalized B12N12 nanocages. <i>Journal of Molecular Liquids</i> , 2021, 334, 116516.	2.3	39
7857	MD, DFT Investigations and Inhibition of the Novel SARS- CoV-2 Mainprotease in Three Cocrystals of Hydrochloro- thiazide. <i>Analytical Chemistry Letters</i> , 2021, 11, 450-468.	0.4	3
7858	The effect of ring aromaticity on ESIPT behavior and photophysical properties of 2-(2-hydroxyphenyl)-4-chloromethylthiazole derivatives: A TD-DFT study. <i>Journal of Molecular Liquids</i> , 2021, 334, 116517.	2.3	15
7859	Argon Adsorption on Cationic Gold Clusters Au ⁿ⁺ (n = 20). <i>Molecules</i> , 2021, 26, 4082.	1.7	2
7860	Understanding the aqueous chemistry of quinoline and the diazaphthalenes: insight from DFT study. <i>Heliyon</i> , 2021, 7, e07531.	1.4	13
7861	Regulation of Thermally Activated Delayed Fluorescence to Room-Temperature Phosphorescent Emission Channels by Controlling the Excited States Dynamics via π - and H-Aggregation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 18059-18064.	7.2	109
7862	Tunable Optical Absorption of Graphene Quantum Dots with Transition Metal Adatom. , 2021, , .		0
7863	Strain-controlled DHP-graphene for ultrahigh-performance hydrogen purification. <i>Applied Surface Science</i> , 2021, 553, 149575.	3.1	3
7864	Cis and trans isomers of 1-(5-bromothiophen-2-yl)-3-(10-chloroanthracen-9-yl)prop-2-en-1-one: Synthesis and characterization. <i>Journal of Molecular Structure</i> , 2021, 1236, 130228.	1.8	8
7865	Study of electronic structure, stabilities and electron localization behavior of AgPbn (n=1-14) nanoclusters: A first principal investigation. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 131, 114725.	1.3	16
7866	Electronic Structure of Superoxidized Radical Cationic Dodecaborate-Based Clusters. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6141-6150.	1.1	2
7867	An IrVO ₄ Cluster Catalytically Oxidizes Four CO Molecules: Importance of Ir-V Multiple Bonding. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6519-6525.	2.1	9
7868	Fluoride ion-induced gas sensor based on the dipyrromethene boron difluoride derivative: A theoretical investigation. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4265.	0.9	2
7869	The process and mechanism for cesium and rubidium extraction with saponified 4-tert-butyl-2-(1-methylbenzyl) phenol. <i>Chinese Journal of Chemical Engineering</i> , 2022, 46, 31-39.	1.7	6
7870	Synthesis and application of low-cost layered double hydroxides intercalated by gluconic acid anion for flame retardancy and tensile strength conservation of high filling epoxy resin. <i>Journal of Colloid and Interface Science</i> , 2021, 594, 791-801.	5.0	26
7871	Racemic Bisindole Alkaloids: Structure, Bioactivity, and Computational Study. <i>Chinese Journal of Chemistry</i> , 2021, 39, 2588-2598.	2.6	9
7872	A novel ICT-based chemosensor for F ⁻ and its application in real samples and bioimaging. <i>Journal of Hazardous Materials</i> , 2021, 413, 125384.	6.5	10
7873	Regulation of Novel Multi-Center Ionic Liquids for Synergetically Catalyzing CO ₂ Conversion into Cyclic Carbonates. <i>ChemistrySelect</i> , 2021, 6, 6380-6387.	0.7	8

#	ARTICLE	IF	CITATIONS
7874	Organic ligand mediated evolution from aluminum-based superalkalis to superatomic molecules and one-dimensional nanowires. <i>Nano Research</i> , 2022, 15, 1162-1170.	5.8	11
7875	Solvent Effect on the Stability and Reverse Substituent Effect in Nitropurine Tautomers. <i>Symmetry</i> , 2021, 13, 1223.	1.1	3
7876	Theoretical study on the noncovalent interactions involving triplet diphenylcarbene. <i>Journal of Molecular Modeling</i> , 2021, 27, 224.	0.8	0
7877	CONI-Net: Machine Learning of Separable Intermolecular Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4996-5006.	2.3	5
7878	Aggregation Behavior of Asphalt on the Natural Gas Hydrate Surface with Different Surfactant Coverages. <i>Journal of Physical Chemistry C</i> , 2021, 125, 16378-16390.	1.5	28
7880	Bi(III) halometallate ionic liquids: Interactions and speciation. <i>Journal of Chemical Physics</i> , 2021, 155, 014501.	1.2	10
7881	Theoretical calculation on the interaction mechanism between 2,6-diamino-3,5-dinitropyrazine-1-oxide and ammonium perchlorate. <i>Journal of Energetic Materials</i> , 2023, 41, 236-252.	1.0	4
7882	Predicting the substituent effects in the optical and electrochemical properties of N,N ² -substituted isoindigos. <i>Photochemical and Photobiological Sciences</i> , 2021, 20, 927-938.	1.6	5
7883	Molybdenum disulfide monolayer electronic structure information as explored using density functional theory and quantum theory of atoms in molecules. <i>Applied Surface Science</i> , 2021, 555, 149545.	3.1	11
7884	On the Potentiality of X-T-X ₃ Compounds (T = C, Si, and Ge, and X = F, Cl, and Br) as Tetrel- and Halogen-Bond Donors. <i>ACS Omega</i> , 2021, 6, 19330-19341.	1.6	11
7885	Chiral Thermally Activated Delayed Fluorescence Materials Based on <i>N,N</i> -bis(2-diphenyl-1,1'-binaphthalene)-2,2'-diamine Donor with Narrow Emission Spectra for Highly Efficient Circularly Polarized Electroluminescence. <i>Advanced Functional Materials</i> , 2021, 31, 2103875.	7.8	61
7886	Vibrational spectroscopy, quantum computational and molecular docking studies on 2-chloroquinoline-3-carboxaldehyde. <i>Heliyon</i> , 2021, 7, e07529.	1.4	18
7887	Oxacarbon superalkali C ₃ X ₃ Y ₃ (X = O, S and Y = Li, Na, K) clusters as excess electron compounds for remarkable static and dynamic NLO response. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 106, 107922.	1.3	19
7888	Quasi liquid Schiff bases from trans-2-hexenal and cytosine and l-leucine with potential antieczematic and antiarthritic activities: Synthesis, structure and quantum mechanical studies. <i>Journal of Molecular Liquids</i> , 2021, 334, 116448.	2.3	37
7889	A computational investigation of the activation of allene (H ₂ C=C=CHR; R = H, CH ₃ , CN) by a frustrated phosphorous/boron Lewis pair. <i>Chemical Physics Letters</i> , 2021, 774, 138623.	1.2	14
7890	Plausible Pnictogen Bonding of epi-Cinchonidine as a Chiral Scaffold in Catalysis. <i>Frontiers in Chemistry</i> , 2021, 9, 669515.	1.8	7
7891	Terpenoid-capric acid based natural deep eutectic solvent: Insight into the nature of low viscosity. <i>Cleaner Engineering and Technology</i> , 2021, 3, 100116.	2.1	14
7892	Molecular Modeling Reveals the Mechanism of Ran-RanGAP-Catalyzed Guanosine Triphosphate Hydrolysis without an Arginine Finger. <i>ACS Catalysis</i> , 2021, 11, 8985-8998.	5.5	10

#	ARTICLE	IF	CITATIONS
7893	Molecular dynamics simulation for mechanism revelation of the safety and nutrition of lipids and derivatives in food: State of the art. <i>Food Research International</i> , 2021, 145, 110399.	2.9	12
7894	Experimental and theoretical studies of some propiolate esters derivatives. <i>Journal of Molecular Structure</i> , 2021, 1236, 130281.	1.8	30
7895	Azoimidazole gold(III) complexes: Synthesis, structural characterization and self-assembly in the solid state. <i>Inorganica Chimica Acta</i> , 2021, 522, 120373.	1.2	24
7896	The influence of monomer deformation on triel and tetrel bonds between TrR ₃ /TR ₄ (Tr = Al, Ga, In; T = Si, Ge, Sn). <i>Journal of Organometallic Chemistry</i> , 2021, 911, 100011.	1.1	0
7897	Different cation-anion interaction mechanisms of diamino protic ionic liquids: A density functional theory study. <i>Chemical Physics Letters</i> , 2021, 774, 138615.	1.2	11
7898	Stability and Hydrogen Storage Properties of M ₂ B ₆ H ₆ Complexes (M = Mo, Ru, Ag, x = 1, 2). <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 10868-10881.	3.2	3
7899	Atoms in Highly Symmetric Environments: H in Rhodium and Cobalt Cages, H in an Octahedral Hole in MgO, and Metal Atoms Ca-Zn in C ₂₀ Fullerenes. <i>Symmetry</i> , 2021, 13, 1281.	1.1	0
7900	Efficient Restraint of Intra-Cluster Aggregation Caused Quenching Effect Lighting Room Temperature Photoluminescence. <i>Advanced Optical Materials</i> , 2021, 9, 2100757.	3.6	11
7901	Excited State Resonance Raman of Flavin Mononucleotide: Comparison of Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6171-6179.	1.1	10
7902	Theoretical investigation of impact sensitivity of nitrogen rich energetic salts. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113267.	1.1	7
7903	Accurate Prediction of Absorption Spectral Shifts of Proteorhodopsin Using a Fragment-Based Quantum Mechanical Method. <i>Molecules</i> , 2021, 26, 4486.	1.7	8
7904	Theoretical Insights into Transplutonium Element Separation with Electronically Modulated Phenanthroline-Derived Bis-Triazine Ligands. <i>Inorganic Chemistry</i> , 2021, 60, 10267-10279.	1.9	14
7905	Theoretical and computational insight into the supramolecular assemblies of Schiff bases involving hydrogen bonding and C-H...N interactions: Synthesis, X-ray characterization, Hirshfeld surface analysis, anticancer activity and molecular docking analysis. <i>Journal of Molecular Structure</i> , 2021, 1235, 130223.	1.8	8
7906	Dual XH...F Interaction of Hexafluoroisopropanol with Arenes. <i>Molecules</i> , 2021, 26, 4558.	1.7	7
7907	Two Ongoing Magnetic Transitions Originating from Spin-Peierls Dimerization and Cation Orientation Transformation in an S = 1/2 Spin Chain System. <i>Journal of Physical Chemistry C</i> , 2021, 125, 17493-17500.	1.5	4
7908	Anion-Cation Bonding and Structure-Property Relationships of Three cyclo-Pentazolate Compounds. <i>Crystal Growth and Design</i> , 2021, 21, 4329-4336.	1.4	5
7909	Atomistic insights into uptake of hydrogen peroxide by TiO ₂ particles as a function of humidity. <i>Journal of Molecular Liquids</i> , 2022, 346, 117097.	2.3	1
7910	How Can the 1-Type Fullerene-Metal Bond Survive? A Systematic Survey of Reactions between Mono-EMFs and (M ²⁺ Ln) ₂ Dimers. <i>Inorganic Chemistry</i> , 2021, 60, 11287-11296.	1.9	0

#	ARTICLE	IF	CITATIONS
7911	Surface engineering enables highly reversible lithium-ion storage and durable structure for advanced silicon anode. <i>Cell Reports Physical Science</i> , 2021, 2, 100486.	2.8	2
7912	A novel lysosome-localized fluorescent probe with aggregation-induced emission without alkalinizing effect. <i>SmartMat</i> , 2021, 2, 554-566.	6.4	25
7913	Adsorption properties of amino acid-based ionic liquids (AAILs) on edge fluorinated graphene surface – a DFT study. <i>Molecular Simulation</i> , 2021, 47, 1066-1077.	0.9	3
7914	Transformation of Atrazine to Hydroxyatrazine with Alkali-H ₂ O ₂ Treatment: An Efficient Dechlorination Strategy under Alkaline Conditions. <i>ACS ES&T Water</i> , 2021, 1, 1868-1877.	2.3	9
7915	Mechanism study on the formation of furfural during zinc chloride-catalyzed pyrolysis of xylose. <i>Fuel</i> , 2021, 295, 120656.	3.4	17
7916	Understanding the Catalytic Sites in Porous Hexagonal Boron Nitride for the Epoxidation of Styrene. <i>ACS Catalysis</i> , 2021, 11, 8872-8880.	5.5	20
7917	Metabolic activation mechanism of 2,2,3,3,6,6-hexachlorobiphenyl (PCB136) by cytochrome P450 2B6: A QM/MM approach. <i>Science of the Total Environment</i> , 2021, 776, 145579.	3.9	7
7918	SepPCNET: Deeping Learning on a 3D Surface Electrostatic Potential Point Cloud for Enhanced Toxicity Classification and Its Application to Suspected Environmental Estrogens. <i>Environmental Science & Technology</i> , 2021, 55, 9958-9967.	4.6	22
7919	Curing mechanism, thermal and ablative properties of hexa-(4-amino-phenoxy) cyclotriphosphazene/benzoxazine blends. <i>Composites Part B: Engineering</i> , 2021, 216, 108838.	5.9	31
7920	Dissection of the Origin of ĩ-Holes and the Noncovalent Bonds in Which They Engage. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6514-6528.	1.1	21
7921	First-principles study of hybrid nanostructures formed by deposited phthalocyanine/porphyrin metal complexes on phosphorene. <i>Journal of Molecular Liquids</i> , 2021, 333, 115948.	2.3	9
7922	Non-conventional Behavior of a 2,1-Benzazaphosphole: Heterodiene or Hidden Phosphinidene?. <i>Chemistry - A European Journal</i> , 2021, 27, 13149-13160.	1.7	4
7923	Designing and theoretical study of fluorinated small molecule donor materials for organic solar cells. <i>Journal of Molecular Modeling</i> , 2021, 27, 216.	0.8	31
7924	The influence of fluorinated position on the performance of isoindigo-based polymer solar cells. <i>Synthetic Metals</i> , 2021, 277, 116768.	2.1	2
7925	A DFT study of Se-decorated B12N12 nanocluster as a possible drug delivery system for ciclopirox. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113246.	1.1	28
7926	Radiolysis of cardiovascular drug atenolol in aqueous solution by electron beam: Effect of water components and persulfate addition. <i>Radiation Physics and Chemistry</i> , 2021, 184, 109458.	1.4	4
7927	Concerning the Role of ĩf-Hole in Non-Covalent Interactions: Insights from the Study of the Complexes of ArBeO with Simple Ligands. <i>Molecules</i> , 2021, 26, 4477.	1.7	2
7928	Pyrrrole/thiophene ĩ-bridged two triphenylamine electron donor and substituted thiobarbituric electron acceptor for <sc>D&A&D</sc>-featured <sc>DSSC</sc> applications. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 1842-1851.	0.8	8

#	ARTICLE	IF	CITATIONS
7929	On the Low-Lying Electronically Excited States of Azobenzene Dimers: Transition Density Matrix Analysis. <i>Molecules</i> , 2021, 26, 4245.	1.7	9
7930	Binding of noble gas atoms by superhalogens. <i>Journal of Chemical Physics</i> , 2021, 155, 014304.	1.2	5
7931	A DFT Study on the Mechanism of Catalytic Oxidation Desulfurization Over Ti-MWW Zeolite. <i>Journal of Cluster Science</i> , 2022, 33, 2103-2112.	1.7	3
7932	Computational Investigations on the Transition-Metal-Catalyzed Cross-Coupling of Enynones with Diazo Compounds. <i>Topics in Catalysis</i> , 0, , 1.	1.3	0
7933	Using topological analysis of the electron density to study a geometry-electronic structure relationship in M (d ⁵ â€“10)â€“O and Eâ€“O (E=â€“Se,Te) compounds. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113279.	1.1	1
7934	Deciphering the Mechanistic Details of Manganese-Catalyzed Formic Acid Dehydrogenation: Insights from DFT Calculations. <i>Inorganic Chemistry</i> , 2021, 60, 11038-11047.	1.9	7
7935	Electronic Structure and Donor Ability of an Unsaturated Triphosphorus-Bridged Dimolybdenum Complex. <i>Inorganic Chemistry</i> , 2021, 60, 11548-11561.	1.9	2
7936	Structural stabilities and transformation mechanism of rhynchophylline and isorhynchophylline in aqueous and methanol solution based on high-performance liquid chromatography and density functional theory. <i>Journal of Molecular Structure</i> , 2021, 1236, 130300.	1.8	3
7937	Investigating phosphorescence capability of halogen-substituted metal-free organic molecules: A theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 255, 119642.	2.0	4
7938	Second hyperpolarizability of hexagonal graphene quantum dots: Effects of size and structural defects. <i>Carbon Trends</i> , 2021, 4, 100054.	1.4	5
7939	The Isocyanide Complexes cis-[MCl ₂ (CNC ₆ H ₄ -4-X) ₂] (M = Pd, Pt; X = Cl, Br) as Tectons in Crystal Engineering Involving Halogen Bonds. <i>Crystals</i> , 2021, 11, 799.	1.0	10
7940	A Novel Centrosymmetric Fe(III) Complex with Anionic Bis-pyrazolyl-s-triazine Ligand; Synthesis, Structural Investigations and Antimicrobial Evaluations. <i>Symmetry</i> , 2021, 13, 1247.	1.1	6
7941	Improved color stability of anthocyanins in the presence of ascorbic acid with the combination of rosmarinic acid and xanthan gum. <i>Food Chemistry</i> , 2021, 351, 129317.	4.2	40
7942	Excess properties, spectral analyses and computational chemistry of the binary mixture of polyethylene glycol 200+1,3-propanediamine. <i>Journal of Molecular Liquids</i> , 2022, 346, 117080.	2.3	11
7943	Intramolecular Hydrogen Bond, Hirshfeld Analysis, AIM; DFT Studies of Pyran-2,4-dione Derivatives. <i>Crystals</i> , 2021, 11, 896.	1.0	9
7944	Insights into theoretical detection of CO ₂ , NO, CO, O ₂ , and O ₃ gases molecules using Zinc phthalocyanine with peripheral mono and tetra quinoleinoxy substituents: Molecular geometries, Electronic properties, and Vibrational analysis. <i>Chemical Physics</i> , 2021, 547, 111198.	0.9	9
7945	Combination of FTIR and DFT to study the structure and hydrogen-bond properties of alkylammonium-based ILs and DMSO mixtures. <i>Journal of Molecular Liquids</i> , 2021, 333, 115940.	2.3	7
7946	Interaction of M@Au ₁₂ nanocluster (M=â€“Au, Ag, Pd, and Pt) with different forms of cysteine (uncharged, cationic, anionic, and zwitterion) via the Au-S bond. <i>Journal of Molecular Liquids</i> , 2021, 334, 116090.	2.3	1

#	ARTICLE	IF	CITATIONS
7947	Reaction mechanism and kinetics of Criegee intermediate and hydroperoxymethyl formate. <i>Journal of Environmental Sciences</i> , 2021, 105, 128-137.	3.2	6
7948	Magnetic superatoms in cage doped 13-atom trimetallic Mg _n Li ₁₂ Sc (n = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12). <i>Physics B: Atomic, Molecular and Optical Physics</i> , 2021, 54, 145005.	0.6	0
7949	Group 11 m-Terphenyl Complexes Featuring Metallophilic Interactions. <i>Inorganic Chemistry</i> , 2021, 60, 10114-10123.	1.9	9
7950	Understanding the molecular mechanism of the chlorine atom transfer between ammonia and hypochlorous acid with electron localisation function (ELF). <i>Molecular Physics</i> , 0, , e1961035.	0.8	2
7951	Bifunctional Fe for Induced Graphitization and Catalytic Ozonation Based on a Fe/N-Doped Carbon ₂ O ₃ Framework: Theoretical Calculations Guided Catalyst Design and Optimization. <i>Environmental Science & Technology</i> , 2021, 55, 11236-11244.	4.6	41
7952	A matrix isolation infrared spectroscopic study of thermal isomerisation of 1-butanol. <i>Chemical Physics Letters</i> , 2021, 775, 138617.	1.2	3
7953	Hydroxyl-Assisted Hydrogen Transfer Interaction in Lignin Pyrolysis: An Extended Concerted Interaction Mechanism. <i>Energy & Fuels</i> , 2021, 35, 13170-13180.	2.5	17
7954	Simulation of Negative Ion Photoelectron Spectroscopy Using a Nuclear Ensemble Approach: Implications from a Nuclear Vibration Effect. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6621-6628.	1.1	1
7955	Towards Computational Screening for New Energetic Molecules: Calculation of Heat of Formation and Determination of Bond Strengths by Local Mode Analysis. <i>Frontiers in Chemistry</i> , 2021, 9, 726357.	1.8	4
7956	Dimeric aza-BODIPY and Dichloro-aza-BODIPY: A DFT Study. <i>Gazi University Journal of Science</i> , 2022, 35, 388-402.	0.6	0
7957	Glucose-Lipopeptide Conjugates Reveal the Role of Glucose Modification Position in Complexation and the Potential of Malignant Melanoma Therapy. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 11483-11495.	2.9	5
7958	Are σ -GAPT Charges Really Just Charges?. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3881-3890.	2.5	15
7959	Theoretical exploration of global minima, magnetism, structural stability and growth pattern of holmium-doped silicon HoSi ₁₀ (n = 10-18) nanoclusters. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26776.	1.0	1
7960	Effect of the heteroatom presence in different positions of the model asphaltene structure on the self-aggregation: MD and DFT study. <i>Journal of Molecular Liquids</i> , 2021, 334, 116109.	2.3	27
7961	Tuning fluorescence behavior and ESIPT reaction of 2-(2-Hydroxy-phenyl)-4(3H)-quinazolinone by introducing different groups. <i>Journal of Luminescence</i> , 2021, 235, 118059.	1.5	25
7962	Theoretical insights into the directionality of ESIPT behavior of BTHMB molecule with two proton acceptors in solution. <i>Chemical Physics Letters</i> , 2021, 775, 138670.	1.2	8
7963	Theoretical description of green solvents effect on electronic property and reactivity of Tert-butyl 4-formylpiperidine-1-carboxylate. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113255.	1.1	7
7964	Role of the nucleophilicity of the amino group of benzidines in the synthesis of hemiaminal ethers. <i>Journal of Molecular Structure</i> , 2021, 1236, 130307.	1.8	1

#	ARTICLE	IF	CITATIONS
7965	Synthesis, X-ray structure, Hirshfeld analysis and DFT studies of Ni(II) complexes with pyridine-type ligands and monoanionic (SCN ⁻ , N ₃ ⁻ and NO ₃ ⁻) ligands. <i>Journal of Molecular Structure</i> , 2021, 1236, 130325.	1.8	0
7966	Mechanistic Origins of Stereodivergence in Asymmetric Cascade Allylation and Cyclization Reactions Enabled by Synergistic Cu/Ir Catalysis. <i>ACS Catalysis</i> , 2021, 11, 9008-9021.	5.5	33
7967	Mechanistic Insight into Pd(II)-Catalyzed Late-Stage Nondirected C(sp ²)-H Cyanation of Toluene Using the Dual Ligands MPAA and Quinoxaline: A Density Functional Theory Investigation. <i>Journal of Organic Chemistry</i> , 2021, 86, 10526-10535.	1.7	1
7968	Density functional theory calculations of copper-doped rutile crystals: Local structural, electronic, optical, and electron paramagnetic resonance properties. <i>Magnetic Resonance in Chemistry</i> , 2022, 60, 104-112.	1.1	1
7969	Blue Axially Chiral Biphenyl Based Thermally Activated Delayed Fluorescence Materials for Efficient Circularly Polarized OLEDs. <i>Advanced Optical Materials</i> , 2021, 9, 2100596.	3.6	21
7970	Ternary aromatic and anti-aromatic clusters derived from the hypoh species [Sn ₂ Sb ₅] ³⁺ . <i>Nature Communications</i> , 2021, 12, 4465.	5.8	14
7971	Size-Dependent $\tilde{\epsilon}_g + \tilde{\epsilon}_u$ Combination Band Intensities of Polyynes C _{2n} H ₂ (n = 1-9) Analyzed by the Local CCH Bending and the Linear Response Functions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6404-6419.	1.1	0
7972	Modelling of the adsorption of pharmaceutically active compounds on carbon-based nanomaterials. <i>Journal of Hazardous Materials</i> , 2021, 414, 125554.	6.5	24
7973	On the properties of N-methyl-2-pyrrolidonium hydrogen sulfate ionic liquid and alkanol mixtures. <i>Journal of Molecular Liquids</i> , 2021, 333, 115925.	2.3	2
7974	Influence of bi-alkali metals doping over Al ₁₂ N ₁₂ nanocage on stability and optoelectronic properties: A DFT investigation. <i>Radiation Physics and Chemistry</i> , 2021, 184, 109457.	1.4	15
7975	The high-capacity hydrogen storage of B ₆ Ca ₂ and B ₈ Ca ₂ inverse sandwiches. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 24225-24232.	3.8	10
7976	In silico exploration of O-H...X ₂ ⁺ (X = Cu, Ag, Hg) interaction, targeted adsorption zone, charge density iso-surface, O-H proton analysis and topographic parameters theory for calix[6]arene and calix[8]arene as model. <i>Journal of Molecular Liquids</i> , 2021, 334, 116127.	2.3	13
7977	Singlet/Triplet State Anti/Aromaticity of Cyclopentadienyl Cation: Sensitivity to Substituent Effect. <i>Chemistry</i> , 2021, 3, 765-782.	0.9	6
7978	Influence of fluorine substitution on nonbonding interactions in selected para-halogeno anilines. <i>ChemPhysChem</i> , 2021, 22, 2115-2127.	1.0	3
7979	Role of atomicity in the oxygen reduction reaction activity of platinum sub nanometer clusters: A global optimization study. <i>Journal of Computational Chemistry</i> , 2021, 42, 1944-1958.	1.5	4
7980	Suspect Screening of Fentanyl Analogs Using Matrix-Assisted Ionization and a Miniature Mass Spectrometer with a Custom Expandable Mass Spectral Library. <i>Analytical Chemistry</i> , 2021, 93, 10152-10159.	3.2	14
7981	Influence of 5-Methylation and the 2'- and 3'-Hydroxy Substituents on the Base Pairing Energies of Protonated Cytidine Nucleoside Analogue Base Pairs: Implications for the Stabilities of i-Motif Structures. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5939-5955.	1.1	8
7982	Theoretical and Experimental Study of 3-Pentanol Autoignition: Ab Initio Calculation, Shock Tube Experiments, and Kinetic Modeling. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5976-5989.	1.1	3

#	ARTICLE	IF	CITATIONS
7983	lonâ€“solvent chemistry in lithium battery electrolytes: From mono-solvent to multi-solvent complexes. <i>Fundamental Research</i> , 2021, 1, 393-398.	1.6	50
7984	Efficient responsive ionic liquids with multiple active centers for the transformation of CO ₂ under mild conditions: Integrated experimental and theoretical study. <i>Journal of CO₂ Utilization</i> , 2021, 49, 101573.	3.3	14
7985	Computational simulation and efficient evaluation on corrosion inhibitors for electrochemical etching on aluminum foil. <i>Corrosion Science</i> , 2021, 187, 109492.	3.0	24
7986	Investigation of Glycolic Acid Natural Deep Eutectic Solvents with Strong Proton Donors for Ammonia Capture and Separation. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 11600-11610.	1.8	27
7987	DFT Study of Structure and Radical Scavenging Activity of Natural Pigment Delphinidin and Derivatives. , 0, , .		0
7988	Rapid electron transfer via dynamic coordinative interaction boosts quantum efficiency for photocatalytic CO ₂ reduction. <i>Nature Communications</i> , 2021, 12, 4276.	5.8	69
7989	A lead(II) toluene complex. <i>Mendeleev Communications</i> , 2021, 31, 471-474.	0.6	2
7990	Taming the Antiferromagnetic Beast: Computational Design of Ultrashort Mn ^{II} -Mn Bonds Stabilized by Nâ€“Heterocyclic Carbenes. <i>Chemistry - A European Journal</i> , 2021, 27, 12126-12136.	1.7	6
7991	Group 12 Carbonates and their Binary Complexes with Nitrogen Bases and FH 2 Z Molecules (Z=P, As,) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.6	7
7992	Enhancing the absorption of 1-chloro-1,2,2,2-tetrafluoroethane on carbon nanotubes: an ab initio study. <i>Bulletin of Materials Science</i> , 2021, 44, 1.	0.8	31
7993	Effect of a â€œZn Bridgeâ€“on the Consecutively Tunable Retention Characteristics of Volatile Random Access Memory Materials. <i>Chemistry - A European Journal</i> , 2021, 27, 12526-12534.	1.7	3
7994	Highâ€“Efficiency Solutionâ€“Processable OLEDs by Employing Thermally Activated Delayed Fluorescence Emitters with Multiple Conversion Channels of Triplet Excitons. <i>Advanced Science</i> , 2021, 8, e2101326.	5.6	43
7995	Substituent effects and mechanism studies in <sc>CO₂</sc> transformation to benzoxazinone derivatives as worthwhile Nâ€“containing heterocycles: Insight from <sc>Density functional theory</sc>. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26784.	1.0	3
7996	Theoretical investigation on conversion of CO ₂ with epoxides to cyclic carbonates by bifunctional metal-salen complexes bearing ionic liquid substituents. <i>Molecular Catalysis</i> , 2021, 511, 111733.	1.0	5
7997	A Crystalline B₄N₂ Dewar Benzene as a Building Block for Conjugated B,N-Chains. <i>Journal of the American Chemical Society</i> , 2021, 143, 11152-11159.	6.6	10
7998	Regulation of Thermally Activated Delayed Fluorescence to Roomâ€“Temperature Phosphorescent Emission Channels by Controlling the Excitedâ€“States Dynamics via Jâ€“and Hâ€“Aggregation. <i>Angewandte Chemie</i> , 2021, 133, 18207-18212.	1.6	15
7999	Element-specific contributions to improved magnetic heating of theranostic CoFe ₂ O ₄ nanoparticles decorated with Pd. <i>Scientific Reports</i> , 2021, 11, 15843.	1.6	5
8000	Study on the molecular structure and chemical properties of the polyoxypregnane derivatives 11â€“O-2-methylbutyryl-12â€“O-tigloyl tenacigenin B and 11â€“,12â€“-O-ditigloyl tenacigenin B by combining experimental and theoretical methods. <i>Journal of Molecular Structure</i> , 2021, 1237, 130350.	1.8	0

#	ARTICLE	IF	CITATIONS
8001	Probing nano-QSAR to assess the interactions between carbon nanoparticles and a SARS-CoV-2 RNA fragment. <i>Ecotoxicology and Environmental Safety</i> , 2021, 219, 112357.	2.9	15
8002	Chitosanâ€“ZnO nanocomposite from a circular economy perspective: in situ cotton-used fabric recycling and the nanocomposite recovering. <i>Polymer Bulletin</i> , 2022, 79, 7491-7529.	1.7	2
8003	A potential insensitive-highly-energetic material through conjugation-promoted N-oxidation strategy. <i>Chemical Engineering Journal</i> , 2022, 436, 131990.	6.6	18
8004	Evolution of the structural and electronic properties, and dynamical fluxionality of B ₂ Ge _n (<i>n</i> = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12) clusters: emergence of B ₂ unit endohedral pentagonal structure and aromaticity at <i>n</i> = 10. <i>Molecular Physics</i> , 2021, 119, .	0.8	0
8005	Polyoxometalate Interlayered Zincâ€“Metallophthalocyanine Molecular Layer Sandwich as Photocoupled Electrocatalytic CO ₂ Reduction Catalyst. <i>Journal of the American Chemical Society</i> , 2021, 143, 13721-13730.	6.6	49
8006	Diastereomeric Ni(II) Schiff-base cysteine derivatives: Non-covalent interactions and redox activity. <i>Electrochimica Acta</i> , 2021, 388, 138537.	2.6	3
8007	Tin Metal Cluster Compounds as New Third-Order Nonlinear Optical Materials by Computational Study. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7537-7544.	2.1	13
8008	Elucidation of the structure, spectroscopic techniques and quantum chemical investigations on nonlinear optical material 2â€“hydroxy-5-methylbenzaldehyde. <i>Journal of Molecular Structure</i> , 2021, 1238, 130426.	1.8	1
8009	Relating Bond Strength and Nature to the Thermodynamic Stability of Hypervalent Togniâ€“Type Iodine Compounds. <i>ChemPlusChem</i> , 2021, 86, 1199-1210.	1.3	5
8010	Hydration of Simple Model Peptides in Aqueous Osmolyte Solutions. <i>International Journal of Molecular Sciences</i> , 2021, 22, 9350.	1.8	5
8011	Indole Alkaloids from a Soil-Derived <i>Clonostachys rosea</i> . <i>Journal of Natural Products</i> , 2021, 84, 2468-2474.	1.5	15
8012	Photoinduced charge transfer in two-photon absorption. <i>Results in Optics</i> , 2021, 4, 100099.	0.9	2
8013	Catalytic S _N Ar Hydroxylation and Alkoxylation of Aryl Fluorides. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20391-20399.	7.2	22
8014	Intermolecular [5+2] Annulation between Î“Indanones and Internal Alkynes by Rhodiumâ€“Catalyzed Câ€“C Activation. <i>Angewandte Chemie</i> , 2021, 133, 20639-20645.	1.6	4
8015	The conglomerate crystal formation of methoxetamine salts in the presence of some organic achiral anions: a theoretical approach. <i>Supramolecular Chemistry</i> , 2021, 33, 183-193.	1.5	0
8016	Accurate machine learning models based on small dataset of energetic materials through spatial matrix featurization methods. <i>Journal of Energy Chemistry</i> , 2021, 63, 364-375.	7.1	7
8017	Studies of Nature of Uncommon Bifurcated Î“Î“-(<i>l</i>)-M(<i>l</i>)-Metal-Involving Noncovalent Interaction in Palladium(II) and Platinum(II) Isocyanide Cocrystals. <i>Inorganic Chemistry</i> , 2021, 60, 13200-13211.	1.9	16
8018	Mechanism and Selectivities in Ru-Catalyzed Anti-Markovnikov Formal Hydroalkylation of 1,3-Dienes and Enynes: A Computational Study. <i>Journal of Organic Chemistry</i> , 2021, 86, 11895-11904.	1.7	2

#	ARTICLE	IF	CITATIONS
8019	Synthesis of luminescent cocrystals based on fluoranthene and the analysis of weak interactions and photophysical properties. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 551-560.	0.2	2
8020	Solvent-Dependent Spectral Properties in Diverse Solvents, Light Harvesting and Antiviral Properties of Mono-Azo Dye (Direct Yellow-27): A Combined Experimental and Theoretical Study. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 619-630.	1.0	3
8021	Unraveling the Ultrafast Self-assembly and Photoluminescence in Zero-Dimensional Mn ²⁺ -Based Halides with Narrow-Band Green Emissions. <i>ACS Applied Electronic Materials</i> , 2021, 3, 4144-4150.	2.0	16
8022	The distance between g-tensors of nitroxide biradicals governs MAS-DNP performance: The case of the bTurea family. <i>Journal of Magnetic Resonance</i> , 2021, 329, 107026.	1.2	11
8023	Molecular Orbital Insight into the Near-Threshold Photoionization Cross Sections of Monocyclic Substituted Aromatic Compounds. <i>Energy & Fuels</i> , 2021, 35, 14051-14062.	2.5	3
8025	High performance task-specific ionic liquid in uranium extraction endowed with negatively charged effect. <i>Journal of Molecular Liquids</i> , 2021, 336, 116601.	2.3	7
8026	Computational design of photoswitchable anion receptors: Red-shifted and bistable di-ortho-fluoro di-ortho-chloro azobenzene derivatives. <i>Chemical Physics</i> , 2021, 548, 111246.	0.9	2
8027	Intermolecular [5+2] Annulation between 1-Indanones and Internal Alkynes by Rhodium-Catalyzed C-C Activation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20476-20482.	7.2	25
8028	The Catalysis Effect of Na and Point Defect on NO Heterogeneous Adsorption on Carbon during High-Sodium Zhundong Coal Reburning: Structures, Interactions and Thermodynamic Characteristics. <i>Catalysts</i> , 2021, 11, 1046.	1.6	4
8029	Nature and Strength of the π -Hole Chalcogen Bonded Complexes between Substituted Pyridines and SO ₃ Molecule. <i>ChemistrySelect</i> , 2021, 6, 7514-7524.	0.7	6
8030	Improved Reliability of Silver Nanowire-Based Composites by Electroplating: A Theoretical and Experimental Study. <i>ACS Applied Electronic Materials</i> , 2021, 3, 3329-3337.	2.0	4
8031	Mesomorphic Behaviour and DFT Insight of Arylidene Schiff Base Liquid Crystals and Their Pyridine Impact Investigation. <i>Crystals</i> , 2021, 11, 978.	1.0	9
8032	Atomic Clusters: Structure, Reactivity, Bonding, and Dynamics. <i>Frontiers in Chemistry</i> , 2021, 9, 730548.	1.8	14
8033	Organocatalytic enantioselective dearomatization of thiophenes by 1,10-conjugate addition of indole imine methides. <i>Nature Communications</i> , 2021, 12, 4881.	5.8	36
8034	Magnetic Core-Shell-Structured FeO/CN Catalyst Mediated Peroxymonosulfate Activation for Degradation of 2,4-Dichlorophenol via Non-Radical Pathway. <i>ACS ES&T Water</i> , 2021, 1, 2217-2232.	2.3	12
8035	Quantum computational, spectroscopic, Hirshfeld surface, electronic state and molecular docking studies on sulfanilic acid: An anti-bacterial drug. <i>Journal of Molecular Liquids</i> , 2022, 346, 117150.	2.3	25
8036	Structural (monomer and dimer), wavefunctional, NCI analysis in aqueous phase, electronic and excited state properties in different solvent atmosphere of 3-((E)-[(3,4-dichlorophenyl)imino]methyl)benzene-1,2-diol. <i>Journal of Molecular Liquids</i> , 2021, 336, 116335.	2.3	26
8037	Revealing dissolution behavior of o-methoxybenzoic acid in twelve pure solvents using thermodynamic analysis and molecular simulation. <i>Journal of Molecular Liquids</i> , 2021, 336, 116242.	2.3	15

#	ARTICLE	IF	CITATIONS
8056	Decorating BODIPY with Electron-Withdrawing NO Group: Spectroelectrochemical Consequences and Computational Investigation. <i>ChemElectroChem</i> , 2021, 8, 2921-2934.	1.7	0
8057	Natural Syringyl Mediators Accelerate Laccase-Catalyzed 2-O-4 Cleavage and C ₁ -Oxidation of a Guaiacyl Model Substrate via an Aggregation Mechanism. <i>ACS Omega</i> , 2021, 6, 22578-22588.	1.6	7
8058	Structural and physical properties of trichloroethylene under an external electric field. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4269.	0.9	2
8059	Iron Pentazolate Complex: Isoelectronic Species of Ferrocene but with a Planer Structure. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3903.	1.0	0
8060	3D-printed smartphone-based device for fluorimetric diagnosis of ketosis by acetone-responsive dye marker and red emissive carbon dots. <i>Mikrochimica Acta</i> , 2021, 188, 306.	2.5	8
8061	Double-Regio-determining-Stages Mechanistic Model Explaining the Regioselectivity of Pd-Catalyzed Hydroaminocarbonylation of Alkenes with Carbon Monoxide and Ammonium Chloride. <i>Journal of Organic Chemistry</i> , 2021, 86, 12988-13000.	1.7	4
8062	Easy preparation of novel 3,3-dimethyl-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide: Molecular structure, Hirshfeld surface, NCI analyses and molecular docking on AMPA receptors. <i>Journal of Molecular Structure</i> , 2021, 1238, 130435.	1.8	9
8063	<sc>Intra-Ring</sc> Bridging: A Strategy for Molecular Design of Highly Energetic Nitramines. <i>Chinese Journal of Chemistry</i> , 2021, 39, 2857-2864.	2.6	6
8064	A Covalent-Like Feature of Intermolecular Hydrogen Bonding in Energetic Molecules 3,6-Dihydrazino- <i>s</i> -s-tetrazine (DHT). <i>Advanced Theory and Simulations</i> , 2021, 4, 2100179.	1.3	2
8065	Enhanced catalytic performance of oxidized Ru supported on N-doped mesoporous carbon for acetylene hydrochlorination. <i>Applied Catalysis A: General</i> , 2021, 623, 118236.	2.2	11
8066	Hydrophobic phosphonium-based ionic liquids as novel extractants for palladium(II) recovery from alkaline cyanide solutions. <i>Journal of Molecular Liquids</i> , 2021, 336, 116358.	2.3	15
8067	Interaction between organic molecules and a gold nanoparticle: a quantum chemical topological analysis. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	3
8068	Catalytic Formation of Cyclic Carbonates using Gallium Aminotrisphenolate Compounds and Comparison to their Aluminium Congeners: A Combined Experimental and Computational Study. <i>ChemCatChem</i> , 2021, 13, 4099-4110.	1.8	14
8069	All-Liquid-Phase Reaction Mechanism Enabling Cryogenic Li-S Batteries. <i>ACS Nano</i> , 2021, 15, 13847-13856.	7.3	55
8070	Tunable Intramolecular Charge Transfer Effect on Diphenylpyrazine-Based Linear Derivatives and Their Expected Performance in Blue Emitters. <i>Advanced Optical Materials</i> , 2021, 9, 2101085.	3.6	12
8071	Heteroleptic cuprous complexes of a diimine MePBO ligand and their structure influence on phosphorescent color: Syntheses, structure characterizations, properties and TD-DFT calculations. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2021, 647, 1896.	0.6	9
8072	Structure activity relationships and the binding mode of quinolinone-pyrimidine hybrids as reversal agents of multidrug resistance mediated by P-gp. <i>Scientific Reports</i> , 2021, 11, 16856.	1.6	19
8073	Structural stability and thermodynamic properties of (Y ₂ O ₃) _n (n = 1-15) clusters based on density functional theory. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26802.	1.0	3

#	ARTICLE	IF	CITATIONS
8074	Weak interaction-alleviated toxicity of aromatic compounds in EPS matrices: Quantifying the noncovalent bonding-to-EPS ecoservice chain. <i>Journal of Hazardous Materials</i> , 2021, 416, 125824.	6.5	5
8075	Interaction between Curcumin and β -Casein: Multi-Spectroscopic and Molecular Dynamics Simulation Methods. <i>Molecules</i> , 2021, 26, 5092.	1.7	10
8076	Quantum Mechanical Investigation of the Oxidative Cleavage of the C-C Backbone Bonds in Polyethylene Model Molecules. <i>Polymers</i> , 2021, 13, 2730.	2.0	8
8077	Dithiane Based Boronic Acid as a Carbohydrate Sensor in an Aqueous Solution at pH 7.5: Theoretical and Experimental Approach. <i>Journal of Fluorescence</i> , 2021, 31, 1683-1703.	1.3	5
8078	Kick-Fukui: A Fukui Function-Guided Method for Molecular Structure Prediction. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3955-3963.	2.5	14
8079	Insights into the electronic structure and mechanism of norcaradiene hydroxylation by OxoMn(V) porphyrin complexes: A density functional theory study. <i>Journal of Computational Chemistry</i> , 2021, 42, 1920-1928.	1.5	2
8080	Quantum mechanical simulation of Molnupiravir drug interaction with Si-doped C60 fullerene. <i>Computational and Theoretical Chemistry</i> , 2021, 1202, 113336.	1.1	13
8081	Effect of alkali atom doping on the electronic structure and aromatic character of planar and quasi-planar Al ₁₃ ⁺ clusters. <i>Journal of Molecular Modeling</i> , 2021, 27, 235.	0.8	2
8082	Revisiting the energy treatment of the density of molecular crystals: an interrelation between intermolecular interaction energies and changes of molecular volume. <i>Russian Chemical Bulletin</i> , 2021, 70, 1429-1437.	0.4	5
8083	PCM-ROKS for the Description of Charge-Transfer States in Solution: Singlet-Triplet Gaps with Chemical Accuracy from Open-Shell Kohn-Sham Reaction-Field Calculations. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8470-8480.	2.1	23
8084	Toward Quantum Confinement in Graphitic Carbon Nitride-Based Polymeric Monolayers. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7597-7606.	1.1	5
8085	Group 14 Central Atoms and Halogen Bonding in Different Dielectric Environments: How Germanium Outperforms Silicon. <i>ChemPlusChem</i> , 2021, 86, 1387-1396.	1.3	1
8086	Different degradation mechanisms of carbamazepine and diclofenac by single-atom Barium embedded g-C ₃ N ₄ : the role of photosensitization-like mechanism. <i>Journal of Hazardous Materials</i> , 2021, 416, 125936.	6.5	43
8087	Unraveling the Mechanism of Aerobic Alcohol Oxidation by a Cu/pyridyl- β -Cyclodextrin/TEMPO Catalytic System under Air in Neat Water. <i>Inorganic Chemistry</i> , 2021, 60, 14132-14141.	1.9	4
8088	Preparation of magnetic powdered carbon/nano-Fe ₃ O ₄ composite for efficient adsorption and degradation of trichloropropyl phosphate from water. <i>Journal of Hazardous Materials</i> , 2021, 416, 125765.	6.5	15
8089	DFT molecular modeling studies of D-A-D type cyclopentadithiophene-diketopyrrolopyrrole based small molecules donor materials for organic photovoltaic cells. <i>Optik</i> , 2021, 239, 166787.	1.4	48
8090	A mutant T1 lipase homology modeling, and its molecular docking and molecular dynamics simulation with fatty acids. <i>Journal of Biotechnology</i> , 2021, 337, 24-34.	1.9	25
8091	Colour-tunable dual-mode afterglows and helical-array-induced mechanoluminescence from AIE enantiomers: Effects of molecular arrangement on formation and decay of excited states. <i>Chemical Engineering Journal</i> , 2021, 418, 129167.	6.6	50

#	ARTICLE	IF	CITATIONS
8092	Conformational changes for porphyrinoid derivatives: an information-theoretic approach study. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	8
8093	Surface Reactivity of Carbonaceous Nanoparticles: The Importance of Surface Pocket. <i>Frontiers in Mechanical Engineering</i> , 2021, 7, .	0.8	0
8094	Time-dependent atomistic simulations of the CP29 light-harvesting complex. <i>Journal of Chemical Physics</i> , 2021, 155, 055103.	1.2	10
8095	Pyrolyzed carbon derived from red soil as an efficient catalyst for cephalixin removal. <i>Chemosphere</i> , 2021, 277, 130339.	4.2	6
8096	A first-principles evaluation on the interaction of 1,3,4-oxadiazole with pristine and B-, Al-, Ga-doped C60 fullerenes. <i>Journal of Molecular Liquids</i> , 2021, 335, 116181.	2.3	34
8098	Nonadiabatic Dynamics Mechanism of Chalcone Analogue Sunscreen FPPO-HBr: Excited State Intramolecular Proton Transfer Followed by Conformation Twisting. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9572-9578.	1.2	15
8099	Covalently linked hydrogen bond donors: The other side of molecular frustration in deep eutectic solvents. <i>Journal of Chemical Physics</i> , 2021, 155, 084502.	1.2	3
8100	Structural, spectral, electronic and optical investigations of D-(-)-alpha-Phenylglycine: protease kinase inhibitor. <i>Spectroscopy Letters</i> , 0, , 1-17.	0.5	2
8101	Methyl groups as widespread Lewis bases in noncovalent interactions. <i>Nature Communications</i> , 2021, 12, 5030.	5.8	21
8102	Carbon nanotube-based titanium and zirconium doped [N ₄] type ORR catalysts. First principle study. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26809.	1.0	5
8103	Investigating the Bismuth Complexes with Benzoazacrown Tri- and Tetraacetates. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3344-3354.	1.0	6
8104	π-hole interactions of group III-VI elements with π-systems and Lewis bases: a comparative study. <i>Structural Chemistry</i> , 2022, 33, 9-21.	1.0	9
8105	Investigating the property and strength of intermolecular interaction in saturated and unsaturated cyclic cations constructed ionic liquids. <i>Journal of Molecular Liquids</i> , 2021, 335, 116253.	2.3	5
8106	Theoretical study of the formation and nucleation mechanism of highly oxygenated multi-functional organic compounds produced by α -pinene. <i>Science of the Total Environment</i> , 2021, 780, 146422.	3.9	12
8107	Tris-isopropyl-sily-ethynyl anthracene based small molecules for organic solar cells with efficient photovoltaic parameters. <i>Computational and Theoretical Chemistry</i> , 2021, 1202, 113305.	1.1	8
8108	Investigation of interfacial composition and thermodynamic stability of 14-n-14/alcohol/oil/water microemulsions by dilution method. <i>Journal of Molecular Liquids</i> , 2021, 336, 116333.	2.3	2
8109	Photo-induced electron transfer of [C60%+Abacavir] nano-complex and feasibility of C60 fullerene application as a chemical shift reagent: a DFT/TD-DFT insights. <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 937-956.	1.2	2
8110	Hydrogen bonding effect on the thermal behavior of acidic ionic liquids. <i>Journal of Molecular Structure</i> , 2021, 1238, 130416.	1.8	5

#	ARTICLE	IF	CITATIONS
8111	<i>In Situ</i> Synthesis of Vacancy-Rich Titanium Sulfide Confined in a Hollow Carbon Nanocage as an Efficient Sulfur Host for Lithium–Sulfur Batteries. <i>ACS Applied Energy Materials</i> , 2021, 4, 10104-10113.	2.5	15
8112	Comprehensive investigations of interaction properties of polylactic Acid–Attapulgitite composite by reactive molecular dynamics simulations and dispersion corrected DFT calculations. <i>Current Applied Physics</i> , 2021, 28, 78-86.	1.1	3
8113	Tris isocyanide copper(I) complex enabling copper azide–alkyne cycloaddition in neat conditions. <i>Applied Organometallic Chemistry</i> , 2021, 35, e6401.	1.7	7
8114	The Interplay between Diradical Character and Stability in Organic Molecules. <i>Symmetry</i> , 2021, 13, 1448.	1.1	1
8115	Anti-Electrostatic Main Group Metal–Metal Bonds That Activate CO ₂ . <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7545-7552.	2.1	2
8116	Molecular insight into photoresponsive surfactant regulated reversible emulsification and demulsification processes. <i>Journal of Molecular Liquids</i> , 2021, 335, 116218.	2.3	8
8117	Simple, reliable, and universal metrics of molecular planarity. <i>Journal of Molecular Modeling</i> , 2021, 27, 263.	0.8	90
8118	STRUCTURE AND CATALYTIC PROPERTIES OF (ACETYLACETONATO- η^2 O, η^2)BIS(TRI(2-FURYL)PHOSPHINE) PALLADIUM(II) TETRAFLUOROBORATE. <i>Journal of Structural Chemistry</i> , 2021, 62, 1218-1228.	0.3	3
8119	Catalytic S _N Ar Hydroxylation and Alkoxylation of Aryl Fluorides. <i>Angewandte Chemie</i> , 2021, 133, 20554-20562.	1.6	4
8120	A cosolvent pretreatment: effect of solvent–water on enzymatic hydrolysis of glucan, lignin structure, and dynamics. <i>Cellulose</i> , 2021, 28, 9051-9067.	2.4	5
8121	Sulphur-Bridged BAl ₅ S ₅ ⁺ with 17 Counting Electrons: A Regular Planar Pentacoordinate Boron System. <i>Molecules</i> , 2021, 26, 5205.	1.7	4
8122	Quantum Chemical Approach of Donor–Acceptor Based Arylborane–Arylamine Macrocycles with Outstanding Photovoltaic Properties Toward High-Performance Organic Solar Cells. <i>Energy & Fuels</i> , 2021, 35, 15018-15032.	2.5	66
8123	Facile access to highly flexible and mesoporous structured silica fibrous membranes for tetracyclines removal. <i>Chemical Engineering Journal</i> , 2021, 417, 129211.	6.6	34
8124	Binding Sites, Vibrations and Spin–Lattice Relaxation Times in Europium(II)-Based Metallofullerene Spin Qubits. <i>Chemistry - A European Journal</i> , 2021, 27, 13242-13248.	1.7	7
8125	Nucleophilic Activation of Sulfur Hexafluoride by N-Heterocyclic Carbenes and N-Heterocyclic Olefins: A Computational Study. <i>Chemistry - an Asian Journal</i> , 2021, 16, 2687-2693.	1.7	9
8126	A DFT study on carbon dioxide reduction of low-valent diuranium complex supported by a polypyrrolic macrocycle. <i>Chemical Physics Letters</i> , 2021, 776, 138652.	1.2	3
8127	Fine-diameter Si–B–C–N ceramic fibers enabled by polyborosilazanes with N–methyl pendant group. <i>Journal of the European Ceramic Society</i> , 2021, 41, 5016-5025.	2.8	12
8128	Isomerization energies and surface electrostatic potential analyses on nitriles and isocyanides. <i>Journal of Molecular Modeling</i> , 2021, 27, 257.	0.8	2

#	ARTICLE	IF	CITATIONS
8129	Excited States Symmetry Breaking and In-Plane Polarization Cause Chiral Reversal in Diastereomers. <i>Molecules</i> , 2021, 26, 4680.	1.7	1
8130	Synthesis and Characterization of Azido Esters as Green Energetic Plasticizers. <i>Propellants, Explosives, Pyrotechnics</i> , 2021, 46, 1537-1546.	1.0	4
8131	Performance and Mechanism of Alkylimidazolium Ionic Liquids as Corrosion Inhibitors for Copper in Sulfuric Acid Solution. <i>Molecules</i> , 2021, 26, 4910.	1.7	8
8132	Gas-phase structure, bonding, and fragmentation chemistry of the An (IV)-TMPDCAM complexes studied using mass spectrometry and theoretical calculation (An=Th and U). <i>Rapid Communications in Mass Spectrometry</i> , 2021, 35, e9168.	0.7	1
8133	Manganese peroxidase mediated oxidation of sulfamethoxazole: Integrating the computational analysis to reveal the reaction kinetics, mechanistic insights, and oxidation pathway. <i>Journal of Hazardous Materials</i> , 2021, 415, 125719.	6.5	35
8136	Remote effect of substituents on the properties of phenyl thienyl thioether-based oxime esters as LED-sensitive photoinitiators. <i>Dyes and Pigments</i> , 2021, 192, 109435.	2.0	26
8137	Anomeric and Perlin Effect Ladders for 2-Substituted 2-Fluorotetrahydro-2H-pyrans Using Sensitive Structural, Energetic, and NMR Probes. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7457-7472.	1.1	2
8138	Solid-liquid equilibrium behavior, thermodynamic analysis and molecular simulation of dimetridazole in twelve organic solvents. <i>Journal of Molecular Liquids</i> , 2021, 336, 116252.	2.3	18
8139	Towards the design of ideal electrochromic materials with low driving voltage based on phthalate derivatives. <i>Organic Electronics</i> , 2021, 95, 106189.	1.4	2
8140	Insights into vitamin B3, B6 and C as inhibitor of steel reinforcement: A DFT study. <i>Construction and Building Materials</i> , 2021, 294, 123571.	3.2	17
8141	Endohedral functionalization of chiral metal-organic cages for encapsulating achiral dyes to induce circularly polarized luminescence. <i>CheM</i> , 2021, 7, 2771-2786.	5.8	74
8142	Structure and properties of Be- and Mg-doped cyclo[18]carbon. <i>European Physical Journal D</i> , 2021, 75, 1.	0.6	6
8143	Competitive processes of tributyl phosphate degradation in HNO ₃ -saturated solution in Isopar-M during radiolysis and aging. <i>Radiation Physics and Chemistry</i> , 2021, 185, 109495.	1.4	12
8144	Two new spongian diterpene derivatives from the aquaculture sponge <i>Spongia officinalis</i> Linnaeus, 1759. <i>Natural Product Research</i> , 2021, , 1-11.	1.0	0
8145	Covalence and π -electron delocalization influence on hydrogen bonds in proton transfer process of <i>o</i> -hydroxy aryl Schiff bases: A combined NMR and QTAIM analysis. <i>Journal of Chemical Physics</i> , 2021, 155, 054307.	1.2	2
8146	Direct Attack and Indirect Transfer Mechanisms Dominated by Reactive Oxygen Species for Photocatalytic H ₂ O ₂ Production on g-C ₃ N ₄ Possessing Nitrogen Vacancies. <i>ACS Catalysis</i> , 2021, 11, 11440-11450.	5.5	132
8147	2-METHYLPYRIDINIUM SALT OF PENTAIODOBENZOIC ACID: ROLE OF THE HALOGEN BOND IN THE FORMATION OF A CRYSTAL PACKING. <i>Journal of Structural Chemistry</i> , 2021, 62, 1237-1242.	0.3	0
8148	Study of the Redox Potentials of Benzoquinone and Its Derivatives by Combining Electrochemistry and Computational Chemistry. <i>Journal of Chemical Education</i> , 2021, 98, 3019-3025.	1.1	4

#	ARTICLE	IF	CITATIONS
8149	Photochromic Semiconductors with Record-High Dielectric Permittivity Gain at Room Temperature. ACS Applied Electronic Materials, 2021, 3, 3301-3305.	2.0	3
8150	Mechanism and Selectivity of Cyclopropanation of 3-Alkenyl-oxindoles with Sulfoxonium Ylides Catalyzed by a Chiral N,N -Dioxide-Mg(II) Complex. Journal of Organic Chemistry, 2021, 86, 11683-11697.	1.7	7
8151	Theoretical investigation on tautomerism and NLO properties of salicylideneaniline derivatives. Canadian Journal of Physics, 2021, 99, 1095-1104.	0.4	1
8152	Mechanism of urea decomposition catalyzed by <i>Sporosarcina pasteurii</i> urease based on quantum chemical calculations. Molecular Simulation, 2021, 47, 1335-1348.	0.9	7
8153	Pyrrrolizinone-Fused BOPYINs: Characterization and Selective C=O Bond Formation Mechanism. ChemistrySelect, 2021, 6, 7894-7900.	0.7	0
8154	Tuning the metal-ligand bond in the σ -complexes of stannylenes and azabenzenes. Journal of Computational Chemistry, 2021, 42, 2103-2115.	1.5	2
8155	Halogen Bonding Mediated Hierarchical Supramolecular Chirality. ACS Nano, 2021, 15, 15306-15315.	7.3	23
8156	Antiproliferative activity on <i>Trypanosoma cruzi</i> (Y strain) of the triterpene $3\beta,6\beta,16\beta$ -trihydroxylup-20 (29)-ene isolated from <i>Combretum leprosum</i> . Journal of Biomolecular Structure and Dynamics, 2022, 40, 12302-12315.	2.0	3
8157	Modeling the DFT structural and reactivity studies of a pyrimidine -6-carboxylate derivative with reference to its wavefunction-dependent, MD simulations and evaluation for potential antimicrobial activity. Journal of Molecular Structure, 2021, 1237, 130397.	1.8	20
8158	Acetaminophen degradation by hydroxyl and organic radicals in the peracetic acid-based advanced oxidation processes: Theoretical calculation and toxicity assessment. Journal of Hazardous Materials, 2021, 416, 126250.	6.5	17
8159	Selectively Fluorinated Furan-Phenylene Co-Oligomers Pave the Way to Bright Ambipolar Light-Emitting Electronic Devices. Advanced Functional Materials, 2021, 31, 2104638.	7.8	12
8160	A conjugated piper-linked nano-spacing graphite network for sodium-ion battery. Energy Storage Materials, 2021, 39, 70-80.	9.5	18
8161	Highly selective and sensitive chiral recognition to deoxynucleosides by calixarene oligomers modified silver nanoparticles. Sensors and Actuators B: Chemical, 2021, 341, 130044.	4.0	6
8162	Visible-light-driven photoelectrocatalytic degradation of p-chloronitrobenzene by BiOBr/TiO ₂ nanotube arrays photoelectrodes: Mechanisms, degradation pathway and DFT calculation. Separation and Purification Technology, 2021, 268, 118699.	3.9	28
8163	Cationic effect on properties related to thermal stability and ignition delay for hypergolic ionic liquids. Journal of Molecular Liquids, 2021, 336, 116572.	2.3	5
8164	QM/MD study on the ability of phosphorene for selective detection of amino acids. Journal of Molecular Liquids, 2021, 336, 116865.	2.3	5
8166	Viologen-Decorated TEMPO for Neutral Aqueous Organic Redox Flow Batteries. Energy Material Advances, 2021, 2021, .	4.7	29
8167	Experimental and molecular dynamics study of graphene oxide quantum dots interaction with solvents and its aggregation mechanism. Journal of Molecular Liquids, 2021, 335, 116136.	2.3	5

#	ARTICLE	IF	CITATIONS
8168	Solvent effect on the excited-state intramolecular double proton transfer of 1,3-bis(2-pyridylimino)-4,7-dihydroxyisoindole. <i>Photochemical and Photobiological Sciences</i> , 2021, 20, 1183-1194.	1.6	12
8169	Novel Sulfonamide-Based Carbamates as Selective Inhibitors of BChE. <i>International Journal of Molecular Sciences</i> , 2021, 22, 9447.	1.8	11
8170	Hydrophobic Moiety of Capsaicinoids Haptens Enhancing Antibody Performance in Immunoassay: Evidence from Computational Chemistry and Molecular Recognition. <i>Journal of Agricultural and Food Chemistry</i> , 2021, 69, 9957-9967.	2.4	23
8171	Interpretation of the differential UV-visible absorbance spectra of metal-NOM complexes based on the quantum chemical simulations for the model compound esculetin. <i>Chemosphere</i> , 2021, 276, 130043.	4.2	10
8172	Potential Energy Surfaces of Vinylogous Wolff Rearrangement: NBO Analysis and Molecular Dynamic Simulation. <i>ChemistryOpen</i> , 2021, 10, 949-953.	0.9	0
8173	A hybrid molecular peapod of sp ² - and sp ³ -nanocarbons enabling ultrafast terahertz rotations. <i>Nature Communications</i> , 2021, 12, 5062.	5.8	12
8174	Nitrene-Mediated P=C-N Coupling Under Iron Catalysis. <i>CCS Chemistry</i> , 2022, 4, 2258-2266.	4.6	17
8175	Hydrogen-bonding regulated supramolecular chirality with controllable biostability. <i>Nano Research</i> , 2022, 15, 2226-2234.	5.8	11
8176	Theoretical research on cage-like furazan-based energetic compounds and its derivatives. <i>Journal of Molecular Modeling</i> , 2021, 27, 243.	0.8	4
8177	Electrochemical sensing behavior of graphdiyne nanoflake towards uric acid: a quantum chemical approach. <i>Journal of Molecular Modeling</i> , 2021, 27, 244.	0.8	4
8178	Intermolecular charge-transfer aggregates enable high-efficiency near-infrared emissions by nonadiabatic coupling suppression. <i>Science China Chemistry</i> , 2021, 64, 1786-1795.	4.2	25
8179	Polycyclic Arene-Fused Selenophenes via Site Selective Selenocyclization of Arylethynyl Substituted Polycyclic Arenes. <i>Journal of Organic Chemistry</i> , 2021, 86, 12494-12506.	1.7	7
8180	Noble Gas in a Ring. <i>Molecules</i> , 2021, 26, 4677.	1.7	2
8181	Nitrogen-Doped Buckybowls as Potential Scaffold Material for Lithium-Sulfur Battery: A DFT Study. <i>Electrocatalysis</i> , 2021, 12, 678-690.	1.5	8
8182	Efficient tuning of small acceptor chromophores with A1- π -A2- π -A1 configuration for high efficacy of organic solar cells via end group manipulation. <i>Journal of Saudi Chemical Society</i> , 2021, 25, 101305.	2.4	53
8183	Substituted Stilbene-based D- π -A and A- π -A type oxime esters as photoinitiators for LED photopolymerization. <i>European Polymer Journal</i> , 2021, 156, 110617.	2.6	13
8184	Design, synthesis, DFT calculations, molecular docking and antimicrobial activities of novel cobalt, chromium metal complexes of heterocyclic moiety-based 1,3,4-oxadiazole derivatives. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-14.	2.0	1
8185	Linear Group 13 E ₂ Triple Bonds in E ₂ Li ₆ 2+. <i>ChemPhysChem</i> , 2021, 22, 1996-2003.	1.0	0

#	ARTICLE	IF	CITATIONS
8186	Ylide-Substituted Phosphines with a Cyclic Ylide-Backbone: Angle Dependence of the Donor Strength. <i>Organometallics</i> , 2021, 40, 2888-2900.	1.1	11
8187	Solvents Hinder the Interlocking Rotation between Molecular Gears, as Revealed by Torque Calculations. <i>Journal of Physical Chemistry C</i> , 2021, 125, 17612-17621.	1.5	5
8188	High-pressure structural and optical property evolution of a hybrid indium halide perovskite. <i>Journal of Solid State Chemistry</i> , 2021, 300, 122262.	1.4	3
8189	Theoretical study of enantioenriched aminohydroxylation of styrene catalyzed by an engineered hemoprotein. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, e4280.	0.9	1
8190	Efficient synthesis of bepotastine and cloperastine intermediates using engineered alcohol dehydrogenase with a hydrophobic pocket. <i>Applied Microbiology and Biotechnology</i> , 2021, 105, 5873-5882.	1.7	4
8191	Hydration of selenolate moiety: Ab initio investigation of properties of $\text{H}_3\text{Se}^-(\text{H}_2\text{O})_n$ clusters. <i>Journal of Computational Chemistry</i> , 2021, 42, 2014-2023.	1.5	3
8192	Tuning the optoelectronic properties of triphenylamine (TPA) based small molecules by modifying central core for photovoltaic applications. <i>Journal of Molecular Modeling</i> , 2021, 27, 237.	0.8	60
8193	NONLINEAR OPTICAL AND SPECTRAL PROPERTIES OF HYDROQUINONE & FULLERENE SYSTEMS. <i>Eskişehir Teknik Üniversitesi Bilim Ve Teknoloji Dergisi B - Teorik Bilimler</i> , 2021, 9, 47-53.	0.0	0
8194	Long Carbon-Carbon Bonding beyond 2 Å... in Tris(9-fluorenylidene)methane. <i>Journal of the American Chemical Society</i> , 2021, 143, 14360-14366.	6.6	19
8195	Mechanism and regio- and stereoselectivity in NHC-catalyzed reaction of 2-bromoaldehydes with β -ketoamides. <i>Molecular Catalysis</i> , 2021, 513, 111790.	1.0	2
8196	Tetradentate Platinum(II) and Palladium(II) Complexes Containing Fused 6/6/6 or 6/6/5 Metallocycles with Azacarbazolylicarbazole-Based Ligands. <i>Inorganic Chemistry</i> , 2021, 60, 12972-12983.	1.9	17
8197	Defect-Engineering of Anionic Porous Aromatic Frameworks for Ammonia Capture. <i>ACS Applied Polymer Materials</i> , 2021, 3, 4534-4542.	2.0	7
8198	Two amino acid derivatives as high efficient green inhibitors for the corrosion of carbon steel in CO ₂ -saturated formation water. <i>Corrosion Science</i> , 2021, 189, 109596.	3.0	94
8199	Unveiling the Intramolecular Ionic Diels-Alder Reactions within Molecular Electron Density Theory. <i>Chemistry</i> , 2021, 3, 834-853.	0.9	0
8200	Therapeutic potential of graphyne as a new drug-delivery system for daunorubicin to treat cancer: A DFT study. <i>Journal of Molecular Liquids</i> , 2021, 336, 116327.	2.3	48
8201	Construction of Coplanar Bicyclic Backbones for 1,2,4-Triazole-1,2,4-Oxadiazole-Derived Energetic Materials. <i>Chemistry - A European Journal</i> , 2021, 27, 13807-13818.	1.7	17
8202	Kinetics and mechanisms of phenolic compounds by Ferrate(VI) assisted with density functional theory. <i>Journal of Hazardous Materials</i> , 2021, 415, 125563.	6.5	24
8203	Mechanical insight into the formation of H ₂ S from thiophene pyrolysis: The influence of H ₂ O. <i>Chemosphere</i> , 2021, 279, 130628.	4.2	9

#	ARTICLE	IF	CITATIONS
8204	Sulfanion-initiated open-vessel anionic ring-opening polymerization (AROP) of N-sulfonyl aziridines. <i>Science China Chemistry</i> , 2021, 64, 1778-1785.	4.2	3
8205	Prediction of Multicomponent Reaction Yields Using Machine Learning. <i>Chinese Journal of Chemistry</i> , 2021, 39, 3231-3237.	2.6	19
8206	A comprehensive investigation of the intermolecular interactions between CH_2N_2 and $\text{X}_{12}\text{Y}_{12}$ (X = B, Al, Ga; Y = N, P, As) nanocages. <i>Canadian Journal of Chemistry</i> , 2021, 99, 733-741.	0.6	30
8207	Properties of a furan ring-opening reaction in aqueous micellar solutions for selective sensing of mesalazine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 258, 119846.	2.0	2
8208	Regulation mechanism of the solvent coligands on the magnetic properties of azido-Cu(II) complexes by mixed carboxylate/alkanols ligands: A theoretical exploration. <i>Polyhedron</i> , 2021, 205, 115312.	1.0	5
8209	Energy and reactivity profile and proton affinity analysis of rimegepant with special reference to its potential activity against SARS-CoV-2 virus proteins using molecular dynamics. <i>Journal of Molecular Modeling</i> , 2021, 27, 276.	0.8	12
8210	Electronically excited state structures and stabilities of organic small molecules: A DFT study of triphenylamine derivatives. <i>Chemical Physics</i> , 2021, 549, 111256.	0.9	3
8211	Halogen Interactions in Halogenated Oxindoles: Crystallographic and Computational Investigations of Intermolecular Interactions. <i>Molecules</i> , 2021, 26, 5487.	1.7	3
8212	Metal Effect Meets Volcano Plots: A DFT Study on Tris(phosphino)borane-Transition Metal Complexes Catalyzed H ₂ Activation. <i>Chemistry - an Asian Journal</i> , 2021, 16, 3427-3436.	1.7	2
8213	On the radical behavior of large polycyclic aromatic hydrocarbons in soot formation and oxidation. <i>Combustion and Flame</i> , 2022, 235, 111692.	2.8	24
8214	Fluorescence turn off mechanism of selective chemosensor for hydrogen sulfide: A theoretical perspective. <i>Journal of Molecular Liquids</i> , 2021, 338, 116679.	2.3	5
8215	Closer look into the structures of tetrabutylammonium bromide-glycerol-based deep eutectic solvents and their mixtures with water. <i>Journal of Molecular Liquids</i> , 2021, 338, 116676.	2.3	13
8216	Rational design of AIE-based fluorescent probes for hypochlorite detection in real water samples and live cell imaging. <i>Journal of Hazardous Materials</i> , 2021, 418, 126243.	6.5	47
8217	Complexes of criegee intermediate CH_2OO with CO , CO_2 , H_2O , SO_2 , NO_2 , CH_3OH , HCOOH and $\text{CH}_3\text{CH}_3\text{CO}$ molecules: A DFT study on bonding, energetics and spectra. <i>Computational and Theoretical Chemistry</i> , 2021, 1203, 113341.	1.1	5
8218	Adsorption performance of boron nitride nanomaterials as effective drug delivery carriers for anticancer drugs based on density functional theory. <i>Computational and Theoretical Chemistry</i> , 2021, 1203, 113360.	1.1	13
8219	Catalytic decomposition of N_2O on iron-embedded C_2N monolayer: A DFT study. <i>Materials Today Communications</i> , 2021, 28, 102585.	0.9	4
8220	A single palladium atom immerses in magnesium clusters: PdMg_n ($n = 2-20$) clusters DFT study. <i>New Journal of Physics</i> , 2021, 23, 103002.	1.2	14
8221	Organic Semiconductor Single Crystals for X-ray Imaging. <i>Advanced Materials</i> , 2021, 33, e2104749.	11.1	43

#	ARTICLE	IF	CITATIONS
8222	UV-fluorescence probe for detection Ni ²⁺ with colorimetric/spectral dual-mode analysis method and its practical application. <i>Bioorganic Chemistry</i> , 2021, 114, 105103.	2.0	43
8223	Benzothiazole-based chemosensor: a quick dip into its anion sensing mechanism. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, e4283.	0.9	2
8224	Evaluation of the excited state dynamics, photophysical properties, and the influence of donor substitution in a donor- π -acceptor system. <i>Journal of Molecular Modeling</i> , 2021, 27, 284.	0.8	34
8225	Photoregulated Morphological Transformation of Spiropyran Derivatives Achieving the Tunability of Interfacial Hydrophilicity. <i>Langmuir</i> , 2021, 37, 11170-11175.	1.6	6
8226	Neutral and charged thorium impurity in solid argon. <i>Physical Review A</i> , 2021, 104, .	1.0	2
8227	Exploration of experimental and theoretical properties of 5,5-dimethyl 3-amino-cyclohex-2-en-1-one (AMINE DIMEDONE) by DFT/TD-DFT with ethanol and DMSO as solvents and molecular docking studies. <i>Journal of Molecular Liquids</i> , 2021, 338, 116551.	2.3	40
8228	Predicting Solvent-Dependent Nucleophilicity Parameter with a Causal Structure Property Relationship. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4890-4899.	2.5	16
8229	Achieve 100% transmission via grafting hydroxyl groups on CNT nanomotors. <i>Current Applied Physics</i> , 2021, 29, 59-65.	1.1	3
8230	Accurate Modeling of Excitonic Coupling in Cyanine Dye Cy3. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7852-7866.	1.1	13
8231	Charge ρ -Skin Behavior of Gold Superatoms. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8713-8719.	2.1	10
8232	Role of the Weak Interactions during the 2,4,6-Trinitrophenol Detecting Process of a Fluorescein-Based Sensor. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7867-7875.	1.1	5
8233	Synergistic Dissociation and Trapping Effect to Promote Li ⁺ Ion Conduction in Polymer Electrolytes via Oxygen Vacancies. <i>Small</i> , 2021, 17, e2102039.	5.2	38
8234	Theoretical study on pentiptycene molecular brake: photoinduced isomerization and photoinduced electron transfer. <i>Journal of Molecular Modeling</i> , 2021, 27, 289.	0.8	0
8235	Octanuclear Organotin Copper Sulfide Cage [(RSnCu) ₄ (I ^{1/4} 3-S) ₈]·2CHCl ₃ (R ¹ =2-phenylazophenyl) Assembled using Intramolecular Coordination Approach: Synthesis, Structure and DFT-NBO-AIM Analysis. <i>Journal of Molecular Structure</i> , 2021, 1239, 130458.	1.8	6
8236	Synergistic desulfurization over graphitic N and enzyme-like Fe-N sites of Fe-N-C. <i>Chemical Engineering Journal</i> , 2022, 430, 132657.	6.6	20
8237	Bending for Better: Flexible Organic Single Crystals with Controllable Curvature and Curvature-Related Conductivity for Customized Electronic Devices. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 22424-22431.	7.2	38
8238	Molecular modeling and biological activity analysis of new organic-inorganic hybrid: 2-(3,4-dihydroxyphenyl) ethanaminium nitrate. <i>Journal of King Saud University - Science</i> , 2021, 33, 101616.	1.6	53
8239	Probing the structural and electronic properties of neutral and anionic strontium-doped magnesium clusters. <i>Computational Materials Science</i> , 2021, 197, 110605.	1.4	21

#	ARTICLE	IF	CITATIONS
8240	High performance SACs for HER process using late first-row transition metals anchored on graphyne support: A DFT insight. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 37814-37823.	3.8	49
8241	Molecular modeling study of structures, Hirschfield surface, NBO, AIM, RDG, IGM and 1HNMR of thymoquinone/hydroxypropyl- β -cyclodextrin inclusion complex from QM calculations. <i>Journal of Molecular Structure</i> , 2022, 1249, 131565.	1.8	19
8242	Introducing Secondary Acceptors into Conjugated Polymers to Improve Photocatalytic Hydrogen Evolution. <i>Macromolecules</i> , 2021, 54, 8839-8848.	2.2	31
8243	Transmetalation Reactions of Aromatic Dilithionickelole: Synthesis of Heterobimetallic Complexes Featuring Metalloles as Diene Ligands. <i>Chemistry - A European Journal</i> , 2021, 27, 15967-15972.	1.7	2
8244	π - π Noncovalent Interaction Involving 1,2,4- and 1,3,4-Oxadiazole Systems: The Combined Experimental, Theoretical, and Database Study. <i>Molecules</i> , 2021, 26, 5672.	1.7	32
8245	Molecular Cage-Mediated Radial Gradient Porous Sponge Nanofiber for Selective Adsorption of a Mustard Gas Simulant. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 47835-47844.	4.0	10
8246	Surface Local Polarization Induced by Bismuth δ -Oxygen Vacancy Pairs Tuning Non δ -Covalent Interaction for CO ₂ Photoreduction. <i>Advanced Energy Materials</i> , 2021, 11, 2102389.	10.2	109
8247	Electronic structure investigation of the stability, reactivity, NBO analysis, thermodynamics, and the nature of the interactions in methyl-substituted imidazolium-based ionic liquids. <i>Journal of Molecular Liquids</i> , 2021, 337, 116458.	2.3	68
8248	Solvent Effect on Excited-State Intramolecular Proton-Coupled Charge Transfer Reaction in Two Seven-Membered Ring Pyrrole-Indole Hydrogen Bond Systems. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11275-11284.	1.2	9
8249	Assessing citric acid-derived luminescent probes for pH and ammonia sensing: A comprehensive experimental and theoretical study. <i>Analytica Chimica Acta</i> , 2021, 1186, 339125.	2.6	6
8250	Atomistic insights into heterogeneous reaction of formic acid on mineral oxide particles. <i>Chemosphere</i> , 2022, 287, 132430.	4.2	6
8251	Theoretical study of the adsorption of BMSF-BENZ drug for osteoporosis disease treatment on Al-doped carbon nanotubes (Al-CNT) as a drug delivery vehicle. <i>European Journal of Chemistry</i> , 2021, 12, 314-322.	0.3	12
8252	Irradiation δ -Wavelength Directing Circularly Polarized Luminescence in Self δ -Organized Helical Superstructures Enabled by Hydrogen δ -Bonded Chiral Fluorescent Molecular Switches. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 27158-27163.	7.2	66
8253	Spectroscopically Guided Simulations Reveal Distinct Strategies for Positioning Substrates to Achieve Selectivity in Nonheme Fe(II)/ β -Ketoglutarate-Dependent Halogenases. <i>ACS Catalysis</i> , 2021, 11, 12394-12408.	5.5	20
8254	Computational and theoretical study of graphitic carbon nitride (g-C ₃ N ₄) as a drug delivery carrier for lonidamine drug to treat cancer. <i>Computational and Theoretical Chemistry</i> , 2021, 1206, 113459.	1.1	10
8255	Molecular conformation dependence of phosphorescence lifetime in organic aggregates. <i>Dyes and Pigments</i> , 2021, 193, 109520.	2.0	11
8256	Exploring an aggregation induced emission behaviour of neutral iridium complexes consisting of salicylaldimine ligand with dibenzosuberane core. <i>Journal of Organometallic Chemistry</i> , 2021, 949, 121954.	0.8	2
8257	Ultrasound-assisted theophylline polymorphic transformation: Selective polymorph nucleation, molecular mechanism and kinetics analysis. <i>Ultrasonics Sonochemistry</i> , 2021, 77, 105675.	3.8	7

#	ARTICLE	IF	CITATIONS
8258	Intermolecular weak interaction of imidacloprid investigated by terahertz spectroscopy and theoretical calculation. <i>Optik</i> , 2021, 241, 167063.	1.4	2
8259	Metal-Involving Chalcogen Bond. The Case of Platinum(II) Interaction with Se/Te-Based π -Hole Donors. <i>Journal of the American Chemical Society</i> , 2021, 143, 15701-15710.	6.6	28
8260	Effects of functionalization of Y6 end-groups with electron-withdrawing groups on the photovoltaic properties at the donor-acceptor interfaces of PM6/Y6 OSCs: A theoretical insight. <i>Organic Electronics</i> , 2021, 96, 106235.	1.4	12
8261	Methane conversion by transition metal-doped vanadium oxide clusters. <i>Chemical Physics Letters</i> , 2021, 779, 138829.	1.2	5
8262	Can the Antivirals Remdesivir and Favipiravir Work Better Jointly? In Silico Insights. <i>Drug Research</i> , 2022, 72, 34-40.	0.7	6
8263	Effect of formic-acid-to-acetic-acid ratio on the structure and spinnability of aqueous aluminium sol of alumina fibre. <i>Ceramics International</i> , 2021, 47, 26034-26041.	2.3	10
8264	Mechanism of reactivation of the peroxidase catalytic activity of human cyclooxygenases by reducing cosubstrate quercetin. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 107, 107941.	1.3	6
8265	Breaking Classic Heavy-Atom Effect to Achieve Heavy-Atom-Induced Dramatic Emission Enhancement of Silole-Based AlEgens with Through-Bond and Through-Space Conjugation. <i>Advanced Optical Materials</i> , 2021, 9, 2101228.	3.6	18
8266	Light-Activated Biodegradable Covalent Organic Framework-Integrated Heterojunction for Photodynamic, Photothermal, and Gaseous Therapy of Chronic Wound Infection. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 42396-42410.	4.0	59
8267	Molecular Insights on the Dihydrogen Bond Properties of Metal Borohydride Complexes upon Ammoniation. <i>ECS Journal of Solid State Science and Technology</i> , 2021, 10, 091006.	0.9	1
8268	Variational tight-binding method for simulating large superconducting circuits. <i>Physical Review Research</i> , 2021, 3, .	1.3	2
8269	Umpolung Strategy for Arene C-H Etherification Leading to Functionalized Chromanes Enabled by I(III) π -Ligated Hypervalent Iodine Reagents. <i>Advanced Synthesis and Catalysis</i> , 2021, 363, 4867-4875.	2.1	4
8270	Copper(II)-Mediated Iodination of 1-Nitroso-2-naphthol. <i>Molecules</i> , 2021, 26, 5708.	1.7	1
8271	Theoretical Insight into $20d$ -Electron Transition Metal Complexes ($C_{5v}H_{5v}O_2TM(E_1E_2)_{22}$) ($TM = Cr, Tj, ET, Qq, 1, 0, 7, 8$) Bonding Nature. <i>Physica Status Solidi (B): Basic Research</i> , 2021, 258, 2100417.	0.7	1
8272	Study of the Ribavirin drug adsorption on the surfaces of carbon nanotube and graphene nanosheet using density functional theory calculations. <i>Bulletin of the Korean Chemical Society</i> , 2021, 42, 1446-1457.	1.0	6
8273	Comprehensive in silico study on lithiated Triazine isomers and its H ₂ storage efficiency. <i>Journal of the Indian Chemical Society</i> , 2021, 98, 100134.	1.3	5
8274	Distorted Copper(II) Complex with Unusually Short CF ₃ -Cu Distances. <i>Inorganic Chemistry</i> , 2021, 60, 14759-14764.	1.9	1
8275	Way to Enforce Selectivity via Steric Hindrance: Improvement of Am(III)/Eu(III) Solvent Extraction by Loaded Diphosphonic Acid Esters. <i>Inorganic Chemistry</i> , 2021, 60, 14563-14581.	1.9	22

#	ARTICLE	IF	CITATIONS
8276	Synthesis and Tetraphenylethylene-Based Aggregation-Induced Emission Probe for Rapid Detection of Nitroaromatic Compounds in Aqueous Media. <i>ACS Omega</i> , 2021, 6, 25447-25460.	1.6	42
8277	Development of ketoprofen-p-aminobenzoic acid co-crystal: formulation, characterization, optimization, and evaluation. <i>Medicinal Chemistry Research</i> , 2021, 30, 2090.	1.1	3
8278	Aqueous picloram degradation by hydroxyl radicals: Unveiling mechanism, kinetics, and ecotoxicity through experimental and theoretical approaches. <i>Chemosphere</i> , 2021, 278, 130401.	4.2	15
8279	Synthesis and Characterization of Bis[$(\text{R}^1\text{O})_2\text{Ti}(\text{R}^2)_2$] (X = H, CH_3 , O , Br) with Symmetry- and Distance-Dependent Vibrational Circular Dichroism Enhancement and Sign Inversion. <i>Inorganic Chemistry</i> , 2021, 60, 14116-14131.	1.9	10
8280	Computational Study on the Mechanisms and Origins of Selectivity in Hydroarylation of 1,3-Diyne Alcohol Catalyzed by Di- and Mononuclear Manganese Complexes. <i>Organometallics</i> , 2021, 40, 3124-3135.	1.1	5
8281	Novel Donor-Acceptor Framework for Higher Charge Transfer and Distance of Charge Transfer through Dipole Engineering. <i>Journal of Physical Chemistry C</i> , 2021, 125, 20219-20229.	1.5	1
8282	Conversion of dinitrogen to ammonia by rhenium doped graphyne. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 33409-33419.	3.8	5
8283	Solubility and thermodynamic properties of flonicamid in pure and binary solvents in the temperature range of 283.15–323.15 K. <i>Journal of Molecular Liquids</i> , 2021, 337, 116233.	2.3	8
8284	Membrane-active La(III) and Ce(III) complexes as potent antibacterial agents: synthesis, characterization, in vitro, in silico, and in vivo studies. <i>Journal of Molecular Structure</i> , 2022, 1249, 131595.	1.8	5
8285	Computational, spectroscopic, Hirshfeld surface, electronic state and molecular docking studies on phthalic anhydride. <i>Journal of Molecular Structure</i> , 2022, 1249, 131571.	1.8	21
8286	Biomimetic Recognition of Quinones in Water by an Endo-Functionalized Cavity with Anthracene Sidewalls. <i>Angewandte Chemie</i> , 0, , .	1.6	7
8287	Revisiting the electronic nature of nanodiamonds. <i>Diamond and Related Materials</i> , 2021, 120, 108627.	1.8	7
8288	Synthesis and characterization of pyrazole- and imidazole- derived energetic compounds featuring ortho azido/nitro groups. <i>FirePhysChem</i> , 2022, 2, 140-146.	1.5	7
8289	Role of O Substitution in Expanded Porphyrins on Uranyl Complexation: Orbital- and Density-Based Analyses. <i>Inorganic Chemistry</i> , 2021, 60, 15351-15363.	1.9	7
8290	Thermal Decomposition Mechanism and Energy Release Law of Novel Cyclo- N_5 -Based Nitrogen-Rich Energetic Salt. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9489-9494.	1.1	8
8291	Pnictogen effects on the electronic interactions in the Lewis pair complexes $\text{Ph}_3\text{EB}(\text{C}_6\text{F}_5)_3$ (E = P, As). <i>Journal of Physical Chemistry A</i> , 2021, 125, 9489-9494.	1.08	4
8292	Benchmark Force Fields for the Molecular Dynamic Simulation of G-Quadruplexes. <i>Molecules</i> , 2021, 26, 5379.	1.7	12
8293	Robust fluorogenic non-porphyrin interaction of Zn(II) and Hg(II) naphthadiazacrown macrocyclic complexes with C60: Spectroscopic and dispersion-corrected DFT study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 418, 113414.	2.0	4

#	ARTICLE	IF	CITATIONS
8294	Dithiocarbamate modified glucose as a novel eco-friendly corrosion inhibitor for copper in sodium chloride media. <i>Sustainable Chemistry and Pharmacy</i> , 2021, 22, 100488.	1.6	12
8295	In Silico Studies on Selected Neutral Molecules, CGa ₂ Ge ₂ , AlGaGe ₂ , and CSiGa ₂ Ge Containing Planar Tetracoordinate Carbon. <i>Atoms</i> , 2021, 9, 65.	0.7	16
8296	Copper(II) Prevents the Saccharine-Dialkylcyanamide Coupling by Forming Mononuclear (Saccharinate)(Dialkylcyanamide)copper(II) Complexes. <i>Inorganics</i> , 2021, 9, 69.	1.2	0
8297	Efficient and stable deep-blue narrow-spectrum electroluminescence based on hybridized local and charge-transfer (HLCT) state. <i>Dyes and Pigments</i> , 2021, 193, 109482.	2.0	28
8298	Insights into the photocatalytic peroxymonosulfate activation over defective boron-doped carbon nitride for efficient pollutants degradation. <i>Journal of Hazardous Materials</i> , 2021, 418, 126338.	6.5	37
8299	Possible coordination modes of copper(II) atom in model silsesquioxanes complexes at various pH conditions: DFT study. <i>Chemical Physics Letters</i> , 2021, 778, 138739.	1.2	2
8300	Insight into molecular interactions between condensed aromatics in high-temperature coal tar and organic solvents by combining experimental, density functional theory, and molecular dynamics. <i>Fuel</i> , 2021, 300, 120942.	3.4	9
8301	An in-depth DFT insight into the mechanism of NHC-catalyzed generation of p-quinodimethanes: Investigation the role of NHC and different substituents on μ -functionalization. <i>Computational and Theoretical Chemistry</i> , 2021, 1203, 113350.	1.1	3
8302	Designing of benzodithiophene (BDT) based non-fullerene small molecules with favorable optoelectronic properties for proficient organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2021, 1203, 113359.	1.1	49
8303	Enhancing the electrocatalytic activity of Fe phthalocyanines for the oxygen reduction reaction by the presence of axial ligands: Pyridine-functionalized single-walled carbon nanotubes. <i>Electrochimica Acta</i> , 2021, 398, 139263.	2.6	27
8304	Novel Oxidovanadium Complexes with Redox-Active R-Mian and R-Bian Ligands: Synthesis, Structure, Redox and Catalytic Properties. <i>Molecules</i> , 2021, 26, 5706.	1.7	26
8305	Intermolecular Forces Driving Hexamethylenetetramine Co-Crystal Formation, a DFT and XRD Analysis. <i>Molecules</i> , 2021, 26, 5746.	1.7	1
8306	Modulation of mechanofluorochromism based on carboxylic acid esters compounds bearing triphenylamine and pyrene with different substituents. <i>Journal of Luminescence</i> , 2022, 241, 118495.	1.5	6
8307	Effect of External Electric Field on Tetrel Bonding Interactions in (FTF ₃) ⁺ ⋯(FH) Complexes (T) Tj ETQq _{1.6} 0.784314 rgBT / 9	1.6	9
8308	Molecular modelling of two coordination states of Zn(II) ion at the active site of human carbonic anhydrase II. <i>Chemical Physics</i> , 2021, 549, 111281.	0.9	3
8309	Naphthyridine derived colorimetric and fluorescent turn off sensors for Ni ²⁺ in aqueous media. <i>Scientific Reports</i> , 2021, 11, 19242.	1.6	11
8310	Ozone oxidation of 2,4,6-TCP in the presence of halide ions: Kinetics, degradation pathways and toxicity evaluation. <i>Chemosphere</i> , 2022, 288, 132343.	4.2	14
8311	Synthesis and Properties of Symmetric Glycerol-Derived 1,2,3-Triethers and 1,3-Diether-2-Ketones for CO ₂ Absorption. <i>Chemical Engineering Science</i> , 2021, 248, 117150.	1.9	9

#	ARTICLE	IF	CITATIONS
8312	Reveal Brønsted–Evans–Polanyi relation and attack mechanisms of reactive oxygen species for photocatalytic H ₂ O ₂ production. <i>Applied Catalysis B: Environmental</i> , 2022, 301, 120757.	10.8	50
8313	Boosting hydrogen evolution over Ni ₆ (SCH ₂ Ph) ₁₂ nanocluster modified TiO ₂ via pseudo-Z-scheme interfacial charge transfer. <i>Applied Catalysis B: Environmental</i> , 2021, 292, 120158.	10.8	18
8314	Probing Limits of a C=C Bond Activation by π -Coordinated Organopnictogen(II) Compounds. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 4030-4041.	1.0	7
8315	BF ₃ -catalyzed oxa-Diels–Alder reaction of ethyl vinyl sulfide and β -methyl- α -phenylacrolein: a molecular electron density theory study. <i>Monatshefte für Chemie</i> , 2021, 152, 1209-1221.	0.9	6
8316	Sustainable afterglow materials from lignin inspired by wood phosphorescence. <i>Cell Reports Physical Science</i> , 2021, 2, 100542.	2.8	21
8317	Charge Transfer Mechanisms Regulated by the Third Component in Ternary Organic Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8982-8990.	2.1	17
8318	Estimation of ground and excited-state dipole moments of three symmetric carbocyanine dyes via the analysis of luminescence properties. <i>Journal of Molecular Liquids</i> , 2021, 337, 116476.	2.3	5
8319	Effect of the side-chain length and NLO properties of the N-ethyl-N,N,N-trialkylammonium ionic liquids – A DFT study. <i>Journal of Molecular Liquids</i> , 2021, 337, 116251.	2.3	1
8320	Tetrahedral Cyclopentadienylmetal Carbonyl Clusters of Manganese and Chromium: A Theoretical Study. <i>Inorganic Chemistry</i> , 2021, 60, 14557-14562.	1.9	0
8321	Examining a Transition from Supramolecular Halogen Bonding to Covalent Bonds: Topological Analysis of Electron Densities and Energies in the Complexes of Bromosubstituted Electrophiles. <i>ACS Omega</i> , 2021, 6, 23588-23597.	1.6	14
8322	Enhancing the Photoelectric Properties of Zinc Porphyrin Dyes by Introducing Five-Membered Heterocyclic Rings into the Electron Donor: A Density Functional Theory and Time-Dependent Density Functional Theory Study. <i>ACS Omega</i> , 2021, 6, 23551-23557.	1.6	6
8323	Bending for Better: Flexible Organic Single Crystals with Controllable Curvature and Curvature-Related Conductivity for Customized Electronic Devices. <i>Angewandte Chemie</i> , 2021, 133, 22598-22605.	1.6	22
8324	Cumene extraction separation from alkanes using DMSO: Influence of the alkane structure. <i>Fluid Phase Equilibria</i> , 2021, 550, 113236.	1.4	9
8325	Optimizing the Cosensitization Effect of SQ02 Dye on BP-2 Dye-Sensitized Solar Cells: A Computational Quantum Chemical Study. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5098-5116.	2.5	16
8326	Revisiting Dehydrothiopheno[12]annulenes: Synthesis, Electronic Properties, and Aromaticity. <i>Journal of Organic Chemistry</i> , 2021, 86, 13198-13211.	1.7	9
8327	Enhanced visible light photo-Fenton-like degradation of tetracyclines by expanded perlite supported FeMo ₃ Ox/g-C ₃ N ₄ floating Z-scheme catalyst. <i>Journal of Hazardous Materials</i> , 2022, 424, 127387.	6.5	83
8328	DFT Study of Microsolvated [NO ₃] ⁻ ·(H ₂ O) _n Clusters and Molecular Dynamics Simulation of Nitrate Solution. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8899-8906.	1.1	6
8329	Tunable copper complexes with functional ligands: A promising strategy for green primary explosives. <i>Chemical Engineering Journal</i> , 2022, 430, 132739.	6.6	12

#	ARTICLE	IF	CITATIONS
8330	<i>Pixel</i> calculations using <i>Orca</i> or <i>GAUSSIAN</i> for electron density automated within the <i>Oscail</i> package. <i>Journal of Applied Crystallography</i> , 2021, 54, 1535-1541.	1.9	4
8331	An ultrasensitive high-performance baicalin sensor based on C3N4-SWCNTs/reduced graphene oxide/cyclodextrin metal-organic framework nanocomposite. <i>Sensors and Actuators B: Chemical</i> , 2022, 350, 130853.	4.0	26
8332	Red emissive two-photon carbon dots: Photodynamic therapy in combination with real-time dynamic monitoring for the nucleolus. <i>Carbon</i> , 2021, 182, 155-166.	5.4	40
8333	Investigations of electronic and nonlinear optical properties of superalkali adsorbed biphenylene based sheets by first-principles calculations. <i>Optik</i> , 2021, 242, 166830.	1.4	4
8334	Stable Noble Gas Compounds Based on Superelectrophilic Anions [B ₁₂ (BO) ₁₁] ⁺ and [B ₁₂ (OBO) ₁₁] ⁺ . <i>ChemPhysChem</i> , 2021, 22, 2240-2246.	1.0	5
8335	Synthesis and Properties of ortho-t-BuSO ₂ C ₆ H ₄ -Substituted Iodonium Ylides. <i>Crystals</i> , 2021, 11, 1085.	1.0	4
8336	Promising small molecule Pechmann dye analogue donors with low interfacial charge recombination for photovoltaic application: A DFT study. <i>Materials Today Communications</i> , 2021, 28, 102555.	0.9	2
8337	Study on Chemical Bond Dissociation and the Removal of Oxygen-Containing Functional Groups of Low-Rank Coal during Hydrothermal Carbonization: DFT Calculations. <i>ACS Omega</i> , 2021, 6, 25772-25781.	1.6	3
8338	Sunlight-controlled CO ₂ separation resulting from a biomass-based CO ₂ absorber. <i>Green Energy and Environment</i> , 2022, 7, 566-574.	4.7	7
8339	Metal Coordinated Tri- and Tetraborane Analogues. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	3
8340	Synthesis, spectral characterization, DFT calculations, pharmacological studies, CT-DNA binding and molecular docking of potential N, O-multidentate chelating ligand and its VO(II), Zn(II) and ZrO(II) chelates. <i>Bioorganic Chemistry</i> , 2021, 114, 105106.	2.0	29
8341	The excited state behaviors of 3-(benzo[d]thiazol-2-yl)-2-hydroxy-5-methoxybenzaldehyde system in aprotic solvents. <i>Chemical Physics</i> , 2021, 549, 111280.	0.9	2
8342	The synthesis of the conjugated polymers based on phenanthroline-5,6-dione and thiophene derivatives, their composites with carbon and the lithium storage performances as anode materials. <i>Journal of Electroanalytical Chemistry</i> , 2021, 900, 115737.	1.9	4
8343	Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties. <i>ACS Omega</i> , 2021, 6, 24602-24613.	1.6	31
8344	Three-Dimensional Symmetry Decides the Description of the Energy of Charge-Transfer State in Organic Solar Cells. <i>ACS Applied Energy Materials</i> , 2021, 4, 8739-8744.	2.5	2
8345	Effect of COF Presence on DNA Molecular Interactions: A QM/MM and MD Simulations Study. <i>ChemistrySelect</i> , 2021, 6, 9541-9551.	0.7	3
8346	Systematical study on electronic properties of monoazaphenanthrene compounds. <i>Chemical Physics</i> , 2021, 552, 111370.	0.9	0
8347	Multi-scale stabilization mechanism of pickering emulsion gels based on dihydromyricetin/high-amylose corn starch composite particles. <i>Food Chemistry</i> , 2021, 355, 129660.	4.2	27

#	ARTICLE	IF	CITATIONS
8348	Reaction Dynamics Study of Hypergolic Bipropellants: Azide Amine and Dinitrogen Tetroxide. Propellants, Explosives, Pyrotechnics, 2021, 46, 1679-1686.	1.0	3
8349	Fluorine-free, blue-emitting cationic iridium complexes with a phenyl-triazole type cyclometalating ligand: Synthesis, characterizations and their use for efficient organic light-emitting diodes. Dyes and Pigments, 2021, 193, 109477.	2.0	6
8350	Catalytic ozonation for metoprolol and ibuprofen removal over different MnO ₂ nanocrystals: Efficiency, transformation and mechanism. Science of the Total Environment, 2021, 785, 147328.	3.9	68
8351	Using general computational chemistry strategy to unravel the reactivity of emerging pollutants: An example of sulfonamide chlorination. Water Research, 2021, 202, 117391.	5.3	13
8352	Perfluoro octanoic acid-modified magnetic hyperbranched polyamideamine as a sorbent for the extraction of fluorine-containing pesticides from water samples. Journal of Separation Science, 2021, 44, 3830-3839.	1.3	1
8353	Extraction of Noncondensed Lignin from Poplar Sawdusts with <i>p</i> -Toluenesulfonic Acid and Ethanol. Journal of Agricultural and Food Chemistry, 2021, 69, 10838-10847.	2.4	20
8354	Synthesis and characterization of tracers and development of a fluorescence polarization immunoassay for amantadine with high sensitivity in chicken. Journal of Food Science, 2021, 86, 4754-4767.	1.5	5
8355	Evolution of Electronic Structure of Cuboid Thiolate-Monolayer-Protected Gold Nanocrystals. Journal of Physical Chemistry C, 2021, 125, 20670-20675.	1.5	3
8356	Methyl Groups as Hydrogen Bond Acceptors via Their sp^3 Carbon Atoms. Crystal Growth and Design, 2021, 21, 5961-5966.	1.4	5
8357	Azepine- or Azocine-Embedded Hexabenzocoronene Derivatives as Nitrogen-Doped Saddle or Saddle-Helix Nanographenes. Angewandte Chemie, 2021, 133, 24683-24688.	1.6	3
8358	Synthesis, characterization, and computational survey of a novel material template <i>o</i> -xylylenediamine. Journal of the Iranian Chemical Society, 2022, 19, 1499-1514.	1.2	2
8359	A DFT investigation of the host-guest interactions between boron-based aromatic systems and β -cyclodextrin. Structural Chemistry, 2022, 33, 195-206.	1.0	8
8360	Quantitative Estimation of the Hydrogen-Atom-Donating Ability of 4-Substituted Hantzsch Ester Radical Cations. ACS Omega, 2021, 6, 23621-23629.	1.6	11
8361	Design, Synthesis, and <i>In Vitro</i> and <i>In Vivo</i> Evaluation of Novel Fluconazole-Based Compounds with Promising Antifungal Activities. ACS Omega, 2021, 6, 24981-25001.	1.6	11
8362	Engineering zwitterionic barrier by squaraine-based porous organic framework fiber for superior lithium-sulfur batteries. Electrochimica Acta, 2021, 397, 139276.	2.6	4
8363	Motivation of reactive oxidation species in peracetic acid by adding nanoscale zero-valent iron to synergic removal of spiramycin under ultraviolet irradiation: Mechanism and N-nitrosodimethylamine formation potential assessment. Water Research, 2021, 205, 117684.	5.3	22
8364	Computational study of therapeutic potential of phosphorene as a nano-carrier for drug delivery of nebulivolol for the prohibition of cardiovascular diseases: a DFT study. Journal of Molecular Modeling, 2021, 27, 306.	0.8	8
8365	Physical Mechanisms on Plasmon-Enhanced Organic Solar Cells. Journal of Physical Chemistry C, 2021, 125, 21301-21309.	1.5	36

#	ARTICLE	IF	CITATIONS
8366	Design and Synthesis of Nitrogen-Rich Azo-Bridged Furoxanylazoles as High-Performance Energetic Materials. <i>Chemistry - A European Journal</i> , 2021, 27, 14628-14637.	1.7	25
8367	Photodegradation, toxicity and density functional theory study of pharmaceutical metoclopramide and its photoproducts. <i>Science of the Total Environment</i> , 2022, 807, 150694.	3.9	11
8368	Vibrational, electronic and reactivity insight on (5-chloro-benzofuran-3-yl)-acetic acid hydrazide: A Spectroscopic and DFT approach. <i>Journal of Molecular Structure</i> , 2021, 1239, 130479.	1.8	11
8369	Artificial Intelligence Designer for Highly-Efficient Organic Photovoltaic Materials. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8847-8854.	2.1	15
8370	Prospects of co-poly(biquinoline-hydrazide-imide)s for separation of benzene-isopropanol mixture via pervaporation. <i>Journal of Applied Polymer Science</i> , 2022, 139, 51646.	1.3	4
8371	Theoretical and experimental comparison of the reactivity of the sulfanyl-closo-decaborate and sulfanyl-closo-dodecaborate anions and their mono-S-substituted derivatives. <i>Polyhedron</i> , 2021, 206, 115347.	1.0	5
8372	Characterization of nitrite degradation by polyphenols in sea buckthorn (<i>Hippophaë rhamnoides</i> L.) by density function theory calculations. <i>LWT - Food Science and Technology</i> , 2021, 149, 111884.	2.5	4
8373	Structures, relative stability, bond dissociation energies, and stabilization energies of alkynes and imines from a homodesmotic reaction. <i>Computational and Theoretical Chemistry</i> , 2021, 1203, 113329.	1.1	13
8374	Theoretical study of Au ₂₀ /WS ₂ composite material as a potential candidate for the capture of XO (X=C, N, S) gases. <i>Computational Condensed Matter</i> , 2021, 28, e00580.	0.9	4
8375	Hydrophilic carbon nanotube membrane enhanced interfacial evaporation for desalination. <i>Chinese Chemical Letters</i> , 2022, 33, 2155-2158.	4.8	33
8376	Mechanisms of Ssp ³ -H functionalization of thiolacetic acid: A density functional theory investigation. <i>Journal of Physical Organic Chemistry</i> , 0, , e4279.	0.9	3
8377	Quantum Chemical Calculation of the Effects of H ₂ O on Oxygen Functional Groups during Coal Spontaneous Combustion. <i>ACS Omega</i> , 2021, 6, 25594-25607.	1.6	9
8378	A Theoretical Insight of Cr Dopant in Tungsten Oxide for Gas Sensor Application. <i>Materials Today Communications</i> , 2021, 28, 102508.	0.9	6
8379	Structural Evolution, Electronic Structures, and Vibrational Properties of Anionic LuGe _n ($n = 5-17$) Clusters: From Lu-Linked to Lu-Encapsulated Configurations. <i>Inorganic Chemistry</i> , 2021, 60, 14446-14456.	1.9	10
8380	Theoretical insight into actinide monometallofullerene Th@C ₇₄ with four-electron-transfer characteristics. <i>Chemical Physics</i> , 2021, 549, 111258.	0.9	2
8381	Theoretical studies of azete based high energy density materials with trinitromethane functional group. <i>Computational and Theoretical Chemistry</i> , 2021, 1203, 113346.	1.1	3
8382	Structural proof of a [C ⁺ F ⁻ C] ⁺ fluoronium cation. <i>Nature Communications</i> , 2021, 12, 5275.	5.8	9
8383	Crystal structures, luminescence, and DFT study of mixed-ligand Zn(II) and Cd(II) complexes with phenyl-containing benzimidazole derivatives with linker C N or N N group. <i>Journal of Luminescence</i> , 2021, 237, 118156.	1.5	25

#	ARTICLE	IF	CITATIONS
8384	Switching of second-order nonlinear response effected by different acceptors: The impacts of environment and frequency dispersion. <i>Dyes and Pigments</i> , 2021, 193, 109502.	2.0	7
8385	How procyanidin C1 sticks to collagen: The role of proline rings. <i>Biophysical Chemistry</i> , 2021, 276, 106627.	1.5	6
8386	Quantum chemical calculations on dissolution of dimethylformamide in ethaline. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 107, 107966.	1.3	3
8387	Structural, surface, and computational analysis of two vitamin-B1 crystals with sulfonimide-based anions. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2021, .	0.4	0
8388	Introducing thiophene and benzothiadiazole groups in triphenylamine-based organic dyes with rigidly fused π -bridge to design high-efficiency solar cells: A theoretical investigation. <i>Solar Energy</i> , 2021, 225, 323-332.	2.9	10
8389	Theoretical research on molecular motors based on 4,5-diazafluorenyl coordination motifs. <i>Journal of Physical Organic Chemistry</i> , 0, , e4277.	0.9	0
8390	3D Hydrazone-Functionalized Covalent Organic Frameworks as pH-Triggered Rotary Switches. <i>Small</i> , 2021, 17, e2102630.	5.2	32
8391	Visualizing Correlation Regions: The Case of the Ammonia Crystal. <i>Chemistry Methods</i> , 0, , .	1.8	2
8392	Os ^{B9} : An Aromatic Osmium-Centered Monocyclic Boron Ring. <i>Frontiers in Chemistry</i> , 2021, 9, 751482.	1.8	1
8393	Anti-Metatype Antibody Screening, Sandwich Immunoassay Development, and Structural Insights for β -Lactams Based on Penicillin Binding Protein. <i>Molecules</i> , 2021, 26, 5569.	1.7	2
8394	Thermochemiluminescence-Based Sensitive Probes: Synthesis and Photophysical Characterization of Acridine-Containing 1,2-dioxetanes Focusing on Fluorophore Push-Pull Effects. <i>ChemPhotoChem</i> , 2022, 6, .	1.5	2
8395	Measurement and comprehensive analysis of the solubility of abacavir in twelve pure solvents. <i>Journal of Molecular Liquids</i> , 2021, 338, 116603.	2.3	7
8396	A pH dependent sulfate formation mechanism caused by hypochlorous acid in the marine atmosphere. <i>Science of the Total Environment</i> , 2021, 787, 147551.	3.9	4
8397	Synthesis, characterization, X-ray structural analysis, DFT and BSA binding study of a Zn(II) complex, [Zn(II)Cl ₂ (nia) ₂]. <i>Journal of Coordination Chemistry</i> , 2021, 74, 2741-2763.	0.8	4
8398	Exploration of Structural insights, spectroscopic assignments of 4-amino-6-methyl-3-thioxo-3,4-dihydro-1,2,4-triazin-5(2H) one. <i>Journal of Molecular Structure</i> , 2021, , 131559.	1.8	1
8399	Designing Well-Organized Donor-Bridge-Acceptor Conjugated Systems Based on Cyclopentadithiophene as Donors in Bulk Heterojunction Organic Solar Cells: DFT-Based Modeling and Calculations. , 0, , .		0
8400	Irradiation-Wavelength Directing Circularly Polarized Luminescence in Self-Organized Helical Superstructures Enabled by Hydrogen Bonded Chiral Fluorescent Molecular Switches. <i>Angewandte Chemie</i> , 0, , .	1.6	6
8401	Delineating Conformation Control in the Photophysical Behaviour of a Molecular Donor-Acceptor-Donor Triad. <i>ChemPhysChem</i> , 2021, 22, 2297-2304.	1.0	6

#	ARTICLE	IF	CITATIONS
8402	2Châ€“2N Square Chalcogen Bonds between Pairs of Radicals: A Case Study of 1,2,3,5-Dichalcogenadiazolyl Derivatives. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8572-8580.	1.1	4
8403	Effect of the Pyrrolic Nitrogen Functional Group in the Selective Adsorption of CO ₂ : GCMC, MD, and DFT Studies. <i>Energy & Fuels</i> , 2021, 35, 15918-15934.	2.5	19
8404	Theaflavin binds to a druggable pocket of TMEM16A channel and inhibits lung adenocarcinoma cell viability. <i>Journal of Biological Chemistry</i> , 2021, 297, 101016.	1.6	18
8405	Theoretical insights into CO ₂ /N ₂ selectivity of the porous ionic liquids constructed by ion-dipole interactions. <i>Journal of Molecular Liquids</i> , 2021, 344, 117676.	2.3	21
8406	Synthesis, Structural Characterizations, and Quantum Chemical Investigations on 1-(3-Methoxy-phenyl)-3-naphthalen-1-yl-propenone. <i>ACS Omega</i> , 2021, 6, 25982-25995.	1.6	16
8407	Theoretical studies on new family of bridged difurazan derivatives with excellent heat of formation. <i>Journal of the Chinese Chemical Society</i> , 0, , .	0.8	0
8408	Unraveling the Bonding Nature Along the Photochemically Activated Paternoâ€“Bâ€“chi Reaction Mechanism. <i>ChemPhysChem</i> , 2021, 22, 2342-2351.	1.0	11
8409	Azepineâ€“or Azocineâ€“Embedded Hexabenzocoronene Derivatives as Nitrogenâ€“Doped Saddle or Saddleâ€“Helix Nanographenes. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24478-24483.	7.2	26
8410	A Novel Phosphorescent Iridium(III) Complex Bearing Formamide for Quantitative Fluorine Anion Detection. <i>Crystals</i> , 2021, 11, 1190.	1.0	6
8411	Plant Sterol Clustering Correlates with Membrane Microdomains as Revealed by Optical and Computational Microscopy. <i>Membranes</i> , 2021, 11, 747.	1.4	4
8412	Toward Controlled Syntheses of Diphosphine-Protected Homochiral Gold Nanoclusters through Precursor Engineering. <i>ACS Nano</i> , 2021, 15, 16019-16029.	7.3	40
8413	Theoretical exploration in the substituent effect on photophysical properties and excited-state intramolecular proton transfer process of benzo[a]imidazo[5,1,2-cd]indolizines. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 422, 113570.	2.0	9
8414	Experimental and theoretical insights into the enhanced intramolecular charge transfer fluorescence of a 3(2H)-furanone based d-â€“A compounds tailored with dialkyl chains. <i>Journal of Molecular Structure</i> , 2021, 1239, 130500.	1.8	2
8415	Cr(VI) removal by cellulose-based composite adsorbent with a double-network structure. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 625, 126963.	2.3	18
8416	Orange-red emissive N-heterocycle carbene (NHC) Cu(I) complexes bearing benzimidazolylidene-type ligands: Synthesis, structures, and photophysical properties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 418, 113370.	2.0	8
8417	Theoretical studies on phthalimide-based efficient thermally activated delayed fluorescence emitters. <i>Chemical Physics Letters</i> , 2021, 778, 138750.	1.2	4
8418	Oxygen defective titanate nanotubes induced by iron deposition for enhanced peroxymonosulfate activation and acetaminophen degradation: Mechanisms, water chemistry effects, and theoretical calculation. <i>Journal of Hazardous Materials</i> , 2021, 418, 126180.	6.5	33
8419	Photoinduced charge transfer in one-photon and two-photon absorption of C ₂ N: Effects of edge-modified with oxygenated groups. <i>Chemical Physics Letters</i> , 2021, 778, 138810.	1.2	3

#	ARTICLE	IF	CITATIONS
8420	Insight into the adsorption of Imidazolium-based ionic liquids on graphene by first principles simulation. <i>Journal of Molecular Liquids</i> , 2021, 338, 116641.	2.3	18
8421	Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Iron-Sulfur Clusters. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5684-5703.	2.3	25
8422	Detection of Heavy Metals in Water Using Graphene Oxide Quantum Dots: An Experimental and Theoretical Study. <i>Molecules</i> , 2021, 26, 5519.	1.7	7
8423	Electronic structure, stability, and cooperativity of chalcogen bonding in sulfur dioxide and hydrated sulfur dioxide clusters: a DFT study and wave functional analysis. <i>Structural Chemistry</i> , 2022, 33, 179-193.	1.0	8
8424	Structural and electronic analysis of bimetallic thiolate complexes of group-5 transition metal ions. <i>Journal of Organometallic Chemistry</i> , 2021, 949, 121943.	0.8	3
8425	Absorption performance and reaction mechanism study on a novel anhydrous phase change absorbent for CO ₂ capture. <i>Chemical Engineering Journal</i> , 2021, 420, 129897.	6.6	27
8426	Mechanisms, challenges, and opportunities of dual Ni-photoredox-catalyzed C(sp ²)-C(sp ³) cross-couplings. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, e1573.	6.2	20
8427	Donor-Acceptor Pairs in Covalent Organic Frameworks Promoting Electron Transfer for Metal-Free Photocatalytic Organic Synthesis. <i>Langmuir</i> , 2021, 37, 11535-11543.	1.6	32
8428	Ultra-stable anti-counterfeiting materials inspired by water stains. <i>Cell Reports Physical Science</i> , 2021, 2, 100571.	2.8	8
8429	A new series of asymmetric bis-isatin derivatives containing urea/thiourea moiety: Preparation, spectroscopic elucidation, antioxidant properties and theoretical calculations. <i>Journal of Molecular Structure</i> , 2021, 1239, 130495.	1.8	19
8430	Color-Tunable Long-Lived Room-Temperature Phosphorescence in a Coordination Polymer Based on a Nonaromatic Ligand and Its Phosphor/Coordination Polymer-Doped Systems. <i>Chemistry of Materials</i> , 2021, 33, 7272-7282.	3.2	19
8431	PCage: Fluorescent Molecular Temples for Binding Sugars in Water. <i>Journal of the American Chemical Society</i> , 2021, 143, 15688-15700.	6.6	23
8432	Benzylidene ketones as visible light radical photoinitiator: The effects of electron-donating group and co-initiator. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 418, 113395.	2.0	15
8433	A smart chitosan nonwoven fabric coated with coumarin-based fluorophore for selective detection and efficient adsorption of mercury (II) in water. <i>Sensors and Actuators B: Chemical</i> , 2021, 342, 130064.	4.0	27
8434	Al-decorated C ₂₄ N ₂₄ fullerene: A robust single-atom catalyst for CO oxidation. <i>Polyhedron</i> , 2021, , 115497.	1.0	5
8435	Improving the Photocatalytic Hydrogen Generation Using Nonaggregated Zinc Phthalocyanines. <i>ACS Applied Energy Materials</i> , 2021, 4, 10222-10233.	2.5	9
8436	PCDTBT ₈ -Doped PffBT ₄ T ₂ OD ₂ -Based Ternary Solar Cells with Enhanced Open-Circuit Voltage, Fill Factor, and Charge Separation Efficiency. <i>Solar Rrl</i> , 2021, 5, 2100670.	3.1	16
8437	Effect of Al- and Ga-doping on the adsorption of H ₂ onto the outer surface of boron nitride nanotube: a DFT study. <i>Comptes Rendus Chimie</i> , 2021, 24, 291-304.	0.2	12

#	ARTICLE	IF	CITATIONS
8438	Nano zero valent iron encapsulated in graphene oxide for reducing uranium. <i>Chemosphere</i> , 2021, 278, 130229.	4.2	23
8439	Effect of hybridized local and charge transfer molecules rotation in excited state on exciton utilization. <i>Scientific Reports</i> , 2021, 11, 17686.	1.6	1
8440	Multipath elimination of bisphenol A over bifunctional polymeric carbon nitride/biochar hybrids in the presence of persulfate and visible light. <i>Journal of Hazardous Materials</i> , 2021, 417, 126008.	6.5	35
8441	Hydrosulfide (HS ⁻) Recognition and Sensing in Water by Halogen Bonding Hosts. <i>Angewandte Chemie</i> , 0, , .	1.6	5
8442	Density Functional Theory Study of Ultrashort Metal–Metal Distances in Diberyllium Complexes Bearing Carbene Ligands. <i>ChemistrySelect</i> , 2021, 6, 8596-8602.	0.7	1
8443	A strong acid-resistant flavanthrone with excellent photophysical properties. <i>Journal of Molecular Liquids</i> , 2021, 337, 116414.	2.3	5
8444	SERS Chemical Enhancement of 2,4,5-Trichlorophenoxyacetic Acid Adsorbed on Silver Substrate. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8529-8541.	1.1	14
8445	Fullerene–phosphorene nanoflake nanostructures: Modulation of their interaction mechanisms and electronic properties through the size of carbon fullerenes. <i>Carbon</i> , 2021, 182, 354-365.	5.4	5
8446	The Influence of Single-Atom Fe ^{2+/3+} /N ₄ Spin State on the Electroreduction of CO ₂ to CO/HCOOH by Analyzing Proton/Electron Transfer Mechanisms and Free Energy Evolutions. <i>Journal of Physical Chemistry C</i> , 2021, 125, 21460-21470.	1.5	8
8447	Strength analysis of noncovalent interactions between lignite and direct liquefaction solvents: A joint study of DFT calculations and swelling ratio determination. <i>Fuel</i> , 2021, 299, 120920.	3.4	11
8448	Synthesis, spectroscopic characterization, structural studies, thermal analysis and molecular docking of <i>N</i> -(2-methyl-5-nitrophenyl)-4-(pyridin-2-yl)pyrimidin-2-amine, a precursor for drug design against chronic myeloid leukemia. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 621-632.	0.2	0
8449	Hydrosulfide (HS ⁻) Recognition and Sensing in Water by Halogen Bonding Hosts. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24048-24053.	7.2	15
8450	Biomimetic Recognition of Quinones in Water by an Endo-Functionalized Cavity with Anthracene Sidewalls. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 25981-25987.	7.2	24
8451	Electronic Structures and Properties of Actinide–Bimetal Compounds An ₂ O ₂ (An=Th to Cf) and U ₂ E ₂ (E=N, F, S). <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3926.	1.0	5
8452	Van der Waals enhanced interfacial interaction in cellulose/zinc oxide nanocomposite coupled by graphitic carbon nitride. <i>Carbohydrate Polymers</i> , 2021, 268, 118235.	5.1	17
8453	Theoretical and photovoltaic investigations of 1,3,5-triazine-based photosensitizers achieving highly efficient DSSCs. <i>Synthetic Metals</i> , 2021, 280, 116882.	2.1	7
8454	Whether the combination of AIE and TADF functional groups produces AIE-type TADF? –A theoretical study on the synergistic effect of TPE and carbazole donor group/thianthrene-tetraoxide acceptor group. <i>Dyes and Pigments</i> , 2021, 194, 109547.	2.0	10
8455	The stacking induced organic room temperature phosphorescence: A compact weak interaction mechanism. <i>Chemical Physics Letters</i> , 2021, 780, 138904.	1.2	1

#	ARTICLE	IF	CITATIONS
8456	Quantum chemical descriptors in quantitative structure–activity relationship models and their applications. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 217, 104384.	1.8	30
8457	Freestanding 3-dimensional macro-porous SnO ₂ electrodes for efficient electrochemical degradation of antibiotics in wastewater. <i>Chemical Engineering Journal</i> , 2021, 422, 130032.	6.6	49
8458	Predicting phase-splitting behaviors of an amine-organic solvent–water system for CO ₂ absorption: A new model developed by density functional theory and statistical and experimental methods. <i>Chemical Engineering Journal</i> , 2021, 422, 130389.	6.6	14
8459	Tuning the Computational Evaluation of Spectroscopic, ELF, LOL, NCI analysis and Molecular Docking of Novel Anti COVID-19 Molecule 4-Dimethylamino Pyridinium 3, 5-Dichlorosalicylate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 259, 119907.	2.0	21
8460	Sorption mechanism of organic dyes on a novel self-nitrogen-doped porous graphite biochar: Coupling DFT calculations with experiments. <i>Chemical Engineering Science</i> , 2021, 242, 116739.	1.9	47
8461	Atomistic insights into heterogeneous reaction of hydrogen peroxide on alumina particles: Combining DFT calculation and ReaxFF molecular dynamics simulations. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 626, 127064.	2.3	2
8462	A citrate-loaded nano-zero-valent iron heterogeneous Fenton system for steroid estrogens degradation under different acidity levels: The effects and mechanisms. <i>Chemical Engineering Journal</i> , 2021, 421, 129967.	6.6	7
8463	Theoretical design study on the origin of the improved phosphorescent efficiency of DPEphos quinoline-substituted derivatives for OLEDs. <i>Organic Electronics</i> , 2021, 97, 106185.	1.4	1
8464	Fluorescence enhancement mechanism of thymolphthalein-based probe by coordination interaction with zinc ion. <i>Journal of Molecular Liquids</i> , 2021, 339, 116275.	2.3	3
8465	Theoretical study on the mechanism of C N and C C coupling to form indole catalyzed by Pd(OAc) ₂ . <i>Molecular Catalysis</i> , 2021, 515, 111895.	1.0	4
8466	Intermolecular interactions in microhydrated ribonucleoside and deoxyribonucleoside: A computational study. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113422.	1.1	4
8467	Theoretical evaluation of central ring doped Hexa-peri-hexabenzocoronene as Gamma-butyrolactone drug sensors. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113412.	1.1	0
8468	Proton transfer reaction of the formamide and its derivatives characterized via the Kohn–Sham potential. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113385.	1.1	0
8469	Quantum chemical exploration on the inhibition performance of indole and some of its derivatives against copper corrosion. <i>Journal of Molecular Liquids</i> , 2021, 340, 117136.	2.3	11
8470	DABCO-mediated [4+4]-domino annulation reactions of ynones and α -cyano- β -unsaturated ketones: Mechanisms and the role of DABCO. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113396.	1.1	2
8471	Highly efficient and reversible low-concentration SO ₂ absorption in flue gas using novel phosphonium-based deep eutectic solvents with different substituents. <i>Journal of Molecular Liquids</i> , 2021, 340, 117228.	2.3	18
8472	Catalytic oxidation of NO to NO ₂ on pure and doped AuPt _{3-n} (n=0–3) clusters: A DFT perspective. <i>Molecular Catalysis</i> , 2021, 515, 111910.	1.0	4
8473	[1,2,4]Triazolo[4,3-b]pyridazine as a building block towards low-sensitivity high-energy materials. <i>Chemical Engineering Journal</i> , 2021, 421, 129635.	6.6	42

#	ARTICLE	IF	CITATIONS
8474	Thermal hazard and pyrolysis mechanism of tetrazolo[1,5-a]pyridine by TG, DSC, ARC, TG-MS and DFT methods. <i>Journal of Analytical and Applied Pyrolysis</i> , 2021, 159, 105299.	2.6	19
8475	First principle calculation of nonlinear optical response of (D/L)-Alanine in chiral carbon nanotube. <i>Carbon</i> , 2021, 183, 820-829.	5.4	6
8476	Experimental and DFT research on role of sodium in NO reduction on char surface under H ₂ O/Ar atmosphere. <i>Fuel</i> , 2021, 302, 121105.	3.4	13
8477	The effect of oxygen-containing functional groups on formaldehyde adsorption in solution on carbon surface: A density functional theory study. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 105987.	3.3	36
8478	Computational study of the electrostatic potential and charges of multivalent ionic liquid molecules. <i>Journal of Molecular Liquids</i> , 2021, 340, 117190.	2.3	9
8479	Molecular insights into the separation mechanism of imidazole-based ionic liquid supported membranes. <i>Journal of Molecular Liquids</i> , 2021, 340, 117173.	2.3	11
8480	Calculations and analyses of molecular features and properties of nitrogen / carbon tetrafluoride mixture. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113411.	1.1	6
8481	Theoretical investigation on influence of protic and aprotic solvents effect and structural (Monomer, Dimer), Van-der Waals and Hirshfeld surface analysis for clonidine molecule. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113397.	1.1	16
8482	Effect of tunable π - π bridge on two-photon absorption property and intramolecular charge transfer process of polycyclic aromatic hydrocarbons. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 259, 119830.	2.0	4
8483	Selective spectrophotometric determination of peroxydisulfate based on a by-product formation. <i>Sensors and Actuators B: Chemical</i> , 2021, 344, 130214.	4.0	6
8484	On the protonation of a polysubstituted 1,2,4-triazole: A structural study of a hexabromotellurate salt. <i>Journal of Molecular Structure</i> , 2021, 1241, 130632.	1.8	8
8485	Rhodanine-based fluorometric sequential monitoring of silver (I) and iodide ions: Experiment, DFT calculation and multifarious applications. <i>Journal of Hazardous Materials</i> , 2021, 419, 126449.	6.5	23
8486	Titanium(IV) complex containing ONO-tridentate Schiff base ligand: Synthesis, crystal structure determination, Hirshfeld surface analysis, spectral characterization, theoretical and computational studies. <i>Journal of Molecular Structure</i> , 2021, 1241, 130653.	1.8	47
8487	Tuning the dehydrogenation performance of dibenzyl toluene as liquid organic hydrogen carriers. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 34788-34796.	3.8	7
8488	Organotin compounds bearing C ₃ -symmetric Schiff base: Microwave-assisted multicomponent synthesis and their photophysical properties. <i>Journal of Organometallic Chemistry</i> , 2021, 954-955, 122111.	0.8	1
8489	Study of H-bonded cyclic dimer of organic linker 5-Bromoisophthalic acid by DFT and vibrational spectroscopy. <i>Journal of Molecular Structure</i> , 2021, 1241, 130613.	1.8	1
8490	Pentavalent P=O-N phosphorus bonding in the heterodimers of POCl ₃ -nitrogen bases: Evidence from matrix isolation infrared spectroscopy and Ab initio computations. <i>Journal of Molecular Structure</i> , 2021, 1241, 130638.	1.8	7
8491	Binary systems of albendazole desmotropes with amino-acids: Experimental and theoretical studies. <i>Journal of Molecular Liquids</i> , 2021, 340, 117282.	2.3	1

#	ARTICLE	IF	CITATIONS
8492	Separation of lithium isotopes by crown ether-room temperature ionic liquid-anisole friendly solvent system. <i>Journal of Molecular Liquids</i> , 2021, 340, 117207.	2.3	7
8493	Effect of fluorination on the adsorption properties of aromatic heterocycles toward methyl halides: A quantum chemical study. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113394.	1.1	19
8494	Tuning optical and electronic properties of graphene oxide by surface adsorption of molecular halogens (X ₂ =I ₂ , Br ₂ , Cl ₂ , and F ₂) for light harvesting. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113379.	1.1	2
8495	Theoretical exploration of optoelectronic performance of PM6:Y6 series-based organic solar cells. <i>Surfaces and Interfaces</i> , 2021, 26, 101385.	1.5	15
8496	Syntheses and nonlinear optical behavior of four-arm star-shaped phthalocyanine indium polymers containing azobenzene. <i>Dyes and Pigments</i> , 2021, 194, 109632.	2.0	6
8497	Synthesis, structures, DFT calculations, and Hirshfeld surface analysis of sulfonium derivatives of the closo-decaborate anion [B ₁₀ X ₉ -cyclo-S(CH ₂) ₄] [−] and [B ₁₀ X ₉ -cyclo-S(CH ₂ CH ₂) ₂ O] [−] (X=H, Cl, Br). <i>Journal of Molecular Structure</i> , 2021, 1241, 130591.	1.8	15
8498	Experimental and theoretical study on the adsorption mechanism of Amino trimethylphosphate (ATMP) functionalized hydroxyapatite on Pb (II) and Cd (II). <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 626, 127029.	2.3	20
8499	Photodynamic therapy: When van der Waals heterojunction meets tumor. <i>Chemical Engineering Journal</i> , 2021, 421, 129773.	6.6	9
8500	Insight into non-covalent interactions in a tetrachlorocadmate salt with promising NLO properties: Experimental and computational analysis. <i>Journal of Molecular Structure</i> , 2021, 1242, 130730.	1.8	73
8501	Crystal structure and optical property of a Cadmium(II) complex based on triphenylamine derivative—Theoretical and experimental investigation. <i>Journal of Luminescence</i> , 2021, 238, 118270.	1.5	2
8502	Excited state trans-cis photoisomerization via non-adiabatic dynamics of novel UVB protective sunscreens. <i>Journal of Luminescence</i> , 2021, 238, 118215.	1.5	2
8503	Effect of the mixture composition of C ₄ mimBF ₄ /acetonitrile on the charge transfer in Coumarin 153: DFT and TD-DFT analysis. <i>Journal of Molecular Liquids</i> , 2021, 339, 116830.	2.3	0
8504	Effect of the addition of deep eutectic solvent to the anthracene separation. <i>Journal of Molecular Liquids</i> , 2021, 339, 116762.	2.3	7
8505	Enhancement of photocatalytic oxidation of benzyl alcohol by edge-functionalized modified carbon nitride: A DFT evaluation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 419, 113452.	2.0	1
8506	The enhanced adsorption of Ampicillin and Amoxicillin on modified montmorillonite with dodecyl dimethyl benzyl ammonium chloride: Experimental study and density functional theory calculation. <i>Advanced Powder Technology</i> , 2021, 32, 3465-3475.	2.0	17
8507	Research Progress of Intramolecular π - π Stacked Small Molecules for Device Applications. <i>Advanced Materials</i> , 2022, 34, e2104125.	11.1	93
8508	Investigation on the interaction behavior of afatinib, dasatinib, and imatinib docked to the BCR-ABL protein. <i>Journal of Molecular Modeling</i> , 2021, 27, 309.	0.8	4
8509	Folic acid functionalized boron nitride oxide as targeted drug delivery system for fludarabine and cytarabine anticancer drugs: A DFT study. <i>Journal of Molecular Liquids</i> , 2021, 339, 116753.	2.3	7

#	ARTICLE	IF	CITATIONS
8510	Tetraphenylethylene-cholesterol conjugates as sensitive aggregation-induced emission probe for selective detection of explosive FOX-7. <i>Journal of Luminescence</i> , 2021, 238, 118318.	1.5	5
8511	Effect of Na on the condensation reaction of naphthalene molecules during coal pyrolysis. <i>Journal of the Energy Institute</i> , 2021, 98, 313-321.	2.7	3
8512	A comparative investigation on the scavenging of 2,2-diphenyl-1-picrylhydrazyl radical by the natural antioxidants (+) catechin and (-) epicatechin. <i>Journal of Molecular Structure</i> , 2021, 1242, 130805.	1.8	14
8513	Enhanced adsorption of CO ₂ on cellulose and chitosan surface by H ₂ O Co-adsorption. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113413.	1.1	2
8514	Molecular-level evaluation of ionic transport under external electric fields in biological dielectric liquids. <i>Journal of Molecular Liquids</i> , 2021, 340, 116883.	2.3	5
8515	Tuning structural preference of negatively charged B16 by ionically or covalently interacting with alkali and coinage metals. <i>Chemical Physics</i> , 2021, 550, 111315.	0.9	1
8516	Mechanistic insights into the ultra-deep desulfurization of liquid fuel on date-seed derived hierarchical porous carbon. <i>Surfaces and Interfaces</i> , 2021, 26, 101413.	1.5	1
8517	Binding studies of known molecules with acetylcholinesterase and bovine serum albumin: A comparative view. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 259, 119856.	2.0	7
8518	Selective determination of epinephrine using electrochemical sensor based on ordered mesoporous carbon / nickel oxide nanocomposite. <i>Talanta</i> , 2021, 233, 122545.	2.9	42
8519	Theoretical study of heteroatom and substituent effects on excited-state intramolecular proton transfers and electronic properties of amino-type hydrogen bonding molecules. <i>Journal of Luminescence</i> , 2021, 238, 118260.	1.5	13
8520	Turning diamondoids into nonlinear optical materials by alkali metal Substitution: A DFT investigation. <i>Optics and Laser Technology</i> , 2021, 142, 107231.	2.2	21
8521	Hydroxycoumarin encapsulated sulfonatothiacalix[4]arene: ¹ H NMR, steady state fluorescence and theory. <i>Journal of Molecular Liquids</i> , 2021, 339, 116760.	2.3	4
8522	The insights into the catalytic performance of rare earth metal ions on lactic acid formation from biomass via microwave heating. <i>Chemical Engineering Journal</i> , 2021, 421, 130014.	6.6	19
8523	A feasible molecular engineering for bright \hat{I} -conjugation free radical photosensitizers with aggregation-induced emission. <i>Dyes and Pigments</i> , 2021, 194, 109651.	2.0	15
8524	Conformational search, structural analysis, vibrational properties, reactivity study and affinity towards DNA of the novel insecticide flonicamid. <i>Journal of Molecular Structure</i> , 2021, 1241, 130628.	1.8	6
8525	Molecular engineering strategy of naphthalimide based small donor molecules for high-performance organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113416.	1.1	43
8526	Computational insight into pnictogen bonds in the self-assembly of caged pnictogen compounds. <i>Chemical Physics</i> , 2021, 550, 111317.	0.9	2
8527	The removal of benzothiazole by combined inorgano-organo-montmorillonite modified with hydroxyl iron pillar and cationic panthenol intercalation: Experimental study and Multiwfn wavefunction analysis. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 626, 127025.	2.3	8

#	ARTICLE	IF	CITATIONS
8528	Rovibrational spectroscopic constants and anharmonic force fields of CH ₃ AsH ₂ and CH ₂ AsH ₃ : An study. <i>Chemical Physics Letters</i> , 2021, 780, 138917.	1.2	1
8529	Examining the interactions of a thermally robust task-specific phosphonium-based ionic compound. <i>Chemical Data Collections</i> , 2021, 35, 100760.	1.1	2
8530	A density functional investigation on the structures, electronic, spectral and fluxional properties of VB ₂₀ - cluster. <i>Journal of Molecular Liquids</i> , 2021, 339, 116764.	2.3	24
8531	Significantly improve the photoinitiation ability of hydroxyalkyl-derived polymerizable β -hydroxyalkylacetophenone photoinitiators by blocking hyperconjugation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 419, 113451.	2.0	8
8532	Theoretical insights into the substitution effect of phenanthroline derivative ligands on the extraction of Mo (VI). <i>Separation and Purification Technology</i> , 2022, 280, 119817.	3.9	11
8533	DFT investigation on electronic structure, chemical bonds and optical properties of Cu ₆ (SR) ₆ nanocluster. <i>Chemical Physics Letters</i> , 2021, 780, 138898.	1.2	3
8534	Infrared spectroscopic and density functional theoretical study on the binary rhodium- ¹⁸⁷ oxygen Rh ₂ O ₉ ⁺ cation. <i>Chemical Physics Letters</i> , 2021, 780, 138926.	1.2	1
8535	Cationic iridium (III) complexes bearing fluorinated Ar-BIAN ligands: Synthesis, structure, electronic, and electrochemical properties. <i>Journal of Organometallic Chemistry</i> , 2021, 951, 122002.	0.8	2
8536	Squaraine organic crystals with strong dipole effect toward stable lithium-organic batteries. <i>Energy Storage Materials</i> , 2021, 41, 240-247.	9.5	16
8537	Novel tetra-arm chemosensor supply π - π collaboration effect for highly sensitive fluorescent and colorimetric sensing of L-Arg. <i>Dyes and Pigments</i> , 2021, 194, 109658.	2.0	2
8538	Peroxymonosulfate activation through 2D/2D Z-scheme CoAl-LDH/BiOBr photocatalyst under visible light for ciprofloxacin degradation. <i>Journal of Hazardous Materials</i> , 2021, 420, 126613.	6.5	150
8539	Uncovering photo-induced hydrogen bonding interaction and proton transfer mechanism for the novel salicylaldehyde azine derivative with para-position electrophilic cyano group. <i>Journal of Luminescence</i> , 2021, 238, 118231.	1.5	23
8540	A novel sulfamethoxazole derivative as an inhibitory agent against HSP70: A combination of computational with in vitro studies. <i>International Journal of Biological Macromolecules</i> , 2021, 189, 194-205.	3.6	7
8541	The alcohol catalytic mechanism for Schiff base 1,3-proton transfer. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113419.	1.1	1
8542	Synthesis, structural investigation, computational study, antimicrobial activity and molecular docking studies of novel synthesized (E)-4-((pyridine-4-ylmethylene)amino)-N-(pyrimidin-2-yl)benzenesulfonamide from pyridine-4-carboxaldehyde and sulfadiazine. <i>Journal of Molecular Structure</i> , 2021, 1241, 130544.	1.8	55
8543	Evaluation of electronic and biological interactions between N-[4-(Ethylsulfamoyl)phenyl]acetamide and some polar liquids (IEFPCM solvation model) with Fukui function and molecular docking analysis. <i>Journal of Molecular Liquids</i> , 2021, 340, 117271.	2.3	61
8544	Adsorption of alkali and alkaline earth ions on nanocages using density functional theory. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113391.	1.1	35
8545	Synthesis, spectral and quantum mechanical studies and molecular docking studies of Schiff base (E)-2-hydroxy-5-(((4-(N-pyrimidin-2-yl)sulfamoyl)phenyl)imino)methyl benzoic acid from 5-formyl salicylic acid and sulfadiazine. <i>Journal of the Indian Chemical Society</i> , 2021, 98, 100144.	1.3	60

#	ARTICLE	IF	CITATIONS
8546	Adsorption behavior of uracil on external surface of MgO nanotubes: A new class of hybrid nano-bio materials. <i>Journal of Molecular Liquids</i> , 2021, 339, 116732.	2.3	6
8547	Inserting EO groups to improve the performance of fatty acid collectors: Flotation and adsorption study performed with calcite, dolomite, and quartz. <i>Separation and Purification Technology</i> , 2021, 272, 118952.	3.9	21
8548	Ultra-Stable, Ultra-Long-Lifespan and Ultra-High-Rate Na-ion Batteries Using Small-Molecule Organic Cathodes. <i>Energy Storage Materials</i> , 2021, 41, 738-747.	9.5	40
8549	Insight into Anticorrosion Mechanism of Ampicillin on Mild Steel in Acidic Environment: A Combined Experimental and Theoretical Approach. <i>Journal of Chemistry</i> , 2021, 2021, 1-12.	0.9	2
8550	Bio-CQDs surface modification BiOCl for the BPA elimination and evaluation in visible light: The contribution of C-localized level. <i>Journal of Colloid and Interface Science</i> , 2021, 602, 1-13.	5.0	28
8551	Microemulsion system constructed with a new cyano-functionalized ionic liquid for the extraction of Pd(II) and preparation of palladium nanoparticles. <i>Separation and Purification Technology</i> , 2021, 275, 119198.	3.9	13
8552	Investigations on experimental, theoretical spectroscopic, electronic excitations, molecular docking of Sulfaguanidine (SG): An antibiotic drug. <i>Chemical Physics Letters</i> , 2021, 783, 139049.	1.2	19
8553	Unraveling weak interactions between fluorinated gases and ionic liquids. <i>Chemical Engineering Science</i> , 2021, 244, 116792.	1.9	12
8554	Dextran derivatives as highly efficient green corrosion inhibitors for carbon steel in CO ₂ -saturated oilfield produced water: Experimental and theoretical approaches. <i>Chemical Engineering Journal</i> , 2021, 424, 130519.	6.6	75
8555	Y-shape structured azo dyes with self-transforming feature to zwitterionic form as sensitizer for DSSC and DFT investigation of their photophysical and charge transfer properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 261, 120062.	2.0	6
8556	Revisiting UF ₆ , NpF ₆ and PuF ₆ for bonding and molecular surface analysis within density functional theory: Comparative study at the different theory levels with the same basis set. <i>Polyhedron</i> , 2021, 209, 115452.	1.0	2
8557	A novel ion-pair strategy for efficient separation of lithium isotopes using crown ethers. <i>Separation and Purification Technology</i> , 2021, 274, 118989.	3.9	23
8558	Investigating the aging mechanism of asphaltene and its dependence on environmental factors through AIMD simulations and DFT calculations. <i>Science of the Total Environment</i> , 2021, 795, 148897.	3.9	23
8559	Understanding the conformational, electronic and vibrational properties of Tetrahydrocannabinol (THC) and Cannabidiol (CBD). Pharmacophoric similarities and differences. <i>Journal of Molecular Structure</i> , 2021, 1244, 130945.	1.8	6
8560	In-depth insight into the synergistic inhibition mechanism of S-benzyl-L-cysteine and thiourea on the corrosion of carbon steel in the CO ₂ -saturated oilfield produced water. <i>Corrosion Science</i> , 2021, 192, 109807.	3.0	28
8561	Computational study for the electrophilic reactivity prediction of crown ethers. <i>Journal of Molecular Liquids</i> , 2021, 341, 117418.	2.3	2
8562	High stability and properties of adsorbed polycyclic aromatic hydrocarbons (PAHs) onto phosphorene: An atomistic DFT study. <i>Journal of Molecular Liquids</i> , 2021, 341, 117465.	2.3	4
8563	Quantum mechanical/molecular mechanical approach for the simulation of UV-Vis absorption spectra of π -conjugated oligomers. <i>Journal of Molecular Liquids</i> , 2021, 341, 117406.	2.3	1

#	ARTICLE	IF	CITATIONS
8564	Reactivity properties and adsorption behavior of a triazole derivative – DFT and MD simulation studies. <i>Journal of Molecular Liquids</i> , 2021, 341, 117439.	2.3	16
8565	Synthesis of three quasi liquid Schiff bases between hexanal and adenine, cytosine, and l-leucine, structural interpretation, quantum mechanical studies and biological activity prediction. <i>Journal of Molecular Liquids</i> , 2021, 341, 117305.	2.3	22
8566	Density functional theory-based analyses on selective gas separation by β -PVDF-supported ionic liquid membranes. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 108, 108004.	1.3	2
8567	The contrastive study of two thiophene-derived symmetrical Schiff bases as fluorescence sensors for Ca^{3+} detection. <i>Sensors and Actuators B: Chemical</i> , 2021, 347, 130497.	4.0	18
8568	Structural, theoretical and biological activity of mono and binuclear nickel(II) complexes with symmetrical and asymmetrical 4,6-diacetylresorcinol-dithiocarbamate ligands. <i>Journal of Inorganic Biochemistry</i> , 2021, 224, 111559.	1.5	7
8569	Thiazolium-based ionic liquids: Synthesis, characterization and physicochemical properties. <i>Journal of Molecular Liquids</i> , 2021, 342, 117553.	2.3	5
8570	A mediated fuel cell using alkaline proof alizarin as an anode mediator. <i>Journal of Power Sources</i> , 2021, 511, 230456.	4.0	0
8571	Silver cluster decorated graphene nanoflakes for selective and accurate detection of nitroaniline isomers; DFT calculations. <i>Materials Science in Semiconductor Processing</i> , 2021, 134, 106023.	1.9	15
8572	Experimental and theoretical investigation on the separation of chalcopyrite from biotite using xanthan gum as a selective depressant. <i>Separation and Purification Technology</i> , 2021, 274, 119012.	3.9	11
8573	Understanding the properties of methyl vinyl ketone and methacrolein at the air-water interface: Adsorption, heterogeneous reaction and environmental impact analysis. <i>Chemosphere</i> , 2021, 283, 131183.	4.2	10
8574	NDMA formation during ozonation of metformin: Roles of ozone and hydroxyl radicals. <i>Science of the Total Environment</i> , 2021, 796, 149010.	3.9	21
8575	Density functional theory-guided drug loading strategy for sensitized tumor-homing phototherapy. <i>Chemical Engineering Journal</i> , 2021, 423, 130146.	6.6	7
8576	Surface enhanced Raman scattering investigation of pioglitazone on silver and silver-gold metal substrates – Experimental analysis and theoretical modeling. <i>Journal of Molecular Structure</i> , 2021, 1244, 130992.	1.8	13
8577	Synthesis, crystal structure, Hirshfeld surface analysis, DFT calculations, 3D energy frameworks studies of Schiff base derivative 2,2'-((1Z,1'-Z)-(1,2-phenylene bis(azanylylidene)) bis(methanylylidene)) diphenol. <i>Journal of Molecular Structure</i> , 2021, 1244, 130910.	1.8	8
8578	Lone pair Halogen (X_2) – π Interactions Stabilizes Molecular Halogens ($\text{X}_2 = \text{I}_2, \text{Br}_2, \text{Cl}_2, \text{and F}_2$) on Reduced Graphene Oxide surface: Structural, Solvent Effect and optical properties. <i>Journal of Molecular Structure</i> , 2021, 1244, 130963.	1.8	0
8579	Intermolecular hydrogen bonds interactions in water clusters of ammonium sulfamate: FTIR, X-ray diffraction, AIM, DFT, RDG, ELF, NBO analysis. <i>Journal of Molecular Liquids</i> , 2021, 342, 117475.	2.3	89
8580	N-[4-(phenyl telluro) butyl] phthalimide: Synthesis, spectral characterization, DFT studies and its complexes with mercury salts. <i>Journal of Molecular Structure</i> , 2021, 1243, 130902.	1.8	0
8581	The influence of intermolecular hydrogen bonds on single fluorescence mechanism of 1-hydroxy-11H-benzo [b]fluoren-11-one and 10-hydroxy-11H-benzo [b]fluoren-11-one. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 260, 119993.	2.0	7

#	ARTICLE	IF	CITATIONS
8582	Highly selective separation of acetic acid and hydrochloric acid by alkylamide based on double hydrogen bond coupling mechanism. <i>Separation and Purification Technology</i> , 2021, 275, 119110.	3.9	9
8583	Desulfurization in high-sulfur bauxite with a novel thioether-containing hydroxamic acid: Flotation behavior and separation mechanism. <i>Separation and Purification Technology</i> , 2021, 275, 119147.	3.9	15
8584	Predicting both lower and upper flammability limits for fuel mixtures from molecular structures with same descriptors. <i>Chemical Engineering Research and Design</i> , 2021, 155, 177-183.	2.7	4
8585	Theoretical prediction of voltage-current behavior and other photovoltaic properties of natural flavonoid-based solar cells. <i>Solar Energy</i> , 2021, 228, 89-99.	2.9	6
8586	New valve-free organosilica nanocontainer for active anticorrosion of polymer coatings. <i>Composites Part B: Engineering</i> , 2021, 224, 109185.	5.9	18
8587	Exchange coupling in a thiocyanato-bridged copper(II) chain: Computational approach to magnetostructural correlations. <i>Polyhedron</i> , 2021, 208, 115406.	1.0	2
8588	Substituents effect on the methanol-assisted excited-state intermolecular proton transfer of 7-Aminoquinoline: A theoretical study. <i>Journal of Molecular Liquids</i> , 2021, 341, 116920.	2.3	3
8589	Sustainable ionic liquid organic solution with efficient recyclability and low regeneration energy consumption for CO ₂ capture. <i>Separation and Purification Technology</i> , 2021, 275, 119123.	3.9	21
8590	Influence of ring structures on optical absorption of trivalent ytterbium in Yb-doped silica fiber. <i>Journal of Luminescence</i> , 2021, 239, 118370.	1.5	1
8591	Stress degradation mechanism of coal macromolecular structure: Insights from molecular dynamics simulation and quantum chemistry calculations. <i>Fuel</i> , 2021, 303, 121258.	3.4	18
8592	Room temperature dissolving cellulose with a metal salt hydrate-based deep eutectic solvent. <i>Carbohydrate Polymers</i> , 2021, 272, 118473.	5.1	37
8593	Predicting adsorption and separation performance indicators of Xe/Kr in metal-organic frameworks via a precursor-based neural network model. <i>Chemical Engineering Science</i> , 2021, 243, 116772.	1.9	6
8594	Simultaneous determination of riboflavin and chloramphenicol by MoS ₂ nanosheets decorated three-dimensional porous carbon: Reaction mechanism insights by computational simulation. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 628, 127291.	2.3	6
8595	Ultrasound-assisted extractive/oxidative desulfurization of oil using environmentally benign trihexyl tetradecyl phosphonium chloride. <i>Environmental Technology and Innovation</i> , 2021, 24, 101965.	3.0	14
8596	Construction strategies for high-nitrogen M8N6O complexes with high detonation heat and controllable stability. <i>Polyhedron</i> , 2021, 209, 115451.	1.0	2
8597	Molecular insight into the role of polyethylene glycol and cholesterol on the performance of graphene-based nanomaterials in Blood-brain barrier delivery. <i>Journal of Molecular Liquids</i> , 2021, 341, 117446.	2.3	6
8598	Effects of B and N doping/codoping on the adsorption behavior of C ₆₀ fullerene towards aspirin: A DFT investigation. <i>Journal of Molecular Liquids</i> , 2021, 342, 117459.	2.3	20
8599	Dual active site tandem catalysis of metal hydroxyl oxides and single atoms for boosting oxygen evolution reaction. <i>Applied Catalysis B: Environmental</i> , 2021, 297, 120451.	10.8	44

#	ARTICLE	IF	CITATIONS
8600	The reduced graphene oxide/WO ₃ : Sensing properties for NO ₂ gas detection at room temperature. <i>Diamond and Related Materials</i> , 2021, 119, 108593.	1.8	10
8601	Molecular structure, covalent and non-covalent interactions of an oxaborole derivative (L-PRO2F3PBA): FTIR, X-ray diffraction and QTAIM approach. <i>Journal of Molecular Structure</i> , 2021, 1243, 130911.	1.8	5
8602	Experimental spectroscopic, Quantum computational, Hirshfeld surface and molecular docking studies on 3-Pyridinepropionic acid. <i>Journal of Molecular Structure</i> , 2021, 1243, 130932.	1.8	12
8603	Spectral profiling, structural, molecular docking and ELF elucidation of bioactive molecule Benzoguanamine. <i>Journal of Molecular Structure</i> , 2021, 1243, 130879.	1.8	2
8604	Computational prediction of polar and non-polar solvent effect on the electronic property of N-BOC-Piperidine-4-Carboxylic acid. <i>Journal of Molecular Liquids</i> , 2021, 341, 117222.	2.3	5
8605	Effective removal of water-soluble methylated arsenic contaminants with phosphorene oxide nanoflakes: A DFT study. <i>Journal of Molecular Liquids</i> , 2021, 341, 117423.	2.3	3
8606	Adsorption mechanism of p-aminophenol over silver-graphene composite: A first principles study. <i>Journal of Molecular Liquids</i> , 2021, 341, 117415.	2.3	39
8607	Planar triple-decker and capped octahedral clusters of group-6 transition metals. <i>Journal of Organometallic Chemistry</i> , 2021, 952, 122023.	0.8	3
8608	Synthesis, characterization, and physicochemical properties of three new nanostructured benzimidazole-based dicationic Brønsted acidic molten salts and comparison of their catalytic and antibacterial activities. <i>Journal of Molecular Liquids</i> , 2021, 342, 117104.	2.3	6
8609	Enhanced singlet oxygen production over a photocatalytic stable metal organic framework composed of porphyrin and Ag. <i>Journal of Colloid and Interface Science</i> , 2021, 602, 300-306.	5.0	15
8610	Structural properties of a novel heterocyclic chalcones derivative, (E)-3-(5-methyl furan-2-yl)-1-phenyl prop-2-en-1-one: A spectroscopic and DFT perception. <i>Journal of Molecular Structure</i> , 2021, 1244, 130973.	1.8	2
8611	Novel Isoxazolone Based Azo Dyes: Synthesis, Characterization, Computational, Solvatochromic UV-Vis Absorption and Biological Studies. <i>Journal of Molecular Structure</i> , 2021, 1244, 130933.	1.8	35
8612	Mono- and binuclear Cu (II) 3,5-diiodosalicylates: Structures and features of non-covalent interactions in crystalline state. <i>Journal of Molecular Structure</i> , 2021, 1244, 130942.	1.8	8
8613	On the important transition of sugar-based surfactant as a microreactor for C-S coupling in water: From micelle to vesicle. <i>Journal of Molecular Liquids</i> , 2021, 342, 117464.	2.3	3
8614	First example of lanthanum as dopant on Al ₁₂ N ₁₂ and Al ₁₂ P ₁₂ nanocages for improved electronic and nonlinear optical properties with high stability. <i>Materials Science in Semiconductor Processing</i> , 2021, 135, 106122.	1.9	22
8615	New insights into ESIPT mechanism of three sunscreen compounds in solution: A combined experimental and theoretical study. <i>Colloids and Surfaces B: Biointerfaces</i> , 2021, 207, 112039.	2.5	21
8616	Enhancing the reactivity of carbon-nanotube for carbon monoxide detection by mono- and co-doping of boron and nitrogen heteroatoms: A DFT and TD-DFT study. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 158, 110230.	1.9	5
8617	Experimental and theoretical studies on the effect of Al(OH) ₃ on the fire-extinguishing performance of superfine ABC dry powder. <i>Powder Technology</i> , 2021, 393, 280-290.	2.1	22

#	ARTICLE	IF	CITATIONS
8618	Unveiling the nonadiabatic photoisomerization mechanism of hemicyanines for UV photoprotection. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 260, 119949.	2.0	2
8619	Mechanistic insight into the reaction pathway of peroxomonosulfate-initiated decomplexation of EDTA-Ni(II) under alkaline conditions: Formation of high-valent Ni intermediate. <i>Applied Catalysis B: Environmental</i> , 2021, 296, 120375.	10.8	28
8620	Ngn (Ng= Ne, Ar, Kr, Xe, and Rn; n=1, 2) encapsulated porphyrin-like porous C ₂₄ N ₂₄ fullerene: A quantum chemical study. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 108, 107986.	1.3	30
8621	Mechanochemically synthesized S-ZVI/m composites for the activation of persulfate in the pH-independent degradation of atrazine: Effects of sulfur dose and ball-milling conditions. <i>Chemical Engineering Journal</i> , 2021, 423, 129789.	6.6	35
8622	A SOCT-ISC type photosensitizer coumarin-BODIPY promoted by AIE effect: Mechanism of singlet oxygen generation, simulated PDT in A-549 cells and fluorescence imaging in zebrafish. <i>Dyes and Pigments</i> , 2021, 195, 109711.	2.0	17
8623	Novel hole transport materials based on triphenylvinyl substituted triarylamine with excellent thermal stability for green OLEDs. <i>Dyes and Pigments</i> , 2021, 195, 109641.	2.0	9
8624	Synthesis, spectra (FT-IR, NMR) investigations, DFT study, in silico ADMET and Molecular docking analysis of 2-amino-4-(4-aminophenyl)thiophene-3-carbonitrile as a potential anti-tubercular agent. <i>Journal of Molecular Structure</i> , 2021, 1244, 130880.	1.8	53
8625	Synthesis, spectral characterization, SC-XRD, HSA, DFT and catalytic activity of a dioxidomolybdenum complex with aminosalicyl-hydrazone Schiff base ligand: An experimental and theoretical approach. <i>Polyhedron</i> , 2021, 208, 115428.	1.0	29
8626	Multi-objective optimization of alkali/alkaline earth metals doped graphyne for ultrahigh-performance CO ₂ capture and separation over N ₂ /CH ₄ . <i>Materials Today Physics</i> , 2021, 21, 100539.	2.9	4
8627	On the potential of all-boron fullerene B ₄₀ as a carrier for anti-cancer drug nitrosourea. <i>Journal of Molecular Liquids</i> , 2021, 342, 117533.	2.3	18
8628	Probing solvent effect and strong and weak interactions in 2-Nitrophenyl-hydrazine using independent gradient model and Hirshfeld from wave function calculation. <i>Journal of Molecular Liquids</i> , 2021, 341, 117345.	2.3	8
8629	Selective enrichment of carbazole from an anthracene slag by extraction: Experiment and simulation. <i>Journal of Molecular Liquids</i> , 2021, 341, 117382.	2.3	3
8630	Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications. <i>Chemical Physics Letters</i> , 2021, 782, 139018.	1.2	39
8631	Designing and comparative analysis of 3D subphthalocyanines based non-fullerene acceptor molecules as an efficient material for organic solar cells. <i>Optik</i> , 2021, 246, 167845.	1.4	13
8632	Structural contribution of cationic groups to water sorption in anion exchange membranes: A combined DFT and MD simulation study. <i>Chemical Engineering Science</i> , 2021, 244, 116791.	1.9	20
8633	Optical and NLO properties of zigzag carbon nanobelt compounds. <i>Journal of Molecular Structure</i> , 2021, 1244, 130936.	1.8	2
8634	Comment on "18 and 12 Member carbon rings (cyclo[n]carbons) – A density functional study". <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2021, 273, 115425.	1.7	109
8635	A DFT and molecular dynamics simulation study of single-walled carbon nanotube as a drug delivery system for few model nitrogen mustard drugs. <i>Journal of Molecular Structure</i> , 2021, 1243, 130877.	1.8	3

#	ARTICLE	IF	CITATIONS
8636	Exploring the OH-initiated reactions of styrene in the atmosphere and the role of van der Waals complex. <i>Chemosphere</i> , 2021, 282, 131004.	4.2	4
8637	Molecular insight into the reversible dispersion and aggregation of graphene utilizing photo-responsive surfactants. <i>Applied Surface Science</i> , 2021, 567, 150840.	3.1	5
8638	Selective removal of Zr(IV) from simulated High-Level liquid waste of metallic fuel reprocessing using hydroxyacetamide Extractant: Insights from solvent extraction and density functional theory computations. <i>Polyhedron</i> , 2021, 208, 115410.	1.0	5
8639	Ionic liquid screening for dichloromethane absorption by multi-scale simulations. <i>Separation and Purification Technology</i> , 2021, 275, 119187.	3.9	16
8640	Theoretical investigation of energetic performance and impact sensitivities of nitro and trinitromethyl substituted ozonides of ethylene and cyclopentene. <i>Computational and Theoretical Chemistry</i> , 2021, 1205, 113425.	1.1	2
8641	Experimental and theoretical studies of new dioxomolybdenum complex: Synthesis, characterization and application as an efficient homogeneous catalyst for the selective sulfoxidation. <i>Inorganica Chimica Acta</i> , 2021, 527, 120568.	1.2	28
8642	Catalyzed stereo-selective hydrogenation of ynamides to give enamines: Ethanol as a hydrogen donor. <i>Journal of Organometallic Chemistry</i> , 2021, 952, 122024.	0.8	2
8643	Structural, optical and photovoltaic properties of unfused Non-Fullerene acceptors for efficient solution processable organic solar cell (Estimated PCE>12.4%): A DFT approach. <i>Journal of Molecular Liquids</i> , 2021, 341, 117428.	2.3	55
8644	Combining 5,6-fused triazolo-triazine with pyrazole: A novel energetic framework for heat-resistant explosive. <i>Chemical Engineering Journal</i> , 2021, 426, 131297.	6.6	20
8645	Insight into the mechanism of asphaltene disaggregation by alkylated treatment: An experimental and theoretical investigation. <i>Journal of Molecular Liquids</i> , 2021, 343, 117576.	2.3	8
8646	Application of terahertz spectroscopy combined with density functional theory to analysis of intermolecular weak interactions for coumarin and 6-methylcoumarin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 263, 120159.	2.0	6
8647	Photocatalytic degradation of sulfamonomethoxine by mesoporous phosphorus-doped titania under simulated solar light irradiation. <i>Chemosphere</i> , 2021, 285, 131553.	4.2	13
8648	Removal of water-soluble inorganic arsenicals with phosphorene oxide nanoadsorbents: A first-principles study. <i>Chemical Engineering Journal</i> , 2021, 426, 131471.	6.6	4
8649	Synthesis and DFT computations on structural, electronic and vibrational spectra, RDG analysis and molecular docking of novel Anti COVID-19 molecule 3, 5 Dimethyl Pyrazolium 3, 5 Dichloro Salicylate. <i>Journal of Molecular Structure</i> , 2021, 1246, 131165.	1.8	28
8650	Molecular mechanism and extraction performance evaluation of ionic liquids for extraction process of n-heptane/n-propanol. <i>Separation and Purification Technology</i> , 2021, 276, 119342.	3.9	21
8651	Spectroscopic, molecular structure, electronic, Hirshfeld surface, molecular docking, and thermodynamic investigations of trans-4-hydroxy-L-proline by DFT method. <i>Journal of Molecular Liquids</i> , 2021, 343, 117549.	2.3	20
8652	Study on the selective separation of methanol and methyl ethyl ketone from the azeotropic system using ionic liquids and their separation mechanism. <i>Journal of Molecular Liquids</i> , 2021, 343, 117571.	2.3	10
8653	Analysis and intensification of energy saving process for separation of azeotrope by ionic liquid extractive distillation based on molecular dynamics simulation. <i>Separation and Purification Technology</i> , 2021, 276, 119254.	3.9	14

#	ARTICLE	IF	CITATIONS
8654	Fluorescent detection mechanism of CO-releasing molecule-3: Competition of inter-/intra-molecular hydrogen bonds. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 263, 120227.	2.0	3
8655	Enhanced uptake of methacrolein at the acidic nanoparticle interface: Adsorption, heterogeneous reaction and impact for the secondary organic aerosol formation. <i>Science of the Total Environment</i> , 2021, 800, 149532.	3.9	8
8656	Solid-liquid phase equilibrium of N, N'-diphenyl thiourea (DPTU) in twelve pure solvents: Solubility determination, correlation, molecular simulation and thermodynamic analysis. <i>Journal of Chemical Thermodynamics</i> , 2021, 163, 106605.	1.0	8
8657	Multiple-H-bonded-zwitterionic tetramer structure for L-(+)-2-chlorophenylglycine, as investigated by UV, IR and Raman spectroscopy and electronic structure calculations. <i>Journal of Molecular Structure</i> , 2021, 1246, 131218.	1.8	3
8658	Density functional theory investigation into the interaction of deep eutectic solvents with amino acids. <i>Journal of Molecular Liquids</i> , 2021, 343, 117624.	2.3	11
8659	DFT study on the interactions between HCN and NO over char. <i>Combustion and Flame</i> , 2021, 234, 111625.	2.8	8
8660	Cadmium isotope fractionation during leaching with nitrilotriacetic acid. <i>Chemical Geology</i> , 2021, 584, 120523.	1.4	1
8661	Solar-assisted electrooxidation process for enhanced degradation of bisphenol A: Performance and mechanism. <i>Separation and Purification Technology</i> , 2021, 277, 119467.	3.9	13
8662	Metal-free Fenton-like photocatalysts based on covalent organic frameworks. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120548.	10.8	36
8663	Structural and electronic properties of neutral and anionic magnesium clusters doped with two barium atoms. <i>Journal of Molecular Liquids</i> , 2021, 343, 117622.	2.3	9
8664	Theoretical (Hirshfeld surface, molecular docking, structural, electronic properties, NBO and NLO) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 of <i>Journal of Molecular Structure</i> , 2021, 1245, 130981.	1.8	5
8665	Synergistic effects of photoinduced electron transfer and heavy atom effect based on BODIPY for efficient triplet photosensitizers. <i>Dyes and Pigments</i> , 2021, 196, 109662.	2.0	6
8666	Quantitative evaluation of coupling effects of pore structures and metal loadings on catalytic hydrogenation of tar model reactants over sulfided NiMo/β-Al ₂ O ₃ catalysts: Role of segmented catalytic active phase volumes. <i>Fuel Processing Technology</i> , 2021, 224, 107008.	3.7	4
8667	Coumarin-Benzothiazole Based Azo Dyes: Synthesis, Characterization, Computational, Photophysical and Biological Studies. <i>Journal of Molecular Structure</i> , 2021, 1246, 131170.	1.8	28
8668	Cyanoborohydride (CBH)-based hypergolic coordination compounds for versatile fuels. <i>Chemical Engineering Journal</i> , 2021, 426, 131866.	6.6	5
8669	Synergistic inhibition effects of hydrophilic monomeric substances on CH ₄ hydrate as revealed by experimental and computational approaches. <i>Chemical Engineering Journal</i> , 2021, 426, 130794.	6.6	10
8670	Electrospinning visible light response Bi ₂ MoO ₆ /Ag ₃ PO ₄ composite photocatalytic nanofibers with enhanced photocatalytic and antibacterial activity. <i>Applied Surface Science</i> , 2021, 569, 150955.	3.1	19
8671	Facilely produced highly adhered, low thermal conductivity and non-combustible coatings for fire safety. <i>Journal of Colloid and Interface Science</i> , 2021, 604, 378-389.	5.0	15

#	ARTICLE	IF	CITATIONS
8672	Kinetics, structural effects and transformation pathways for norfloxacin oxidation using the UV/chlorine process. <i>Journal of Water Process Engineering</i> , 2021, 44, 102324.	2.6	10
8673	Difunctional carbon quantum dots/g-C ₃ N ₄ with in-plane electron buffer for intense tetracycline degradation under visible light: Tight adsorption and smooth electron transfer. <i>Applied Catalysis B: Environmental</i> , 2021, 299, 120694.	10.8	84
8674	Density functional theory study of adsorption of ionic liquids on graphene oxide surface. <i>Chemical Engineering Science</i> , 2021, 245, 116946.	1.9	14
8675	Aqueous solvation study of melatonin using ab initio molecular dynamics. <i>Journal of Molecular Liquids</i> , 2021, 343, 117451.	2.3	4
8676	Crystallographic, spectroscopic, TD/DFT calculations and Hirshfeld surface analysis of cadmium(II) coordination polymer containing pyridine ring. <i>Journal of Molecular Structure</i> , 2021, 1245, 131028.	1.8	16
8677	Influence mechanism of supports for the adsorption and dissociation of H ₂ O and toluene in toluene steam reforming. <i>Applied Surface Science</i> , 2021, 569, 151008.	3.1	9
8678	Adsorption of acetone onto the pristine and Al-doped ZnO nanotubes: A dispersion corrected DFT study. <i>Materials Science in Semiconductor Processing</i> , 2021, 136, 106141.	1.9	3
8679	Crystal structure, IR investigation and interpretation of interactions in cobalt selenate pentahydrate. <i>Chemical Data Collections</i> , 2021, 36, 100776.	1.1	0
8680	Synthesis, spectroscopic analysis and DFT studies of N-(2-methyl-5-nitro-phenyl)benzamide organic single crystal. <i>Journal of Molecular Structure</i> , 2021, 1246, 131172.	1.8	10
8681	Investigating the electronic excitations in Polyoxoniobates: (Nb ₆ O ₁₉) ₈ ⁶⁻ , (Nb ₁₀ O ₂₈) ₆ ⁴⁻ and (XNb ₁₂ O ₄₀) _Y with (X=As, P, Si, Ge) and (Y=15 ⁺ and 16 ⁺). <i>Journal of Molecular Structure</i> , 2021, 1246, 131156.	1.8	6
8682	Recognition and visual detection of ADP and ATP based on a dinuclear Zn(II)-complex with pyrocatechol violet in water. <i>Dyes and Pigments</i> , 2021, 196, 109827.	2.0	2
8683	Sulfonic acid functionalized hierarchical porous covalent organic frameworks as a SALDI-TOF MS matrix for effective extraction and detection of paraquat and diquat. <i>Journal of Colloid and Interface Science</i> , 2021, 603, 172-181.	5.0	33
8684	Quantum computational studies on optimization, donor-acceptor analysis and solvent effect on reactive sites, global descriptors, non-linear optical parameters of Methyl N-Boc-piperidine-3-carboxylate. <i>Journal of Molecular Liquids</i> , 2021, 343, 117608.	2.3	19
8685	Amidoxime modified chitosan/graphene oxide composite for efficient adsorption of U(VI) from aqueous solutions. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 106363.	3.3	40
8686	Quantum Chemical, experimental spectroscopic, Hirshfeld surface and molecular docking studies of the anti-microbial drug Sulfathiazole. <i>Journal of Molecular Structure</i> , 2021, 1245, 131118.	1.8	29
8687	Intrinsic sodium occurrence in Zhundong coal: Experimental observations and molecular modeling. <i>Fuel</i> , 2021, 305, 121491.	3.4	9
8688	Solubility measurement and thermodynamic correlation of (2,4-dichlorophenoxy)acetic acid in fifteen pure solvents. <i>Journal of Chemical Thermodynamics</i> , 2021, 163, 106589.	1.0	12
8689	SERS and resonance Raman of 5-nitrosatin on silver ϵ^{ϵ} The distinction between the coordination and surface complexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 263, 120163.	2.0	0

#	ARTICLE	IF	CITATIONS
8690	Influence of solvent structure on the extraction of aromatics from FCC diesel and computational thermodynamics study. <i>Fuel Processing Technology</i> , 2021, 224, 107021.	3.7	15
8691	Tuning surface inductive electric field in microporous organic polymers for Xe/Kr separation. <i>Chemical Engineering Journal</i> , 2021, 426, 131271.	6.6	13
8692	Catalytic mechanism of Na on coal pyrolysis-derived carbon black formation: Experiment and DFT simulation. <i>Fuel Processing Technology</i> , 2021, 224, 107011.	3.7	51
8693	Experimental study on the separation of quartz from pyrite using alginate as a selective depressant substantiated by theoretical analysis on intermolecular bonding. <i>Separation and Purification Technology</i> , 2021, 276, 119251.	3.9	4
8694	Effect of PO ₄ ³⁻ on the polymerization of polyferric phosphatic sulfate and its flocculation characteristics for different simulated dye wastewater. <i>Separation and Purification Technology</i> , 2021, 276, 119373.	3.9	10
8695	Design a novel type of excess electron compounds with large nonlinear optical responses using group 12 elements (Zn, Cd and Hg). <i>Journal of Molecular Graphics and Modelling</i> , 2021, 109, 108003.	1.3	4
8696	Selective visible light reduction of carbon dioxide over iridium(III)-terpyridine photocatalysts. <i>Materials Today Chemistry</i> , 2021, 22, 100563.	1.7	3
8697	Adsorption of diatomic molecules on nitrogenated holey graphene: Theoretical insights. <i>Surfaces and Interfaces</i> , 2021, 27, 101446.	1.5	1
8698	Characterization, Hirshfeld surface analysis, DFT study and an in vitro α -glucosidase/ α -amylase/radical scavenging profiling of novel 5-styryl-2-(4-tolylsulfonamido) chalcones. <i>Journal of Molecular Structure</i> , 2021, 1245, 131090.	1.8	5
8699	Experimental (X-ray, TGA) and computation (NBO, AIM) studies of Iron(II) complex with thiabendazole and 5-aminoisophthalate. <i>Journal of Molecular Structure</i> , 2021, 1245, 131100.	1.8	1
8700	Experimental spectroscopic and quantum computational analysis of pyridine-2,6-dicarboxylic acid with molecular docking studies. <i>Journal of Molecular Structure</i> , 2021, 1245, 131046.	1.8	18
8701	A combined experimental and quantum chemical study on molecular structure, spectroscopic properties and biological activity of anti-inflammatory Glucocorticosteroid drug, Dexamethasone. <i>Journal of Molecular Structure</i> , 2021, 1245, 130999.	1.8	25
8702	Interfacial catalytic and mass transfer mechanisms of an electro-peroxone process for selective removal of multiple fluoroquinolones. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120608.	10.8	24
8703	Synthesis and characterization of dicationic and monocationic fluorine-containing DBU based ionic liquids: Experimental and quantum chemical approaches. <i>Journal of Molecular Structure</i> , 2021, 1245, 131123.	1.8	2
8704	Insights into the role of hydroxyl group on carboxyl-modified MWCNTs in accelerating atenolol removal by Fe(III)/H ₂ O ₂ system. <i>Chemical Engineering Journal</i> , 2021, 425, 130581.	6.6	25
8705	Palladium determination with a new dye PNBTAN: Structural, UV-VIS, and DFT study. <i>Journal of Molecular Structure</i> , 2021, 1246, 131150.	1.8	4
8706	New insight into the fluorescence mechanism in a fluorescent probe for detecting Zn ²⁺ and CN ⁻ through theoretical calculations. <i>Journal of Molecular Liquids</i> , 2021, 343, 117539.	2.3	2
8707	Boosting Photo-Fenton reactions by amidoxime chelated ferrous iron (Fe(III)) catalyst for highly efficient pollutant control. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120574.	10.8	11

#	ARTICLE	IF	CITATIONS
8708	A supramolecular H ₁₂ SubPcB-OPhCOPh/TiO ₂ Z-scheme hybrid assembled via dimeric concave-ligand π - π interaction for visible photocatalytic oxidation of tetracycline. <i>Applied Catalysis B: Environmental</i> , 2021, 298, 120550.	10.8	43
8709	Molecular-level insights into adsorption of a novel silyl ester donor on essential MgCl ₂ facets of supported Ziegler-Natta catalysts. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 159, 110249.	1.9	3
8710	Novel Ti ₃ C ₂ /Bi@BiOI nanosheets with gradient oxygen vacancies for the enhancement of spatial charge separation and photocatalytic performance: The roles of reactive oxygen and iodine species. <i>Chemical Engineering Journal</i> , 2021, 426, 130764.	6.6	43
8711	Rationally constructing of a novel composite photocatalyst with multi charge transfer channels for highly efficient sulfamethoxazole elimination: Mechanism, degradation pathway and DFT calculation. <i>Chemical Engineering Journal</i> , 2021, 426, 131585.	6.6	89
8712	Explore fused-ring core incorporated A-D-A type acceptors and their application in organic solar cells: Insight into molecular conformation, optical and electrochemical properties, film morphology, and energy loss. <i>Dyes and Pigments</i> , 2021, 196, 109572.	2.0	1
8713	Tuning the optoelectronic properties of naphthodithiophene (NDT) for designing of A-D-A type photovoltaic materials. <i>Optik</i> , 2021, 247, 167892.	1.4	21
8714	A novel bipolar host material based on carbazole and 1,3,5-triazine with an extremely low efficiency roll-off for green PhOLEDs. <i>Dyes and Pigments</i> , 2021, 196, 109808.	2.0	6
8715	Non covalent interactions and molecular docking studies on morphine compound. <i>Journal of King Saud University - Science</i> , 2021, 33, 101606.	1.6	82
8716	Metalloid Chalcogen-pnictogen π -hole bonding competition in stibanyl telluranes. <i>Journal of Organometallic Chemistry</i> , 2021, 954-955, 122092.	0.8	5
8717	Microstructure manipulation in PVDF/SMA/MWCNTs ultrafiltration membranes: Effects of hydrogen bonding and crystallization during the membrane formation. <i>Separation and Purification Technology</i> , 2021, 278, 119523.	3.9	13
8718	Efficient removal of PFOA with an In ₂ O ₃ /persulfate system under solar light via the combined process of surface radicals and photogenerated holes. <i>Journal of Hazardous Materials</i> , 2022, 423, 127176.	6.5	26
8719	Exploring the antibacterial activity of 1, 2 diaminoethane hexanedionic acid by spectroscopic, electronic, ELF, LOL, RDG analysis and molecular docking studies using DFT method. <i>Journal of Molecular Structure</i> , 2022, 1247, 131388.	1.8	38
8720	Evidence of cluster formation of croconic acid with Ag, Au and Cu cages, enhancement of electronic properties and Raman activity. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 264, 120233.	2.0	24
8721	The effect of complexation with metal ions on tetracycline degradation by Fe ^{2+/3+} and Ru ³⁺ activated peroxymonosulfate. <i>Chemical Engineering Journal</i> , 2022, 429, 132178.	6.6	41
8722	The molecular structure and spectroscopic properties of C ₃ H ₂ O and its isomers: An ab initio study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 265, 120388.	2.0	4
8723	Evaluating anti-coronavirus activity of some phosphoramides and their influencing inhibitory factors using molecular docking, DFT, QSAR, and NCI-RDG studies. <i>Journal of Molecular Structure</i> , 2022, 1248, 131481.	1.8	29
8724	Construction of novel MWCNTs/Bi ₄ O ₅ I ₂ nanosheets with enhanced adsorption and photocatalytic performance for the degradation of tetracycline: Efficiency, mechanism and regeneration. <i>Chemical Engineering Journal</i> , 2022, 429, 132398.	6.6	48
8725	A Density Functional Theory study for adsorption and sensing of 5-Fluorouracil on Ni-doped boron nitride nanotube. <i>Materials Science in Semiconductor Processing</i> , 2022, 137, 106183.	1.9	10

#	ARTICLE	IF	CITATIONS
8726	2,3-diaminophenazine as a high-rate rechargeable aqueous zinc-ion batteries cathode. <i>Journal of Colloid and Interface Science</i> , 2022, 607, 1262-1268.	5.0	18
8727	Theoretical insight into electronic and molecular properties of halogenated (F, Cl, Br) and hetero-atom (N, O, S) doped cyclooctane. <i>Materials Chemistry and Physics</i> , 2022, 275, 125239.	2.0	21
8728	Relationship between tertiary amine's physical property and biphasic solvent's CO ₂ absorption performance: Quantum calculation and experimental demonstration. <i>Chemical Engineering Journal</i> , 2022, 428, 131241.	6.6	50
8729	Effect of carbon nitride synthesized by different modification strategies on the performance of carbon nitride/PVDF photocatalytic composite membranes. <i>Journal of Hazardous Materials</i> , 2022, 422, 126877.	6.5	14
8730	Design, synthesis, molecular docking and DFT computational insight on the structure of Piperazine sulfynol derivatives as a new antibacterial contender against superbugs MRSA. <i>Journal of Molecular Structure</i> , 2022, 1247, 131333.	1.8	19
8731	A novel mechanism study of microplastic and As co-contamination on indica rice (<i>Oryza sativa</i> L.). <i>Journal of Hazardous Materials</i> , 2022, 421, 126694.	6.5	61
8732	Synthesis, characterization, DFT and antibacterial studies of a novel vitamin B6 Schiff base and its Cu(II) and Zn(II) complexes. <i>Journal of Molecular Structure</i> , 2022, 1248, 131452.	1.8	6
8733	Tuning the optoelectronic properties of benzodithiophene based donor materials and their photovoltaic applications. <i>Materials Science in Semiconductor Processing</i> , 2022, 137, 106150.	1.9	34
8734	Heteroaggregation of nanoplastics with oppositely charged minerals in aquatic environment: Experimental and theoretical calculation study. <i>Chemical Engineering Journal</i> , 2022, 428, 131191.	6.6	26
8735	Crystal structure, physicochemical, DFT, optical, keto-enol tautomerization, docking, and anti-diabetic studies of (Z)-pyrazol-1(2H)-one derivative. <i>Journal of Molecular Structure</i> , 2022, 1247, 131308.	1.8	13
8736	Low pH-induced lone-pair activity in the hybrid (C ₆ H ₁₀ N ₂)[SnCl ₃]Cl: Chemical study and physical characterizations. <i>Journal of Molecular Structure</i> , 2022, 1248, 131403.	1.8	2
8737	Highly efficient removal of DEET by UV-LED irradiation in the presence of iron-containing coagulant. <i>Chemosphere</i> , 2022, 286, 131613.	4.2	11
8738	Critical influences of metal compounds on the formation and stabilization of environmentally persistent free radicals. <i>Chemical Engineering Journal</i> , 2022, 427, 131666.	6.6	28
8739	A photoswitchable fluorescent chemosensor: Quinoline-naphthalene duo for nanomolar detection of aluminum and bisulfite ions and its multifarious applications. <i>Food Chemistry</i> , 2022, 371, 131130.	4.2	16
8740	Roles of alkali metal dopants and surface defects on polymeric carbon nitride in photocatalytic peroxymonosulfate activation towards water decontamination. <i>Journal of Hazardous Materials</i> , 2022, 424, 127292.	6.5	13
8741	Joint experimental and computational studies of a cyanomethylcarbonyl-bridged pyrene-dinitrobenzene molecular ensemble. <i>Journal of Molecular Structure</i> , 2022, 1247, 131374.	1.8	2
8742	Terahertz spectra and weak intermolecular interactions of nucleosides or nucleoside drugs. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 265, 120344.	2.0	21
8743	Mononuclear copper(I) complexes bearing 1,3-bis(diphenylphosphino)propane and functional 6-Cyano-2,2'-bipyridine ligands. <i>Journal of Molecular Structure</i> , 2022, 1247, 131402.	1.8	1

#	ARTICLE	IF	CITATIONS
8744	Effects of selected functional groups on nanoplastics transport in saturated media under diethylhexyl phthalate co-contamination conditions. <i>Chemosphere</i> , 2022, 286, 131965.	4.2	23
8745	Three-dimension hierarchical composite via in-situ growth of Zn/Al layered double hydroxide plates onto polyaniline-wrapped carbon sphere for efficient naproxen removal. <i>Journal of Hazardous Materials</i> , 2022, 423, 127192.	6.5	65
8746	Mechanochemical bromination of unburned carbon in fly ash and its mercury removal mechanism: DFT study. <i>Journal of Hazardous Materials</i> , 2022, 423, 127198.	6.5	19
8747	Fine-tuning directionality of ESIPT behavior of the asymmetric two proton acceptor system via atomic electronegativity. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 266, 120406.	2.0	14
8748	Hydrogen as an energy currency: Encapsulation of inorganic Ga ₁₂ N ₁₂ with alkali metals for efficient H ₂ adsorption as hydrogen storage materials. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 160, 110352.	1.9	23
8749	Azo-methoxy-calix[4]arene complexes with metal cations for chemical sensor applications: Characterization, QTAIM analyses and dispersion-corrected DFT- computations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 264, 120242.	2.0	15
8750	Molecular structure, spectroscopy, quantum chemical and antibacterial activity investigations of 2-methylbenzylammonium perchlorate. <i>Journal of Molecular Structure</i> , 2022, 1247, 131311.	1.8	14
8751	Understanding the fundamental interaction mechanism of hazardous gases and imidazolium based ionic liquids for efficient gas adsorption. <i>Chemical Engineering Science</i> , 2022, 247, 117031.	1.9	6
8752	The impact of the molecular structure on aggregation and solid state luminescence of 2,3-diarylfumaronitriles. <i>Journal of Molecular Structure</i> , 2022, 1248, 131503.	1.8	4
8753	Highly selective, reversible and ICT-based fluorescent chemosensor for bismuth ions: Applications in bacterial imaging, logic gate and food sample analysis. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 422, 113558.	2.0	6
8754	Introduction of energetic bis-1,2,4-triazoles bridges: A strategy towards advanced heat resistant explosives. <i>Chemical Engineering Journal</i> , 2022, 429, 132416.	6.6	28
8755	The construction and application of asphalt molecular model based on the quantum chemistry calculation. <i>Fuel</i> , 2022, 308, 122037.	3.4	26
8756	Research on separation of aromatics from FCC diesel using organic solvent: A combination of experiments and quantum chemical calculations. <i>Fuel</i> , 2022, 308, 121982.	3.4	17
8757	Thiolation of trimethylantimony: Identification and structural characterization. <i>Journal of Hazardous Materials</i> , 2022, 423, 127259.	6.5	6
8758	Exploring the relationship between the "ON-OFF" mechanism of fluorescent probes and intramolecular charge transfer properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 265, 120339.	2.0	4
8759	Computational biotransformation of polyethylene terephthalate by depolymerase: A QM/MM approach. <i>Journal of Hazardous Materials</i> , 2022, 423, 127017.	6.5	10
8760	How to enhance the regenerability of biphasic absorbents for CO ₂ capture: An efficient strategy by organic alcohols activator. <i>Chemical Engineering Journal</i> , 2022, 429, 132264.	6.6	19
8761	A wide-bandgap, high-mobility electron-transporting material containing a 9,9'-spirobithioxanthene skeleton. <i>Chemical Engineering Journal</i> , 2022, 429, 132215.	6.6	10

#	ARTICLE	IF	CITATIONS
8762	Pivotal role of water molecules in the photodegradation of pymetrozine: New insights for developing green pesticides. <i>Journal of Hazardous Materials</i> , 2022, 423, 127197.	6.5	7
8763	LiN5: A novel pentazolate salt with high nitrogen content. <i>Chemical Engineering Journal</i> , 2022, 429, 132399.	6.6	33
8764	Synthesis and characterization of the layered insensitive pentazolate salts based on two triazolium isomers. <i>Journal of Molecular Structure</i> , 2022, 1249, 131521.	1.8	5
8765	Intramolecular integration of multiple heterocyclic skeletons for energetic materials with enhanced energy & safety. <i>Chemical Engineering Journal</i> , 2022, 428, 131400.	6.6	26
8766	Visible-light degradation of antibiotics catalyzed by titania/zirconia/graphitic carbon nitride ternary nanocomposites: a combined experimental and theoretical study. <i>Applied Catalysis B: Environmental</i> , 2022, 300, 120633.	10.8	82
8767	UV/Fe ³⁺ /NTA as a novel photoreductive system for the degradation of perfluorooctane sulfonate (PFOS) via a photoinduced intramolecular electron transfer mechanism. <i>Chemical Engineering Journal</i> , 2022, 427, 130923.	6.6	18
8768	Selective adsorption and detection of p-arsanilic acid on MOF-on-MOF heterostructure induced by nitrogen-rich self-assembly template. <i>Chemical Engineering Journal</i> , 2022, 427, 131483.	6.6	24
8769	Unravelling the effects of complexation of transition metal ions on the hydroxylation of catechol over the whole pH region. <i>Journal of Environmental Sciences</i> , 2022, 115, 392-402.	3.2	7
8770	A new sensitive structural motif inlaying the azides and tetrazole-based rigid 3D energetic MOFs: Highly sensitive primary explosives with excellent thermal stability. <i>Chemical Engineering Journal</i> , 2022, 429, 132451.	6.6	30
8771	Understanding delivery and adsorption of Flutamide drug with ZnONS based on: Dispersion-corrected DFT calculations and MD simulations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 135, 114937.	1.3	27
8772	A first principles study on electrochemical sensing of highly toxic pesticides by using porous C4N nanoflake. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 160, 110345.	1.9	34
8773	Crystal structure, chemical bonds nature and thermodynamic functions for the new ionic liquid pyridinium bis(dihydrogen phosphate). <i>Journal of Molecular Structure</i> , 2022, 1247, 131363.	1.8	1
8774	π-Stacking interactions in new arylsulphonylamine-substituted derivatives of imidazo[2,1-b]thiazol. <i>Journal of Molecular Structure</i> , 2022, 1248, 131423.	1.8	1
8775	Low-bandgap nonfullerene acceptor based on thieno[3,2-b]indole core for highly efficient binary and ternary organic solar cells. <i>Chemical Engineering Journal</i> , 2022, 427, 131674.	6.6	27
8776	The effect of heavy atoms replacement sites on the luminescent ways of D-A-D type diphenyl sulfone molecules: Thermally activated delayed fluorescence and phosphorescence. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 264, 120249.	2.0	7
8777	Face specific doping of Janus all-cis-1,2,3,4,5,6-hexafluorocyclohexane with superalkalis and alkaline earth metals leads to enhanced static and dynamic NLO responses. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 160, 110361.	1.9	22
8778	Enhanced degradation of organic water pollutants by photocatalytic in-situ activation of sulfate based on Z-scheme g-C3N4/BiPO4. <i>Chemical Engineering Journal</i> , 2022, 428, 132116.	6.6	48
8779	Positional isomerism for strengthening intermolecular interactions: Toward monocyclic nitramino oxadiazoles with enhanced densities and energies. <i>Chemical Engineering Journal</i> , 2022, 427, 130912.	6.6	29

#	ARTICLE	IF	CITATIONS
8780	Theoretical research on mercury-laden halogenated activated carbon adsorbent bonding nature. <i>Chemical Engineering Journal</i> , 2022, 428, 131076.	6.6	8
8781	Synthesis, characterization and DFT studies of luminescent copper(I) complexes containing pyridine-imidazole ligands with tunable π -conjugation system via variation of polyaromatic groups. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 422, 113566.	2.0	0
8782	Prediction and evaluation of the 3D structure of <i>Macadamia integrifolia</i> antimicrobial protein 2 (MiAMP2) and its interaction with palmitoleic acid or oleic acid: An integrated computational approach. <i>Food Chemistry</i> , 2022, 367, 130677.	4.2	22
8783	Visible-light-driven photocatalytic degradation of ofloxacin by g-C ₃ N ₄ /NH ₂ -MIL-88B(Fe) heterostructure: Mechanisms, DFT calculation, degradation pathway and toxicity evolution. <i>Chemical Engineering Journal</i> , 2022, 427, 131594.	6.6	105
8784	Exploring degradation mechanism of tetracycline via high-effective peroxymonosulfate catalysts of montmorillonite hybridized CoFe composites and safety assessment. <i>Chemical Engineering Journal</i> , 2022, 427, 130930.	6.6	22
8785	Effectively controlling the ESIPT behavior and fluorescence feature of 2-(2-hydroxyphenyl)-4-chloromethylthiazole by changing its π -conjugation: A theoretical exploration. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 422, 113548.	2.0	9
8786	Fast dechlorination of trichloroethylene by a bimetallic Fe(OH) ₂ /Ni composite. <i>Separation and Purification Technology</i> , 2021, 278, 119597.	3.9	4
8787	The role of H ₂ O in structural nitrogen migration during coal devolatilization under oxy-steam combustion conditions. <i>Fuel Processing Technology</i> , 2022, 225, 107040.	3.7	14
8788	UPLC-Triple-TOF/MS characterization of phenolic constituents and the influence of natural deep eutectic solvents on extraction of <i>Carya cathayensis</i> Sarg. peels: Composition, extraction mechanism and in vitro biological activities. <i>Food Chemistry</i> , 2022, 370, 131042.	4.2	44
8789	Construction of new framework of 1,3,4-oxadiazole energetic compounds using 1,1-dichloro-2-nitroethylene: design of high-performance molten-cast explosives. <i>Chemical Engineering Journal</i> , 2022, 429, 132503.	6.6	3
8790	Degradation and mechanism of hexafluoropropylene oxide dimer acid by thermally activated persulfate in aqueous solutions. <i>Chemosphere</i> , 2022, 286, 131720.	4.2	13
8791	Synergistic dual-functionalities of starch-grafted-styrene hydrophilic porous resin for efficiently removing bisphenols from wastewater. <i>Chemical Engineering Journal</i> , 2022, 429, 132350.	6.6	14
8792	Encapsulated hydroxychloroquine and chloroquine into cyclic oligosaccharides are the potential therapeutics for COVID-19: insights from first-principles calculations. <i>Journal of Molecular Structure</i> , 2022, 1247, 131371.	1.8	12
8793	A density functional theory study on favipiravir drug interaction with BN-doped C ₆₀ heterofullerene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 135, 114950.	1.3	22
8794	Density functional theory study of ZnIn _n (n = 10) alloy clusters. <i>Journal of Molecular Structure</i> , 2022, 1247, 131345.	1.8	3
8795	Solvent polarity dependent ESIPT behavior for the novel flavonoid-based solvatochromic chemosensors. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 265, 120383.	2.0	18
8796	Computational, spectroscopic and molecular docking investigation on a bioactive anti-cancer drug: 2-Methyl-8-nitro quinoline. <i>Journal of Molecular Structure</i> , 2022, 1247, 131414.	1.8	19
8797	Underlying mechanisms for the impacts of molecular structures and water chemistry on the enrichment of poly/perfluoroalkyl substances in aqueous aerosol. <i>Science of the Total Environment</i> , 2022, 803, 150003.	3.9	5

#	ARTICLE	IF	CITATIONS
8798	Peroxymonosulfate activation by Fe ₃ O ₄ -MnO ₂ /CNT nanohybrid electroactive filter towards ultrafast micropollutants decontamination: Performance and mechanism. <i>Journal of Hazardous Materials</i> , 2022, 423, 127111.	6.5	62
8799	Structure, morphology and modelling studies of polyvinylalcohol nanocomposites reinforced with nickel oxide nanoparticles and graphene quantum dots. <i>Environmental Research</i> , 2022, 203, 111842.	3.7	28
8800	Diametrically opposite effect of Cu ²⁺ on sulfamerazine and ciprofloxacin adsorption-photodegradation in g-C ₃ N ₄ /visible light system: behavior and mechanism study. <i>Chemical Engineering Journal</i> , 2022, 428, 131065.	6.6	20
8801	Amorphous type FeOOH modified defective BiVO ₄ photoanodes for photoelectrochemical water oxidation. <i>Chemical Engineering Journal</i> , 2022, 428, 131027.	6.6	204
8802	Designing stable closo-B ₁₂ dianions in silico for Li- and Mg-ion battery applications. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 5201-5208.	3.0	0
8803	Chemistry of group 5 metallaboranes with heterocyclic thiol ligands: a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2021, 50, 4036-4044.	1.6	4
8804	The potential mechanism of atmospheric new particle formation involving amino acids with multiple functional groups. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10184-10195.	1.3	9
8805	On the CN [≡] K coordination modes in K _n [M ⁿ (CN) ₆] _n ·xH ₂ O: first evidence of CN [≡] K electron-deficient bonding. <i>Dalton Transactions</i> , 2021, 50, 2510-2520.	1.6	1
8806	Synthesis of Chiral Helic[1]tritycene[3]arenes and Their Enantioselective Recognition towards Chiral Guests Containing Aminoindan Groups. <i>Molecules</i> , 2021, 26, 536.	1.7	8
8807	Comparative studies of the noncovalent interactions in the single-crystal packing of pyrene, pyrene-4,5-dione, and pyrene-4,5,9,10-tetraone. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4192.	0.9	7
8808	Synthesis of tautomerization-inhibited diamino substituted tetraphenylethene derivatives with different mechanochromisms: the vital role of chlorine. <i>Materials Chemistry Frontiers</i> , 2021, 5, 2387-2398.	3.2	5
8809	The effect of external electric field and metal impurities on the interaction of HF and boraphene: a computational study. <i>Journal of Molecular Modeling</i> , 2021, 27, 50.	0.8	0
8810	Enantioselective synthesis of chiral tetrasubstituted allenes: harnessing electrostatic and noncovalent interactions in a bifunctional activation model for N-triflylphosphoramidate catalysis. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1510-1519.	2.3	4
8811	From luminescence quenching to high-efficiency phosphorescence: a theoretical study on the monomeric and dimeric forms of platinum(II) complexes with both 2-pyridylimidazol-2-ylidene and bipyrazolate chelates. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5652-5664.	1.3	5
8812	Cadmium oxide nanoparticles/graphene composite: synthesis, theoretical insights into reactivity and adsorption study. <i>RSC Advances</i> , 2021, 11, 27027-27041.	1.7	43
8813	Metal-centered monocyclic carbon wheel clusters with record coordination numbers in planar species. <i>RSC Advances</i> , 2021, 11, 27193-27198.	1.7	10
8814	Imino-bridged N-rich energetic materials: C ₄ H ₃ N ₁₇ and their derivatives assembled from the powerful combination of four tetrazoles. <i>CrystEngComm</i> , 2021, 23, 5377-5384.	1.3	5
8815	Enhancing the Am ³⁺ /Cm ³⁺ separation ability by weakening the binding affinity of N donor atoms: a comparative theoretical study of N, O combined extractants. <i>Dalton Transactions</i> , 2021, 50, 3559-3567.	1.6	13

#	ARTICLE	IF	CITATIONS
8816	Physicochemical Characterization of a Co-Amorphous Atorvastatin-Irbesartan System with a Potential Application in Fixed-Dose Combination Therapy. <i>Pharmaceutics</i> , 2021, 13, 118.	2.0	23
8817	Adsorption of 1-chloro-1,2,2,2-tetrafluoroethane on pristine, Al, Ga-doped boron nitride nanotubes: a study involving PBC-DFT, NBO analysis, and QTAIM. <i>Canadian Journal of Chemistry</i> , 2021, 99, 51-62.	0.6	27
8818	Understanding the different reactivity of (<i>Z</i>)- and (<i>E</i>)-1 ² -nitrostyrenes in [3+2] cycloaddition reactions. An MEDT study. <i>RSC Advances</i> , 2021, 11, 9698-9708.	1.7	7
8819	A study on the characteristics of saturated triglycerides under electric field. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, .	0.2	0
8820	A computational scheme for evaluating the phosphorescence quantum efficiency: applied to blue-emitting tetradentate Pt(<sc>ii</sc>) complexes. <i>Materials Horizons</i> , 2022, 9, 334-341.	6.4	15
8821	Chalcogen bonding interactions in chelating, chiral bis(selenocyanates). <i>New Journal of Chemistry</i> , 2021, 45, 76-84.	1.4	13
8822	Insights into the mechanism and regioselectivity of the [3+2] cycloaddition reactions of cyclic nitron to nitrile functions with a molecular electron density theory perspective. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	13
8823	Non-covalent interactions involving remote substituents influence the topologies of supramolecular chains featuring hydroxyl-Oâ€“Hâ€“O(hydroxyl) hydrogen bonding in crystals of (HOCH ₂ CH ₂) ₂ NC(=N)(H)(C ₆ H ₄ -Y) for Y = H, Me, Cl and NO ₂ . <i>CrystEngComm</i> , 2021, 23, 1723-1743.	1.3	6
8824	A screening of properties and application based on dimerized fused-ring non-fullerene acceptors: influence of C=C, C=C, <i>spiro</i>-C linkers. <i>Journal of Materials Chemistry C</i> , 2021, 9, 13162-13171.	2.7	4
8825	Regioselectivity of aminomethylation in 3-acetyl-7-hydroxycoumarins: Mannich bases and Betti bases. <i>New Journal of Chemistry</i> , 2021, 45, 9864-9871.	1.4	6
8826	Single-crystal X-ray structural characterization, Hirshfeld surface analysis, electronic properties, NBO, and NLO calculations and vibrational analysis of the monomeric and dimeric forms of 5-nitro-2-oxindole. <i>New Journal of Chemistry</i> , 2021, 45, 10070-10088.	1.4	0
8827	A study of the interaction of cationic dyes with gold nanostructures. <i>RSC Advances</i> , 2021, 11, 17694-17703.	1.7	1
8828	Luminescent cyclometalated platinum(<sc>ii</sc>) complexes with acyclic diaminocarbene ligands: structural, photophysical and biological properties. <i>Dalton Transactions</i> , 2021, 50, 4539-4554.	1.6	25
8829	The structural properties of a ZnCl ₂ â€“ethylene glycol binary system and the peculiarities at the eutectic composition. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13136-13147.	1.3	15
8830	The molecular behavior of pyridinium/imidazolium based ionic liquids and toluene binary systems. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13300-13309.	1.3	19
8831	Synthesis, structural characterization, and bonding analysis of two-coordinate copper(i) and silver(i) complexes of pyrrole-based bis(phosphinimine): new metalâ€“pyrrole ring Î€-interactions. <i>Dalton Transactions</i> , 2021, 50, 8036-8044.	1.6	6
8832	Molecular adduct of amantadine ferulate presents a pathway for slowing<i> in vitro</i>/<i> vivo</i> releases and raising synergistic antiviral effects<i> via</i> dual optimization salification strategy. <i>CrystEngComm</i> , 2021, 23, 4389-4401.	1.3	3
8833	Discovery of the EL-0052 as a potential anesthetic drug. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 710-718.	1.9	4

#	ARTICLE	IF	CITATIONS
8834	Substituent-dependent absorption and fluorescence properties of perylene bisimide radical anions and dianions. <i>Materials Horizons</i> , 2022, 9, 350-359.	6.4	38
8835	Gas-phase hydration of nopinone: the interplay between theoretical methods and experiments unveils the conformational landscape. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18137-18144.	1.3	6
8836	The influence mechanism of the molecular structure on the peak current and peak potential in electrochemical detection of typical quinolone antibiotics. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13873-13877.	1.3	7
8837	Photoluminescence Dynamics Defined by Exciton Trapping Potential of Coupled Defect States in DNA-Functionalized Carbon Nanotubes. <i>ACS Nano</i> , 2021, 15, 923-933.	7.3	15
8838	Acridin-9(10 <i>H</i>)-one based thermally activated delayed fluorescence material: simultaneous optimization of RISC and radiation processes to boost luminescence efficiency. <i>Journal of Materials Chemistry C</i> , 2021, 9, 5885-5892.	2.7	27
8839	Design and synthesis of yellow- to red-emitting gold(III) complexes containing isomeric thienopyridine and thienoquinoline moieties and their applications in operationally stable organic light-emitting devices. <i>Materials Horizons</i> , 2022, 9, 281-293.	6.4	12
8840	Molecular design of efficient yellow- to red-emissive alkynylgold(III) complexes for the realization of thermally activated delayed fluorescence (TADF) and their applications in solution-processed organic light-emitting devices. <i>Chemical Science</i> , 2021, 12, 9516-9527.	3.7	13
8841	Transition-metal-like bonding behaviors of a boron atom in a boron-cluster boronyl complex [(⁷ B-BO) ⁺]. <i>Chemical Science</i> , 2021, 12, 8157-8164.	3.7	11
8842	A DFT study on the adsorption of nucleobases with Au ₂₀ . <i>Journal of Molecular Modeling</i> , 2021, 27, 29.	0.8	4
8843	Mechanism of iron complexes catalyzed in the <i>N</i> -formylation of amines with CO ₂ and H ₂ : the superior performance of σ -H ligand methylated complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16675-16689.	1.3	3
8844	Interaction topologies of the S=O chalcogen bond: the conformational equilibrium of the cyclohexanol-SO ₂ cluster. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10799-10806.	1.3	8
8845	Comment on "Theoretical investigation on bond and spectrum of cyclo[18]carbon (C ₁₈) with sp-hybridized". <i>Journal of Molecular Modeling</i> , 2021, 27, 42.	0.8	23
8846	Iodonium salts as efficient iodine(III)-based noncovalent organocatalysts for Knorr-type reactions. <i>RSC Advances</i> , 2021, 11, 4574-4583.	1.7	32
8847	Tricyclic nitrogen-rich explosives with a planar backbone: bis(1,2,4-triazolyl)-1,2,3-triazoles as potential stable green gas generants. <i>New Journal of Chemistry</i> , 2021, 45, 7758-7765.	1.4	7
8848	Substituted aromatic pentaphosphole ligands "a journey across the p-block. <i>Chemical Science</i> , 2021, 12, 13037-13044.	3.7	10
8849	Determining Partial Atomic Charges for Liquid Water: Assessing Electronic Structure and Charge Models. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 889-901.	2.3	15
8850	Synthesis of an expanded pincer ligand and its bimetallic coinage metal complexes. <i>Dalton Transactions</i> , 2021, 50, 11909-11917.	1.6	7
8851	High energy density aqueous zinc-benzoquinone batteries enabled by carbon cloth with multiple anchoring effects. <i>Journal of Materials Chemistry A</i> , 2021, 9, 6131-6138.	5.2	22

#	ARTICLE	IF	CITATIONS
8852	Cocrystals of Propylthiouracil and Nutraceuticals toward Sustained-Release: Design, Structure Analysis, and Solid-State Characterization. <i>Crystal Growth and Design</i> , 2021, 21, 1202-1217.	1.4	40
8853	Strong intermolecular interaction induced methylene-bridged asymmetric heterocyclic explosives. <i>CrystEngComm</i> , 2021, 23, 7635-7642.	1.3	4
8854	Deep eutectic solvent-based green absorbents for the effective removal of volatile organochlorine compounds from biogas. <i>Green Chemistry</i> , 2021, 23, 4814-4827.	4.6	24
8855	Antioxidant product analysis of <i>Hulu Tea</i> (<i>Tadehagi triquetrum</i>). <i>New Journal of Chemistry</i> , 2021, 45, 20257-20265.	1.4	7
8856	V enhancement of thienobenzofuran and benzotriazole backboned photovoltaic polymer by side chain sulfuration or fluoridation. <i>Dyes and Pigments</i> , 2021, 184, 108775.	2.0	3
8857	Efficient evaluation of electrostatic potential with computerized optimized code. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20323-20328.	1.3	664
8858	Endohedral group-14-element clusters $TM@E_{9}$ ($TM = Co, Ni, Cu; E = Ge, Sn, Pb$) and their low-dimensional nanostructures: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20654-20665.	1.3	6
8859	Alkyl chain regulation: distinctive odd-even effects of mechano-luminescence and room-temperature phosphorescence in alkyl substituted carbazole amide derivatives. <i>Journal of Materials Chemistry C</i> , 2021, 9, 12124-12132.	2.7	16
8860	On the nature of bonding in the photochemical addition of two ethylenes: C-C bond formation in the excited state?. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20598-20606.	1.3	10
8861	Disentangling the complex network of non-covalent interactions in fenchone hydrates via rotational spectroscopy and quantum chemistry. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20686-20694.	1.3	12
8862	London dispersion dominating diamantane packing in helium nanodroplets. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21833-21839.	1.3	2
8863	Isatin-derived non-fullerene acceptors for efficient organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2021, 121, 105345.	1.9	38
8864	A cyclopenta-fused dibenzo[<i>b</i>], [<i>d</i>]thiophene- <i>co</i> -phenanthrene macrocyclic tetradicaloid. <i>Chemical Science</i> , 2021, 12, 3952-3957.	3.7	15
8865	Anion-anion and anion-neutral triel bonds. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4818-4828.	1.3	19
8866	Orientation effects on C2(5)-C2(5) linked bioazole isomers synthesized via regioselective and sequential C H arylation. <i>Chinese Chemical Letters</i> , 2021, 32, 425-428.	4.8	3
8867	Hybridized local and charge-transfer excited state fluorophores enabling organic light-emitting diodes with record high efficiencies close to 20%. <i>Chemical Science</i> , 2021, 12, 5171-5176.	3.7	66
8868	Synthesis, Spectroscopic (FT-IR, FT-Raman, NMR & UV-Vis), Reactive (ELF, LOL, Fukui), Drug likeness and Molecular Docking insights on novel 4-[3-(3-methoxy-phenyl)-3-oxo-propenyl]-benzoxonitrile by Experimental and Computational Methods. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
8869	A phosphine-free Mn(<i>scp</i>)-NNS catalyst for asymmetric transfer hydrogenation of acetophenone: a theoretical prediction. <i>Dalton Transactions</i> , 2021, 50, 14738-14744.	1.6	7

#	ARTICLE	IF	CITATIONS
8870	Oxygen Molecule Activation on Single-Atom Catalysts with Cu, Ag, and Au: A Cluster Model Study. <i>Journal of Materials Science and Chemical Engineering</i> , 2021, 09, 46-59.	0.2	0
8871	Problems of Visualization and 3d Modeling in Chemistry: Analysis of Electronodonor Properties and Spatial Complex-Forming Structure of the Obtained Sulfocationite. <i>Advances in Intelligent Systems and Computing</i> , 2021, , 262-271.	0.5	0
8872	The inspiration and challenge for through-space charge transfer architecture: from thermally activated delayed fluorescence to non-linear optical properties. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15881-15898.	1.3	11
8873	Highly phosphorescent platinum(ⁱⁱ) complexes supported by (2-(1 <i>H</i> -benzimidazole)-phenyl)diphosphine oxide ancillary ligands. <i>Journal of Materials Chemistry C</i> , 2021, 9, 9627-9636.	2.7	7
8874	Tetranuclear copper(ii) cubane complexes derived from self-assembled 1,3-dimethyl-5-(<i>o</i> -phenolate-azo)-6-aminouracil: structures, non-covalent interactions and magnetic property. <i>New Journal of Chemistry</i> , 2021, 45, 2742-2753.	1.4	9
8875	Quantitative and systematic designing of fluorophores enables ultrasensitive distinguishing carbonyls. <i>New Journal of Chemistry</i> , 2021, 45, 12661-12668.	1.4	3
8876	From Y6 to BTPT-4F: a theoretical insight into the influence of the individual change of fused-ring skeleton length or side alkyl chains on molecular arrangements and electron mobility. <i>New Journal of Chemistry</i> , 2021, 45, 12247-12259.	1.4	9
8877	Insights into the nucleophilic substitution of pyridine at an unsaturated carbon center. <i>RSC Advances</i> , 2021, 11, 24238-24246.	1.7	4
8878	Gas-phase preparation and the stability of superatomic Nb ₁₁ O ₁₅ ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15766-15773.	1.3	6
8879	Solvation effect on the ESIPT mechanism of nitrile-substituted <i>ortho</i> -hydroxy-2-phenyl-oxazolines. <i>RSC Advances</i> , 2021, 11, 25795-25800.	1.7	21
8880	From an electride-like super alkali earth atom to a superalkalide or superalkali electride: M(HF) ₃ M (M = Na or Li) as field-induced excellent inorganic NLO molecular switches. <i>Journal of Materials Chemistry C</i> , 2021, 9, 14885-14896.	2.7	13
8881	Lithium–bromine exchange reaction on C ₆₀ : first theoretical proposal of a stable singlet fullerene carbene without the heteroatom. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1551-1562.	2.3	3
8882	Optimization of signal amplification by reversible exchange for polarization of tridentate chelating bis[(2-pyridyl)alkyl]amine. <i>Analyst</i> , The, 2021, 146, 2368-2373.	1.7	1
8883	Probing the origin of the stereoselectivity and enantioselectivity of cobalt-catalyzed [2 + 2] cyclization of ethylene and enynes. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1531-1543.	2.3	8
8884	A mechanistic study of the manganese porphyrin-catalyzed C–H isocyanation reaction. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1858-1866.	2.3	7
8885	Second-order nonlinear optical properties of two chalcone derivatives: insights from sum-over-states. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6128-6140.	1.3	16
8886	Impact of noncovalent interactions on structural and photophysical properties of zero-dimensional tellurium(^{iv}) perovskites. <i>Journal of Materials Chemistry C</i> , 2021, 9, 3271-3286.	2.7	9
8887	Chemical Bonding as a New Avenue for Controlling Excited-State Properties and Excitation Energy-Transfer Processes in Zinc Phthalocyanine–Fullerene Dyads. <i>Chemistry - A European Journal</i> , 2021, 27, 4159-4167.	1.7	10

#	ARTICLE	IF	CITATIONS
8888	Surface modification of polyamide reverse osmosis membranes with small-molecule zwitterions for enhanced fouling resistance: a molecular simulation study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6623-6631.	1.3	7
8889	Theoretical insight into dihydrogen activation with \hat{I}^2 -diketiminato ligand supported Group 13 and 14 elements: mechanism and activity difference. <i>New Journal of Chemistry</i> , 2021, 45, 14789-14796.	1.4	0
8890	Computational study on the mechanism of hydroboration of CO_2 catalysed by POCOP pincer nickel thiolate complexes: concerted catalysis and hydride transfer by a shuttle. <i>Dalton Transactions</i> , 2021, 50, 2903-2914.	1.6	11
8891	Oxidative addition, reduction and reductive coupling: the versatile reactivity of subvalent gallium cations. <i>Dalton Transactions</i> , 2021, 50, 15103-15110.	1.6	13
8892	Theoretical Study on the Structure and Properties of Al_nP_n ($n = 2-9$) Clusters. <i>Modern Physics</i> , 2021, 11, 41-51.	0.1	0
8893	The structure of isolated thalidomide as reference for its chirality-dependent biological activity: a laser-ablation rotational study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13705-13713.	1.3	11
8894	Tunable charge-transport polarity in thienothiophene- <i>bis</i> oxindolinylidene-benzodifurandione copolymers for high-performance field-effect transistors. <i>Journal of Materials Chemistry C</i> , 2022, 10, 2671-2680.	2.7	5
8895	Are all charge-transfer parameters created equally? A study of functional dependence and excited-state charge-transfer quantification across two dye families. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20583-20597.	1.3	3
8896	Design of thermally activated delayed fluorescent emitters for organic solid-state microlasers. <i>Journal of Materials Chemistry C</i> , 2021, 9, 7400-7406.	2.7	18
8897	1,3-Dipolar Cycloadditions by a Unified Perspective Based on Conceptual and Thermodynamics Models of Chemical Reactivity. <i>Journal of Physical Chemistry A</i> , 2021, 125, 801-815.	1.1	8
8898	Theoretical Insight into Molecular Orientation for Thermally Activated Delayed Fluorescence Emitters in Vacuum Deposition. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1665-1672.	1.5	5
8899	Expanding the Family of Octahedral Chiral-at-Metal Cobalt(III) Catalysts by Introducing Tertiary Amine Moiety into the Ligand. <i>Catalysts</i> , 2021, 11, 152.	1.6	14
8900	Predicting the catalytic activity of azolium-based halogen bond donors: an experimentally-verified theoretical study. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 7611-7620.	1.5	21
8901	Visible-light photocatalytic selective oxidation of amine and sulfide with $CsPbBr_3$ as photocatalyst. <i>New Journal of Chemistry</i> , 2021, 45, 13317-13322.	1.4	9
8902	Unveiling the regioselectivity in electrophilic aromatic substitution reactions of deactivated benzenes through molecular electron density theory. <i>New Journal of Chemistry</i> , 2021, 45, 13626-13638.	1.4	10
8903	Noncovalent bond between tetrel σ -hole and hydride. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10536-10544.	1.3	2
8904	High-efficiency solution-processed light-emitting diode based on a phosphorescent Ag_3Cu_5 cluster complex. <i>Journal of Materials Chemistry C</i> , 2021, 9, 5528-5534.	2.7	14
8905	The role of zero-field splitting and π -stacking interaction of different nitrogen-donor ligands on the optical properties of luminescent rhenium tricarbonyl complexes. <i>New Journal of Chemistry</i> , 2021, 45, 11192-11201.	1.4	7

#	ARTICLE	IF	CITATIONS
8906	Anion ⁻ anion (MX ₃) ⁺ ₂ dimers (M = Zn, Cd, Hg; X = Cl, Br, I) in different environments. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13853-13861.	1.3	16
8907	Design of C-H-N-O based new hetero-cyclic high energy density molecules: a theoretical survey. <i>Structural Chemistry</i> , 2021, 32, 1095-1104.	1.0	7
8908	Redox-inactive metal single-site molecular complexes: a new generation of electrocatalysts for oxygen evolution?. <i>Catalysis Science and Technology</i> , 2021, 11, 6411-6424.	2.1	4
8909	Ionic liquid decoration for the hole transport improvement of PEDOT. <i>Materials Advances</i> , 2021, 2, 2009-2020.	2.6	8
8910	Oxymetalation or oxidative cyclization? mechanism of Pd-catalyzed annulation of enynones. <i>Chemical Communications</i> , 2021, 57, 8316-8319.	2.2	0
8911	Access to fused π -extended acridone derivatives through a regioselective oxidative demethylation. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 6985-6989.	1.5	1
8912	Nitrogen as a pnictogen?: evidence for π -hole driven novel pnictogen bonding interactions in nitromethane ⁺ ammonia aggregates using matrix isolation infrared spectroscopy and <i>ab initio</i> computations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6286-6297.	1.3	18
8913	How Long Can A C ⁺ C π -Single Bond Be?. <i>Journal of Physical Chemistry A</i> , 2021, 125, 933-942.	1.1	2
8914	Computational study of the copolymerization mechanism of ethylene with methyl 2-acetamidoacrylate catalyzed by phosphine-sulfonate palladium complexes. <i>New Journal of Chemistry</i> , 2021, 45, 16670-16678.	1.4	13
8915	Theoretical study on the sensing mechanism of chalcone-based fluorescence probe for detecting hydrogen sulfide and biothiols. <i>New Journal of Chemistry</i> , 2021, 45, 16906-16912.	1.4	11
8916	Construction of a Z-scheme 1D/2D FeV ₃ O ₈ /g-C ₃ N ₄ composite for ibuprofen degradation: mechanism insight, theoretical calculation and degradation pathway. <i>Catalysis Science and Technology</i> , 2021, 11, 3466-3480.	2.1	17
8917	Modulation of supramolecular self-assembly of BODIPY tectons <i>via</i> halogen bonding. <i>CrystEngComm</i> , 2021, 23, 6365-6375.	1.3	6
8918	Comparison of σ^* -hole and σ^* -R ⁺ -hole interactions formed by tetrel-containing complexes: a computational study. <i>RSC Advances</i> , 2021, 11, 4011-4021.	1.7	9
8919	Cospatial π -Hole and Lone Pair Interactions of Square-Pyramidal Pentavalent Halogen Compounds with π -Systems: A Quantum Mechanical Study. <i>ACS Omega</i> , 2021, 6, 3319-3329.	1.6	12
8920	The modulation effect of electron-rich solvents on the supramolecular networks and photochromic properties of naphthalene diimide molecules. <i>CrystEngComm</i> , 2021, 23, 3356-3363.	1.3	14
8921	Fused 1,2-Diboraoxazoles Based on closo-Decaborate Anion ⁻ Novel Members of Diboroheterocycle Class. <i>Molecules</i> , 2021, 26, 248.	1.7	22
8922	On the structure of Au ₁₁ (SR) ₉ and Au ₁₃ (SR) ₁₁ clusters. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19636-19646.	1.3	3
8923	Experimental and theoretical investigations of methyl orange adsorption using boron nitride nanosheets. <i>Soft Matter</i> , 2021, 17, 2640-2651.	1.2	44

#	ARTICLE	IF	CITATIONS
8924	Multicomponent crystals of clotrimazole: a combined theoretical and experimental study. <i>CrystEngComm</i> , 2021, 23, 6977-6993.	1.3	6
8925	Analysis of Oxygen–Pnictogen Bonding with Full Bond Path Topological Analysis of the Electron Density. <i>Inorganic Chemistry</i> , 2021, 60, 1846-1856.	1.9	22
8926	Design, synthesis, biological evaluation and molecular modelling of substituted pyrrolo[2,1-a]isoquinolinone derivatives: discovery of potent inhibitors of AChE and BChE. <i>New Journal of Chemistry</i> , 2021, 45, 8321-8334.	1.4	3
8927	Theoretically modelling graphene-like carbon matryoshka with strong stability and particular three-center two-electron π bonds. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11907-11916.	1.3	3
8928	TD-DFT simulations of K-edge resonant inelastic X-ray scattering within the restricted subspace approximation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1835-1848.	1.3	20
8929	Ambiphilic boryl groups in a neutral Ni(η^2) complex: a new activation mode of H_2 . <i>Chemical Science</i> , 2021, 12, 2540-2548.	3.7	11
8930	Bifurcated Halogen Bonding Involving Diaryliodonium Cations as Iodine(III)-Based Double- π -Hole Donors. <i>Crystal Growth and Design</i> , 2021, 21, 1136-1147.	1.4	36
8931	Host–guest complex properties of calix[4]arene derivatives: a DFT study of adsorption and sensing of an anticancer drug, 5-fluorouracil. <i>Monatshefte für Chemie</i> , 2021, 152, 217-228.	0.9	7
8932	On the Catalytic Effects of the Thiazolium Salt in the Oxa-Diel-Alder Reaction between Benzaldehyde and Danishefsky's Diene: A Molecular Electron Density Theory Study. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 9306-9317.	1.5	0
8933	$\hat{\rho}^2$ -Trioxopyrrocorphins: pyrrocorphins of graded aromaticity. <i>Chemical Science</i> , 2021, 12, 12292-12301.	3.7	4
8934	Arylamine organic dye-functionalized $g-C_3N_4$ formed through cycloaddition reactions and its application in photocatalytic hydrogen evolution. <i>Catalysis Science and Technology</i> , 2021, 11, 7316-7325.	2.1	4
8935	Iridium-catalyzed highly stereoselective deoxygenation of tertiary cycloalkanol: stereoelectronic insights and synthetic applications. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 9004-9011.	1.5	7
8936	Tunable Dimroth rearrangement of versatile 1,2,3-triazoles towards high-performance energetic materials. <i>Journal of Materials Chemistry A</i> , 2021, 9, 12291-12298.	5.2	62
8937	Efficient and organic host–guest room-temperature phosphorescence: tunable triplet–singlet crossing and theoretical calculations for molecular packing. <i>Chemical Science</i> , 2021, 12, 6518-6525.	3.7	83
8938	Understanding the Nanoconfinement Effect on the Ethanol-to-Propene Mechanism Catalyzed by Acidic ZSM-5 and FAU Zeolites. <i>Journal of Physical Chemistry C</i> , 2021, 125, 310-334.	1.5	9
8939	Novel carbazole-based multifunctional materials with a hybridized local and charge-transfer excited state acting as deep-blue emitters and phosphorescent hosts for highly efficient organic light-emitting diodes. <i>Journal of Materials Chemistry C</i> , 2021, 9, 5899-5907.	2.7	28
8940	Exploration of high-performance light-conversion agents based on cyanostillbene and phenanthrenecarbonitrile backbones: E/Z and position isomerism, high-contrast Michael addition reaction activity and intramolecular photocyclization. <i>Journal of Materials Chemistry C</i> , 2021, 9, 12681-12693.	2.7	8
8941	The physical nature of the interaction in DMSO extraction separation of C_8H_{10} isomer/ n -decane systems. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22629-22639.	1.3	1

#	ARTICLE	IF	CITATIONS
8942	Mechanical single-molecule potentiometers with large switching factors from ortho-pentaphenylene foldamers. <i>Nature Communications</i> , 2021, 12, 167.	5.8	39
8943	Enantioselective Inverse Electron Demand (3 + 2) Cycloaddition of Palladium-Oxyallyl Enabled by a Hydrogen-Bond-Donating Ligand. <i>Journal of the American Chemical Society</i> , 2021, 143, 1038-1045.	6.6	68
8944	An insight into the reaction mechanism of CO ₂ photoreduction catalyzed by atomically dispersed Fe atoms supported on graphitic carbon nitride. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4690-4699.	1.3	22
8945	In Situ Polymerized Conjugated Poly(pyrene-4,5,9,10-tetraone)/Carbon Nanotubes Composites for High-Performance Cathode of Sodium Batteries. <i>Advanced Energy Materials</i> , 2021, 11, 2002917.	10.2	69
8946	Coaxial Triple-Layered versus Helical Be ₆ B ₁₁ Clusters: Dual Structural Fluxionality and Multifold Aromaticity. <i>Angewandte Chemie</i> , 2017, 129, 10308-10311.	1.6	17
8947	NIR-Absorbing Extended Azulene: Non-Alternant Isomer of Terrylene Bisimide. <i>Angewandte Chemie</i> , 2020, 132, 16042-16046.	1.6	16
8948	A Stable All-Thiophene-Based Core-Modified [38]Octaphyrin Diradicaloid: Conformation and Aromaticity Switch at Different Oxidation States. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 7414-7418.	7.2	23
8949	NIR-Absorbing Extended Azulene: Non-Alternant Isomer of Terrylene Bisimide. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15908-15912.	7.2	52
8950	Chitosan/P3HT biohybrid films as polymer matrices for the in situ synthesis of CdSe quantum dots. Experimental and theoretical studies. <i>Journal of Applied Polymer Science</i> , 2020, 137, 49075.	1.3	2
8951	Coupling Reactions of Alkynyl Indoles and CO ₂ by Bicyclic Guanidine: Origin of Catalytic Activity?. <i>Chemistry - an Asian Journal</i> , 2017, 12, 1780-1789.	1.7	16
8952	Mechanistic Insights into the Regio- and Stereoselectivities of Testosterone and Dihydrotestosterone Hydroxylation Catalyzed by CYP3A4 and CYP19A1. <i>Chemistry - A European Journal</i> , 2020, 26, 6214-6223.	1.7	7
8953	Metallacarboranes as Photoredox Catalysts in Water. <i>Chemistry - A European Journal</i> , 2020, 26, 5027-5036.	1.7	29
8954	Electron-Rich Phenothiazine Congeners and Beyond: Synthesis and Electronic Properties of Isomeric Dithieno[1,4]thiazines. <i>Chemistry - A European Journal</i> , 2020, 26, 12111-12118.	1.7	15
8955	The Atomic Partial Charges Arboretum: Trying to See the Forest for the Trees. <i>ChemPhysChem</i> , 2020, 21, 688-696.	1.0	43
8956	Conformational Equilibria of 2-Methoxypyridine...CO ₂ : Cooperative and Competitive Tetrel and Weak Hydrogen Bonds. <i>ChemPhysChem</i> , 2021, 22, 154-159.	1.0	6
8957	On the N-Arylation of Acetamide Using 2- and 3-Substituted Iodoferrocenes**. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 377-391.	1.0	4
8958	Mechanism, Chemoselectivity, and Stereoselectivity of NHC-Catalyzed Asymmetric Desymmetrization of Enal-ethered Cyclohexadienones. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 3726-3733.	1.2	8
8959	<sc>IOData</sc>: A python library for reading, writing, and converting computational chemistry file formats and generating input files. <i>Journal of Computational Chemistry</i> , 2021, 42, 458-464.	1.5	17

#	ARTICLE	IF	CITATIONS
8960	An Asymmetric Furan/Thieno[3,2- <i>b</i>]Thiophene Diketopyrrolopyrrole Building Block for Annealing-Free Green Solvent Processable Organic Thin-Film Transistors. <i>Macromolecular Rapid Communications</i> , 2018, 39, e1800225.	2.0	28
8961	A DFT study on the mechanism of the formation of 1,4,2,3-dithiadiazinanes by head-to-head [3 + 3] cycloaddition of thiocarbonyl imides. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4170.	0.9	9
8962	Sensing of toxic Lewisite (L_{1} , L_{2} , and L_{3}) molecules by graphdiyne nanoflake using density functional theory calculations and quantum theory of atoms in molecule analysis. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4181.	0.9	18
8963	Theoretical insights on the luminescent mechanism of an efficient aggregation-induced nondoped delayed fluorescence emitter using QM / MM method. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26490.	1.0	3
8964	Synthesis, Structure, and DFT Analysis of the THF Solvate of 2-Picolylithium: A 2-Picolylithium Solvate with Significant Carbanionic Character. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 726-733.	0.6	5
8965	The X-C-Y Carbon Bond. Challenges and Advances in Computational Chemistry and Physics, 2015, , 323-356.	0.6	9
8966	Influence of halogen atom substitution and neutral HCN/anion CN^{-} Lewis base on the triel-bonding interactions. <i>Journal of Molecular Modeling</i> , 2021, 27, 93.	0.8	2
8967	Extending the Marcus $\lambda^{1/4}$ -Scale of Solvent Softness Using Conceptual Density Functional Theory and the Orbital Overlap Distance: Method and Application to Ionic Liquids. <i>Journal of Solution Chemistry</i> , 2020, 49, 614-628.	0.6	2
8968	Achieving white-light emission in a single-component polymer with halogen-assisted interaction. <i>Science China Chemistry</i> , 2021, 64, 467-477.	4.2	10
8969	Adsorption of fluoroquinolone by carbon nanotubes: a combined experimental and density functional theory study. <i>Chemical Papers</i> , 2020, 74, 3847-3856.	1.0	13
8970	A novel composite hydrogel for adsorption and photocatalytic degradation of bisphenol A by visible light irradiation. <i>Chemical Engineering Journal</i> , 2018, 334, 1679-1690.	6.6	74
8971	BeMg9: A tower-like type doped magnesium clusters with high stability. <i>Computational Materials Science</i> , 2020, 182, 109795.	1.4	22
8972	DFT study of 2,9-bis(1,2,4-triazin-3-yl)-1,10-phenanthroline (BTPPhen) and its derivatives complexation with lanthanide series. <i>Computational and Theoretical Chemistry</i> , 2020, 1175, 112729.	1.1	5
8973	Density functional theory investigation on the mechanism of dehydrogenation of cyclohexane catalyzed by heteronuclear NiTi+. <i>Computational and Theoretical Chemistry</i> , 2020, 1184, 112820.	1.1	3
8974	Comparison of biotransformation mechanisms of 2, 4, 6-trinitrotoluene and its hydride-Meisenheimer metabolite by the old yellow enzyme family of flavoproteins. <i>Energetic Materials Frontiers</i> , 2020, 1, 216-226.	1.3	5
8975	Theoretical studies on the antioxidant activity of pinobanksin and its ester derivatives: Effects of the chain length and solvent. <i>Food Chemistry</i> , 2018, 240, 323-329.	4.2	56
8976	Efficient catalytic removal of COS and H ₂ S over graphitized 2D micro-meso-macroporous carbons endowed with ample nitrogen sites synthesized via mechanochemical carbonization. <i>Green Energy and Environment</i> , 2022, 7, 983-995.	4.7	25
8977	Low-energy-gap organic photosensitizers with phenalenothiophene and benzoindothiophene as primary electron-donors for durable dye-sensitized solar cells. <i>Journal of Power Sources</i> , 2020, 451, 227748.	4.0	12

#	ARTICLE	IF	CITATIONS
8978	Spectroscopic constants and spin-orbit coupling in the low-lying electronic states of AsBr. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2020, 251, 107049.	1.1	5
8979	A theoretical investigation of the effects of metal substituted boron subphthalocyanine chloride on the performance of subPC/C60 organic solar cells. <i>Materials Chemistry and Physics</i> , 2020, 243, 122590.	2.0	7
8980	Insight into the formation mechanism of C C chain in ethanol synthesis at the interface of partially hydroxylated β -Al ₂ O ₃ (110D) surface and polyethylene glycol solvent. <i>Molecular Catalysis</i> , 2018, 455, 164-178.	1.0	3
8981	Thermal decomposition mechanisms of some amino acid ionic liquids: Molecular approach. <i>Journal of Molecular Liquids</i> , 2020, 302, 112505.	2.3	6
8982	Exploring the physicochemical properties of para-xylyl linked DBU-based dicationic ionic liquids consist of various anions: A GCMO6X study. <i>Journal of Molecular Liquids</i> , 2020, 310, 113060.	2.3	8
8983	Straight Z and twisted E isomers from triphenylamine derivatives: Intramolecular charge transfer and second-order nonlinear optical response. <i>Journal of Molecular Liquids</i> , 2020, 311, 113297.	2.3	9
8984	Unraveling the effect of nitrogen doping on graphene nanoflakes and the adsorption properties of ionic liquids: A DFT study. <i>Journal of Molecular Liquids</i> , 2020, 312, 113400.	2.3	16
8985	Structural and physico-chemical evaluation of melatonin and its solution-state excited properties, with emphasis on its binding with novel coronavirus proteins. <i>Journal of Molecular Liquids</i> , 2020, 318, 114082.	2.3	64
8986	Nucleophilic properties of the positively charged metal center in the solid state structure of Palladium(II)-Terpyridine complex. <i>Journal of Molecular Structure</i> , 2020, 1199, 126957.	1.8	3
8987	Investigation of detection and adsorption properties of β -propiolactone with silicon and aluminum doped fullerene C60 using density functional theory. <i>Journal of Molecular Structure</i> , 2020, 1217, 128346.	1.8	8
8988	Conformational landscape and intricate conformational relaxation paths of 4,4,4-trifluoro-1-butanol: Rotational spectroscopy and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2020, 1217, 128359.	1.8	3
8989	Synthesis, co-crystal structure, and DFT calculations of a multicomponent co-crystal constructed from 1H-benzotriazole and tetrafluoroterephthalic acid. <i>Journal of Molecular Structure</i> , 2020, 1219, 128480.	1.8	47
8990	Regioselectivity of reduction of nitro groups in 3, 5-dinitrosalicylic acid monohydrate explored by experimental and theoretical charge density analysis. <i>Journal of Molecular Structure</i> , 2020, 1217, 128483.	1.8	1
8991	XRD structure and vibrational analysis of DL- β -Leucine, as aided by DFT tetramer model and characterized by NBO, AIM and NCI calculations. <i>Journal of Molecular Structure</i> , 2020, 1218, 128495.	1.8	12
8992	Experimental and computational approach on p-toluenesulfonamide and its derivatives. <i>Journal of Molecular Structure</i> , 2020, 1218, 128503.	1.8	3
8993	The linear and non-linear optical absorption and asymmetrical electromagnetic interaction in chiral twisted bilayer graphene with hybrid edges. <i>Materials Today Physics</i> , 2020, 14, 100222.	2.9	52
8994	Probing the effect of substituent groups in Ir(III) bis-tridentate complexes during deep-blue phosphorescent illuminating. <i>Organic Electronics</i> , 2020, 84, 105803.	1.4	3
8995	One- and two-photon absorption properties of quadrupolar A ⁺ D ⁻ A dyes with donors of varying strengths. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 230, 118015.	2.0	10

#	ARTICLE	IF	CITATIONS
8996	The rotational spectrum of acetophenone-CO ₂ : Preferred non-covalent interactions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 238, 118424.	2.0	15
8997	Halogen Bonding Involving Palladium(II) as an XB Acceptor. <i>Crystal Growth and Design</i> , 2021, 21, 1159-1177.	1.4	25
8998	Boosting Self-Trapped Emissions in Zero-Dimensional Perovskite Heterostructures. <i>Chemistry of Materials</i> , 2020, 32, 5036-5043.	3.2	46
8999	Molecular Design of the Amphiphilic Polymer as a Viscosity Reducer for Heavy Crude Oil: From Mesoscopic to Atomic Scale. <i>Energy & Fuels</i> , 2021, 35, 1152-1164.	2.5	25
9000	Understanding CO Heterogeneous Adsorption on the Reduced CaSO ₄ (010) Surface for Chemical-Looping Combustion: A First-Principles Study. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 20022-20032.	1.8	5
9001	Transitioning from Intraligand π,π^* to Charge-Transfer Excited States Using Thiophene-Based Donor-Acceptor Systems. <i>Inorganic Chemistry</i> , 2021, 60, 130-139.	1.9	10
9002	Thermal Growth of Au-Fe Heterometallic Carbonyl Clusters Containing N-Heterocyclic Carbene and Phosphine Ligands. <i>Inorganic Chemistry</i> , 2020, 59, 2228-2240.	1.9	13
9003	Structural Evolution and Electronic Properties of TaSi ₄ (γ) (Tj ETQq1 1 0.784314 rgBT). <i>Journal of Physical Chemistry A</i> , 2020, 124, 9818-9831.	1.1	18
9004	The Relative Stability of Indole Isomers Is a Consequence of the Glidewell-Lloyd Rule. <i>Journal of Physical Chemistry A</i> , 2021, 125, 230-234.	1.1	16
9005	Competition between a Tetrel and Halogen Bond to a Common Lewis Acid. <i>Journal of Physical Chemistry A</i> , 2021, 125, 308-316.	1.1	14
9006	Fluorescence Anisotropy Detection of Barrier Crossing and Ultrafast Conformational Dynamics in the S ₂ State of β -Carotene. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9029-9046.	1.2	10
9007	New Structure-Nonlinear Optical Property Correlation in π -Complexes Formed by Nested Pd(II) Nanorings. <i>Journal of Physical Chemistry C</i> , 2020, 124, 12655-12664.	1.5	10
9008	Effect of Noncovalent Interactions on the Intersystem Crossing Behavior in Charge-Transfer Cocrystals of 3,5-Dinitrobenzene. <i>Journal of Physical Chemistry C</i> , 2021, 125, 120-129.	1.5	9
9009	Designing Organic Semiconductors with Ultrasmall Reorganization Energies: Insights from Molecular Symmetry, Aromaticity and Energy Gap. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4548-4553.	2.1	25
9010	Novel Porous Organic Polymer for the Concurrent and Selective Removal of Hydrogen Sulfide and Carbon Dioxide from Natural Gas Streams. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 47984-47992.	4.0	29
9011	Experimental and Theoretical Investigation of Intrinsic Pyridine Isomer Effects on Physical Property Tuning of Metallo Supramolecular Polymers Bearing Multiple Pyridine Ligands. <i>ACS Applied Polymer Materials</i> , 2020, 2, 2327-2337.	2.0	5
9012	Mechanistic Studies of Copper(I)-Catalyzed Stereoselective [2,3]-Sigmatropic Rearrangements of Diazoesters with Allylic Iodides/Sulfides. <i>ACS Catalysis</i> , 2021, 11, 691-702.	5.5	16
9013	Reversible Absorption of Volatile Organic Compounds by Switchable-Hydrophilicity Solvents: A Case Study of Toluene with <i>N,N</i> -Dimethylcyclohexylamine. <i>ACS Omega</i> , 2021, 6, 253-264.	1.6	21

#	ARTICLE	IF	CITATIONS
9014	Theoretical Density Functional Theory Study of Electrocatalytic Activity of MN ₄ -Doped (M = Cu, Ag,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.6	12
9015	Synthesis of 3,3-disubstituted oxindoles by one-pot integrated Brønsted base-catalyzed trichloroacetimidation of 3-hydroxyoxindoles and Brønsted acid-catalyzed nucleophilic substitution reaction. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 1533.	1.5	41
9016	Fluorescence properties of aurone derivatives: an experimental and theoretical study with some preliminary biological applications. <i>Photochemical and Photobiological Sciences</i> , 2017, 16, 1268-1276.	1.6	18
9017	Metathesis of a U ^V imido complex: a route to a terminal U ^V sulfide. <i>Chemical Science</i> , 2017, 8, 5319-5328.	3.7	25
9018	Self-assembled ionic nanofibers derived from amino acids for high-performance particulate matter removal. <i>Journal of Materials Chemistry A</i> , 2019, 7, 4619-4625.	5.2	40
9019	Computational design of <i>i</i> p <i>-</i> (dimethylamino)benzylidene-derived push-pull polyenes with high first-hyperpolarizabilities. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5090-5104.	1.3	7
9020	Boron-containing D ^A type TADF materials with tiny singlet-triplet energy splittings and high photoluminescence quantum yields for highly efficient OLEDs with low efficiency roll-offs. <i>Journal of Materials Chemistry C</i> , 2020, 8, 3846-3854.	2.7	26
9021	Origin of different chain-end microstructures in ethylene/vinyl halide copolymerization catalysed by phosphine-sulfonate palladium complexes. <i>New Journal of Chemistry</i> , 2020, 44, 16941-16947.	1.4	7
9022	Theoretical and extraction studies on the selectivity of lithium with 14C4 derivatives. <i>New Journal of Chemistry</i> , 2020, 44, 20341-20350.	1.4	9
9023	Perfect cubic La-doped boron clusters La ₆ & [La@B ₂₄] ⁺⁰ as the embryos of low-dimensional lanthanide boride nanomaterials. <i>RSC Advances</i> , 2020, 10, 12469-12474.	1.7	9
9024	Donor-acceptor duality of the transition-metal-like B ₂ core in core-shell-like metallo-borosphenes La ₃ & [B ₂ @B ₁₇] ⁺ and La ₃ & [B ₂ @B ₁₈] ⁺ . <i>RSC Advances</i> , 2020, 10, 34225-34230.	1.7	12
9025	Role of the backbone of nucleic acids in the stability of Hg ²⁺ -mediated canonical base pairs and thymine-thymine mispair: a DFT study. <i>RSC Advances</i> , 2020, 10, 40969-40982.	1.7	5
9026	Unraveling the mechanism of CO ₂ capture and separation by porous liquids. <i>RSC Advances</i> , 2020, 10, 42706-42717.	1.7	22
9027	Extensive removal of thallium by graphene oxide functionalized with aza-crown ether. <i>RSC Advances</i> , 2020, 10, 44470-44480.	1.7	8
9028	Direct observation of o-benzyne formation in photochemical hexadehydro-Diels-Alder (h ^{1/2} -HDDA) reactions. <i>Chemical Science</i> , 2020, 11, 9198-9208.	3.7	11
9029	The role of intermolecular interactions in regulating the thermally activated delayed fluorescence and charge transfer properties: a theoretical perspective. <i>Journal of Materials Chemistry C</i> , 2020, 8, 8601-8612.	2.7	22
9030	Real-space visualization of conformation-independent oligothiophene electronic structure. <i>Journal of Chemical Physics</i> , 2016, 144, 194703.	1.2	5
9031	Unveiling the role of short-range exact-like exchange in the optimally tuned range-separated hybrids for fluorescence lifetime modeling. <i>Journal of Chemical Physics</i> , 2020, 152, 204301.	1.2	8

#	ARTICLE	IF	CITATIONS
9032	Unusual blue to red shifting of C-H stretching frequency of CHCl ₃ in co-operatively P-Cl phosphorus bonded POCl ₃ -CHCl ₃ heterodimers at low temperature inert matrixes. Journal of Chemical Physics, 2020, 153, 174305.	1.2	15
9033	Molecular insights into the loading and dynamics of anticancer drugs on silicene and folic acid-conjugated silicene nanosheets: DFT calculation and MD simulation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 3892-3899.	2.0	11
9034	Elastic electron scattering from A@C _n (A = Ca, Mg, n = 60, 20). Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 205202.	0.6	2
9035	New potential stable structures of XMg _n (X = Ge, C, Sn; n = 2-12) clusters: XMg ₈ with high stability. Journal of Physics Condensed Matter, 2021, 33, 065302.	0.7	12
9036	Hole localization in Fe ₂ O ₃ from density functional theory and wave-function-based methods. Physical Review Materials, 2017, 1, .	0.9	26
9037	Approaching isotropic transfer integrals in crystalline organic semiconductors. Physical Review Materials, 2020, 4, .	0.9	5
9038	Vibrational mode contribution to the dielectric permittivity of disordered small-molecule organic semiconductors. Physical Review Materials, 2020, 4, .	0.9	8
9039	Consistency and variability of cocrystals containing positional isomers: the self-assembly evolution mechanism of supramolecular synthons of cresol-piperazine. IUCr, 2019, 6, 1064-1073.	1.0	18
9040	Insight into the role of pre-assembly and desolvation in crystal nucleation: a case of p-nitrobenzoic acid. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 845-854.	0.5	16
9041	Structure and electrical properties of a one-dimensional polymeric silver thiosaccharinate complex with argentophilic interactions. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 186-193.	0.2	2
9042	Extension of the transferable aspherical pseudoatom data bank for the comparison of molecular electrostatic potentials in structure-activity studies. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 398-408.	0.0	25
9043	Three-orders-of-magnitude variation of carrier lifetimes with crystal phase of gold nanoclusters. Science, 2019, 364, 279-282.	6.0	149
9044	QUANTUM-CHEMICAL INVESTIGATION OF THE COMPLEXATION OF TITANOCENE DICHLORIDE WITH C ₂₀ AND M _n @C ₂₀ (M _n = Li, Na, K) CAGES. Journal of Structural Chemistry, 2020, 61, 1681-1690.	0.3	3
9045	Designing of 5,10-Dihydroindolo [3,2-b] Indole (DINI) Based Donor Materials for Small Molecule Organic Solar Cells. Journal of Computational Biophysics and Chemistry, 2021, 20, 71-84.	1.0	17
9046	Underlying Electrochemical Activity Mechanisms on Tunable Electronic Structures of Graphene Quantum Dots Doped with Nitrogen and Sulfur Heteroatoms. Journal of the Electrochemical Society, 2020, 167, 166518.	1.3	4
9047	Quantum Chemical Study of the Role of the Van Der Waals Interaction (4). Journal of Advances in Physical Chemistry, 2014, 03, 1-10.	0.1	2
9048	A Quantum Chemistry Study of Hydrogen Bonds (1). Journal of Advances in Physical Chemistry, 2015, 04, 84-101.	0.1	3
9049	Generalized Charge Decomposition Analysis (GCDA) Method. Journal of Advances in Physical Chemistry, 2015, 04, 111-124.	0.1	134

#	ARTICLE	IF	CITATIONS
9050	Reactivity Indices related to DFT Theory, the Electron Localization Function (ELF) and Non-Covalent Interactions (NCI) Calculations in the Formation of the non-Halogenated Pyruvic Esters in Solution. <i>Mediterranean Journal of Chemistry</i> , 2019, 8, 476-485.	0.3	18
9051	Molecular polarizability investigation of polar solvents: water, ethanol, and acetone at terahertz frequencies using terahertz time-domain spectroscopy. <i>Applied Optics</i> , 2020, 59, 4775.	0.9	11
9052	Third-order nonlinear optical susceptibility of crystalline oxide yttria-stabilized zirconia. <i>Photonics Research</i> , 2020, 8, 110.	3.4	19
9053	Cloning and Expression of Î²-Defensin from Soiny Mullet (<i>Liza haematocheila</i>), with Insights of its Antibacterial Mechanism. <i>PLoS ONE</i> , 2016, 11, e0157544.	1.1	16
9054	A theoretical and experimental study of the adsorptive removal of hexavalent chromium ions using graphene oxide as an adsorbent. <i>Open Chemistry</i> , 2020, 18, 936-942.	1.0	23
9055	Structure of aqueous sodium acetate solutions by X-Ray scattering and density functional theory. <i>Pure and Applied Chemistry</i> , 2020, 92, 1627-1641.	0.9	4
9056	Halogen bonding in crystals of free 1,2-diiodo-ethene (C ₂ H ₂ I ₂) and its π -complex [CpMn(CO) ₂](π -C ₂ H ₂ I ₂). <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2020, 235, 599-607.	0.4	13
9057	Solvent-dependent photochemical dynamics of a phenoxazine-based photoredox catalyst. <i>Zeitschrift Fur Physikalische Chemie</i> , 2020, 234, 1475-1494.	1.4	10
9058	Structure and redox properties of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) adsorbed on a silica surface. A DFT M05 computational study. <i>VÅsnik DnÅpropetrovsË¹kogo UnÅversitetu: SerÅÅ HÅmÅÅ</i> , 2017, 25, 1-8.	0.1	1
9059	Topological Analysis and Frequency Dependent Hyperpolarizability Calculations of FDDNP: a DFT Study. <i>Chemistry Journal of Moldova</i> , 2016, 11, 84-92.	0.3	1
9060	Topological Analysis of Electron Density in Large Biomolecular Systems. <i>Current Drug Discovery Technologies</i> , 2019, 16, 437-448.	0.6	19
9061	A Combined Topological ELF, NCI and QTAIM Study of Mechanism and Hydrogen Bond Controlling the Selectivity of the IMDC Reaction of Nitron-alkene Obtained from m-allyloxybenzaldehyde. <i>Letters in Organic Chemistry</i> , 2020, 17, 260-267.	0.2	8
9062	Facile Synthesis of 6-Phenyl-6h-chromeno [4, 3-b] Quinoline Derivatives using NaHSO ₄ @SiO ₂ Re-usable Catalyst and Their Antibacterial Activity Study Correlated by Molecular Docking Studies. <i>Letters in Drug Design and Discovery</i> , 2020, 17, 929-938.	0.4	4
9064	A Study of the Detonation Properties, Propellant Impulses, Impact Sensitivities and Synthesis of Nitrated ANTA and NTO Derivatives. <i>Central European Journal of Energetic Materials</i> , 2016, 13, 445-467.	0.5	3
9066	Kinetically Controlled Self-Assembly of PhthalocyanineâPeptide Conjugate Nanofibrils Enabling Superlarge Redshifted Absorption. <i>CCS Chemistry</i> , 2019, 1, 173-180.	4.6	66
9067	Polymorphism-Dependent Dynamic Ultralong Organic Phosphorescence. <i>Research</i> , 2020, 2020, 8183450.	2.8	33
9068	DFT and TD-DFT Study of Bis[2-(5-Amino-[1,3,4]-Oxadiazol-2-yl) Phenol](Diaqua)M(II) Complexes [M = Cu, Ni and Zn]: Electronic Structures, Properties and Analyses. <i>Computational Chemistry</i> , 2015, 03, 29-44.	0.2	19
9069	Conversion of 3,4-Dihydroxypyrrolidine-2,5-Dione to Maleimide through Tosylation and Mechanism Study by DFT. <i>Computational Chemistry</i> , 2018, 06, 47-56.	0.2	2

#	ARTICLE	IF	CITATIONS
9070	Interaction between Metalloporphyrins and Diazine Tautomers. Bulletin of the Korean Chemical Society, 2013, 34, 3727-3732.	1.0	1
9071	A theoretical survey of the ability of nanocarbon layers to deliver anti-cancer drug temozolomide to the target cancer cells. Current Chemistry Letters, 2019, , 53-62.	0.5	5
9072	Hydrogen storage properties of Li-decorated C ₂₄ clusters. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 238102.	0.2	2
9073	Effects of organic cations on performance of halide perovskite solar cell. Wuli Xuebao/Acta Physica Sinica, 2018, 67, 106701.	0.2	5
9074	Study on the ground state properties and excitation properties of C ₁₈ under different external electric fields. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 103101.	0.2	7
9075	New capsaicin analogs as molecular rulers to define the permissive conformation of the mouse TRPV1 ligand-binding pocket. ELife, 2020, 9, .	2.8	10
9076	Theoretical insights into the possible applications of amidoxime-based adsorbents in neptunium and plutonium separation. Dalton Transactions, 2021, 50, 15576-15584.	1.6	5
9077	Revisiting the covalent nature of halogen bonding: a polarized three-center four-electron bond. RSC Advances, 2021, 11, 32852-32860.	1.7	11
9078	Novel polynitro azoxy-pyrazole-based energetic materials with high performance. Dalton Transactions, 2021, 50, 16499-16503.	1.6	3
9079	A Quantum Chemical Screening of Two Imidazole-Chalcone Hybrid Ligands and Their Pd, Pt and Zn Complexes for Charge Transport and Nonlinear Optical (NLO) Properties: A DFT Study. Computational Chemistry, 2021, 09, 215-237.	0.2	5
9080	A square planar silylene nickel four-membered ring. Dalton Transactions, 2021, 50, 14105-14109.	1.6	1
9081	Evaluation of Inhibitive Corrosion Potential of Some Symmetrical Hydrazine Derivatives Containing Nitrophenyl Moiety in Molar Hydrochloric Acid for C38 Steel Metal: Experimental, Chemical Quantum and Molecular Dynamics Studies. SSRN Electronic Journal, 0, , .	0.4	0
9082	Degradation pathways of penthiopyrad by $\hat{\Gamma}$ -MnO ₂ mediated processes: a combined density functional theory and experimental study. Environmental Sciences: Processes and Impacts, 2021, 23, 1977-1985.	1.7	0
9083	Modified mesoporous Y zeolite catalyzed nitration of azobenzene using NO ₂ as the nitro source combined with density functional theory studies. New Journal of Chemistry, 2021, 45, 21389-21394.	1.4	2
9084	Color tuning of di-boron derived TADF emitters: molecular design and property prediction. Journal of Materials Chemistry C, 2021, 9, 15309-15320.	2.7	10
9085	Competitive tetrel bond and hydrogen bond in benzaldehyde-CO ₂ : Characterization by rotational spectroscopy. Physical Chemistry Chemical Physics, 2021, 23, 25784-25788.	1.3	10
9086	Self-assembly of ultra-small-sized carbon nanoparticles in lipid membrane disrupts its integrity. Nanoscale Advances, 2021, 4, 163-172.	2.2	6
9087	Stabilizing orthorhombic CsSn ₃ perovskites with optimized electronic properties by surface ligands with inter-molecular hydrogen bond. Journal of Materials Chemistry A, 2021, 9, 24641-24649.	5.2	9

#	ARTICLE	IF	CITATIONS
9088	Dâ€“â€“A type planar chiral TADF materials for efficient circularly polarized electroluminescence. <i>Materials Horizons</i> , 2021, 8, 3417-3423.	6.4	30
9089	Practical room temperature formaldehyde sensing based on a combination of visible-light activation and dipole modification. <i>Journal of Materials Chemistry A</i> , 2021, 9, 23955-23967.	5.2	16
9090	On the origin of reactivity variation upon sequential ligation: the [Re(CI) ₄]/CH ₄ ($\chi = 1$) couples. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24319-24327.	1.3	1
9091	Lead(II) supramolecular structures formed through a cooperative influence of the hydrazinecarbothioamide derived and ancillary ligands. <i>CrystEngComm</i> , 2022, 24, 368-378.	1.3	7
9092	Computational and solubility equilibrium experimental insight into Ca ²⁺ fluoride complexation and their dissociation behaviors in aqueous solutions: implication for the association constant measured using fluoride ion selective electrodes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24711-24725.	1.3	2
9093	Electrostatic effects in N-heterocyclic carbene catalysis: revealing the nature of catalysed decarboxylation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24627-24633.	1.3	8
9094	An electroactive single-atom copper anchored MXene nanohybrid filter for ultrafast water decontamination. <i>Journal of Materials Chemistry A</i> , 2021, 9, 25964-25973.	5.2	43
9095	Moderate conformational transition promotes the formation of a self-reinforced highly oriented silk fibroin network structure. <i>Soft Matter</i> , 2021, 17, 9576-9586.	1.2	6
9096	Correlations between the ECD spectra and absolute configuration of bridged-ring lactones: revisiting Beecham's rule. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 9266-9275.	1.5	2
9097	Precise Recognition of Palladium Through Interlaminar Chelation in a Covalent Organic Framework. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
9098	High-efficiency formation mechanism of mangiferin/ β -cyclodextrin complex. <i>Food Science and Technology Research</i> , 2021, 27, 735-745.	0.3	2
9099	Revealing the tunability of electronic structures and optical properties of novel SWCNT derivatives, phenine nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24239-24248.	1.3	4
9100	What are the Reaction Laws and Toxicity Effects of Phthalate Acid Esters (PAEs) Ozonation Degradation in the Troposphere?. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
9101	A photoexcited halogen-bonded EDA complex of the thiophenolate anion with iodobenzene for C(sp ³)â€“H activation and thiolation. <i>Chemical Science</i> , 2021, 12, 15655-15661.	3.7	41
9102	Penta graphene: a superior anode material for Mg-ion batteries with high specific theoretical capacity. <i>Ionics</i> , 2021, 27, 4819-4828.	1.2	15
9103	Enhanced formation of trihalomethane disinfection byproducts from halobenzoquinones under combined UV/chlorine conditions. <i>Frontiers of Environmental Science and Engineering</i> , 2022, 16, 1.	3.3	5
9104	Adsorption of doxepin drug on the surface of B12N12 and Al12N12 nanoclusters: DFT and TD-DFT perspectives. <i>Main Group Chemistry</i> , 2022, 21, 69-84.	0.4	9
9105	THEORETICAL INVESTIGATION OF SUPRAMOLECULAR Br-Br AND I-I CONTACTS IN TITANIUM, VANADIUM, AND TANTALUM CHALCOGENIDES. <i>Journal of Structural Chemistry</i> , 2021, 62, 1325-1331.	0.3	2

#	ARTICLE	IF	CITATIONS
9106	Application of borophene as catechol sensor: a computational study. <i>Journal of Molecular Modeling</i> , 2021, 27, 310.	0.8	3
9107	Exploration of efficient electron acceptors for organic solar cells: rational design of indacenodithiophene based non-fullerene compounds. <i>Scientific Reports</i> , 2021, 11, 19931.	1.6	63
9108	Conformation and equilibrium molecular structure of isoniazid in the gas phase. <i>Journal of Molecular Structure</i> , 2022, 1250, 131740.	1.8	1
9109	Direct orange 26 dye environmental degradation: experimental studies (UV, mass, and thermal) in comparison with computational exploration hydrogen bonding analysis of TD-DFT calculations. <i>Journal of Molecular Modeling</i> , 2021, 27, 325.	0.8	1
9110	Probing the Structures, Stabilities and Electronic Properties of Neutral and Anionic PrSin ⁹ (n=9, l=0, Q) Tj ETQq	1.7	2
9111	Experimental and Density Functional Theory Studies on a Zinc(II) Coordination Polymer Constructed with 1,3,5-Benzenetricarboxylic Acid and the Derived Nanocomposites from Activated Carbon. <i>ACS Omega</i> , 2021, 6, 28967-28982.	1.6	20
9112	Theoretical Investigation of Excited-State Intramolecular Double-Proton Transfer Mechanism of Substituent Modified 1, 3-Bis (2-Pyridylimino)-4,7-Dihydroxyisoindole in Dichloromethane Solution. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 707-718.	1.0	5
9113	Exploring the Molecular Basis of Substrate and Product Selectivities of Nocardicin Bifunctional Thioesterase. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2022, 14, 233-244.	2.2	2
9114	Effect of confinement on the behavior of superhalogen and superalkali. <i>Computational and Theoretical Chemistry</i> , 2021, 1206, 113491.	1.1	2
9115	Ab initio investigation for the adsorption of acrolein onto the surface of C ₆₀ , C ₅₉ Si, and C ₅₉ Ge: NBO, QTAIM, and NCI analyses. <i>Structural Chemistry</i> , 2022, 33, 363-378.	1.0	26
9116	Enhanced Long-Term Stability of Organic Electrode Materials by a Trap Filler Strategy. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 49936-49941.	4.0	1
9117	Contrasting the Mechanism of H ₂ Activation by Monomeric and Potassium-Stabilized Dimeric Al ^I Complexes: Do Potassium Atoms Exert any Cooperative Effect?. <i>Chemistry - A European Journal</i> , 2021, 27, 17369-17378.	1.7	9
9118	Two Sides of Quantum-Based Modeling of Enzyme-Catalyzed Reactions: Mechanistic and Electronic Structure Aspects of the Hydrolysis by Glutamate Carboxypeptidase. <i>Molecules</i> , 2021, 26, 6280.	1.7	4
9119	Influence of halogen elements on the optical properties of two-photon fluorescent dyes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 267, 120493.	2.0	0
9120	Lithiation of 2,4,5,7-Tetrabromo-1,8-bis(dimethylamino)naphthalene: Peculiarities of Directing Groups™ Effects and the Possibility of Polymetalation. <i>Organometallics</i> , 2021, 40, 3627-3636.	1.1	5
9121	Redox Potentials of Group 13 Metal-Substituted Dipnictenes: A Comparative Cyclic Voltammetry Study. <i>Organometallics</i> , 2021, 40, 3486-3495.	1.1	4
9122	Interactions of pyridoxine (Vitamin B6) with squaric acid and water. Experimental and theoretical studies. <i>Journal of Molecular Structure</i> , 2022, 1251, 131773.	1.8	4
9123	Tuning the optoelectronic properties of ZOPTAN core-based derivatives by varying acceptors to increase efficiency of organic solar cell. <i>Journal of Molecular Modeling</i> , 2021, 27, 316.	0.8	20

#	ARTICLE	IF	CITATIONS
9124	Designing small organic non-fullerene acceptor molecules with diflorobenzene or quinoline core and dithiophene donor moiety through density functional theory. <i>Scientific Reports</i> , 2021, 11, 19683.	1.6	29
9125	Insights into the Solubility and Structural Features of Four Praziquantel Cocrystals. <i>Crystal Growth and Design</i> , 2021, 21, 6321-6331.	1.4	17
9126	Nature of the Trigger Linkage in Explosive Materials Is a Charge-Shift Bond. <i>Journal of Organic Chemistry</i> , 2021, 86, 15588-15596.	1.7	13
9127	Zinc phthalocyanine absorbance in the near-infrared with application for transparent and colorless dye-sensitized solar cells. <i>Comptes Rendus Chimie</i> , 2021, 24, 157-170.	0.2	2
9128	Control of atroposelectivity via non-covalent interaction in Cu-catalyzed synthesis of axially chiral biaryls from azonaphthalenes and arylboronic acids. <i>Molecular Catalysis</i> , 2021, 515, 111833.	1.0	0
9129	Deciphering non-covalent interactions of 1,3-Benzenedimethanaminium bis(trioxonitrate): Synthesis, empirical and computational study. <i>Journal of Molecular Structure</i> , 2022, 1250, 131720.	1.8	13
9130	Double π -Extended Helicene Derivatives Containing Pentagonal Rings: Synthesis, Crystal Analyses, and Photophysics. <i>Journal of Organic Chemistry</i> , 2021, 86, 17535-17542.	1.7	19
9131	Solid State Characterization of One- and Two-Electron Oxidized Cu ^{II} -salen Complexes with <i>para</i> -Substituents: Geometric Structure-Magnetic Property Relationship. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 4133-4145.	1.0	5
9132	Exploring the sensing mechanism in a dual-mode fluorescent probe responding to tryptamine and fluoride ions. <i>Chemical Physics Letters</i> , 2021, 785, 139142.	1.2	3
9133	Effect of amino acids on formation of pigment precursors in garlic discoloration using UPLC-ESI-Q-TOF-MS analysis. <i>Journal of Food Composition and Analysis</i> , 2022, 105, 104231.	1.9	1
9134	Structural and Vibrational Properties of Amino Acids from Composite Schemes and Double-Hybrid DFT: Hydrogen Bonding in Serine as a Test Case. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9099-9114.	1.1	9
9135	Structural, vibrational, electronic properties, hirshfeld surface analysis topological and molecular docking studies of N-[2-(diethylamino)ethyl]-2-methoxy-5-methylsulfonylbenzamide. <i>Heliyon</i> , 2021, 7, e08186.	1.4	14
9136	Exploring the interaction of ionic liquids with Al ₁₂ N ₁₂ and Al ₁₂ P ₁₂ nanocages for better electrode-electrolyte materials in super capacitors. <i>Journal of Molecular Liquids</i> , 2021, 344, 117828.	2.3	18
9137	Experimental and Theoretical Investigations of Terahertz Spectra of the Structural Isomers: Mannose and Galactose. <i>Journal of Spectroscopy</i> , 2021, 2021, 1-9.	0.6	3
9138	Locating the Reaction Site of 1,2,3,4-Butanetetra-carboxylic Acid Carboxyl and Cellulose Hydroxyl in the Esterification Cross-Linking. <i>ACS Omega</i> , 2021, 6, 28394-28402.	1.6	8
9139	Insights into Organoamine-Catalyzed Asymmetric Synthesis of Axially Chiral Allenates Using Morita-Baylis-Hillman Carbonates and Trisubstituted Allenates: Mechanism and Origin of Stereoselectivity. <i>Journal of Organic Chemistry</i> , 2021, 86, 15276-15283.	1.7	10
9140	Substituent effects on the regium- π stacking interactions between Au ₆ cluster and substituted benzene. <i>Journal of Molecular Modeling</i> , 2021, 27, 328.	0.8	0
9141	Theoretical investigation of emodin conjugated doped B ₁₂ N ₁₂ nanocage by means of DFT, QAIM and PCM analysis. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 136, 115027.	1.3	36

#	ARTICLE	IF	CITATIONS
9142	Structural landscape on a series of rhein: Berberine cocrystal salt solvates: The formation, dissolution elucidation from experimental and theoretical investigations. Chinese Chemical Letters, 2022, 33, 3207-3211.	4.8	17
9143	All-nitrogen spiro-pentadiene- π -N ₅ ⁺ . Journal of Chemical Physics, 2021, 155, 174304.	1.2	1
9144	Ability of Lewis Acids with Shallow π -Holes to Engage in Chalcogen Bonds in Different Environments. Molecules, 2021, 26, 6394.	1.7	9
9145	A strategy for stabilizing of N8 type energetic materials by introducing 4-Nitro-1,2,3-Triazole scaffolds. Chemical Engineering Journal, 2022, 430, 133181.	6.6	12
9146	Impact of non-covalent interactions on FT-IR spectrum and properties of 4-methylbenzylammonium nitrate. A DFT and molecular docking study. Heliyon, 2021, 7, e08204.	1.4	17
9147	Multiscale evaluation of the efficiently separation of phenols using a designed cationic functionalized ionic liquid based on Brønsted/Lewis coordination. Journal of Molecular Liquids, 2022, 345, 117901.	2.3	12
9148	Analysis in silico of chemical reactivity employing the local hyper-softness in some classic aromatic compounds, boron aromatic clusters and all-metal aromatic clusters. Journal of Computational Chemistry, 2022, 43, 29-42.	1.5	1
9149	Rosin imidazoline as an eco-friendly corrosion inhibitor for the carbon steel in CO ₂ -containing solution and its synergistic effect with thiourea. Journal of Molecular Structure, 2022, 1250, 131778.	1.8	16
9150	Rapid Removal of Perfluoroalkanesulfonates from Water by β -Cyclodextrin Covalent Organic Frameworks. ACS Applied Materials & Interfaces, 2021, 13, 48700-48708.	4.0	22
9151	The isomeric effect on structure and photophysical property of organic fluorescent material: synthesis, structures, and photophysical properties of two novel Dâ€¢â€¢â€¢A prototype fluorescent material. Journal of the Iranian Chemical Society, 2022, 19, 1271-1286.	1.2	0
9152	Modeling Spectral Tuning in Red Fluorescent Proteins Using the Dipole Moment Variation upon Excitation. Journal of Chemical Information and Modeling, 2021, 61, 5125-5132.	2.5	2
9153	Synthesis and characterization of a hybrid material (C ₁₀ H ₂₈ N ₄) [CoCl ₄] ₂ using Hirshfeld surface, vibrational and optical spectroscopy, DFT calculations and biological activities. Journal of Molecular Structure, 2022, 1250, 131804.	1.8	5
9154	Is the metal involved or not? A computational study of Cu(I)-catalyzed [4+1] annulation of vinyl indole and carbene precursor. Chinese Chemical Letters, 2022, 33, 2031-2035.	4.8	22
9155	Computational insights into the multi-Diels-Alder reactions of neutral C ₆₀ and its Li ⁺ encapsulated analogue: A density functional theory study. International Journal of Quantum Chemistry, 0, , .	1.0	4
9156	Theoretical studies on the acid-catalyzed decompositions of HCHO and HCOOH: Mechanism and thermochemistry. Computational and Theoretical Chemistry, 2021, 1206, 113482.	1.1	6
9157	Insights into Weak and Covalent Interactions, Reactivity sites and Pharmacokinetic Studies of 4-Dimethylaminopyridinium Salicylate Monohydrate using Quantum Chemical Computation method. Computational and Theoretical Chemistry, 2021, 1206, 113483.	1.1	8
9158	Bifunctional Effect of a Triple-Bond Heterobimetallic Zr/Co System for Hydrogen Activation. ACS Catalysis, 2021, 11, 13452-13462.	5.5	8
9159	2,7-Carbazole Derived Organoboron Compounds: Synthesis and Molecular Fluorescence. Frontiers in Chemistry, 2021, 9, 754298.	1.8	2

#	ARTICLE	IF	CITATIONS
9178	Theoretical Insights into the Separation of Am(III)/Eu(III) by Hydrophilic Sulfonated Ligands. <i>Inorganic Chemistry</i> , 2021, 60, 16409-16419.	1.9	13
9179	Degradation evaluation of acrylamide in advanced oxidation processes based on theoretical method: Mechanisms, kinetics, toxicity evaluation and the role of soil particles. <i>Journal of Hazardous Materials</i> , 2022, 424, 127592.	6.5	12
9180	Efficient improvement of W05-based dyes by inserting auxiliary electron acceptors for dye-sensitized solar cells: A theoretical investigation. <i>Journal of Physical Organic Chemistry</i> , 0, , e4290.	0.9	1
9181	Supramolecular Perspective of Coordination Effects on Fluorine Interactions. <i>Crystal Growth and Design</i> , 2021, 21, 6129-6142.	1.4	2
9182	Defluorination of Omega-Hydroperfluorocarboxylates (Î‰-HPFCAs): Distinct Reactivities from Perfluoro and Fluorotelomeric Carboxylates. <i>Environmental Science & Technology</i> , 2021, 55, 14146-14155.	4.6	12
9183	Synthesis of Schiff base potential, structural features, experimental biological screening and quantum mechanical studies. <i>Journal of Molecular Structure</i> , 2022, 1250, 131762.	1.8	26
9184	Geometric and electronic structures of CrSi ⁿ /O ^m + (n=1-3) clusters from DMRG-CASPT2 calculations. <i>Chemical Physics Letters</i> , 2021, 785, 139166.	1.2	4
9185	Molecular Insights into SO ₂ Absorption by [EMIM][Cl]-Based Deep Eutectic Solvents. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 13831-13841.	3.2	18
9186	The exquisite integration of ESIPT, PET and AIE for constructing fluorescent probe for Hg(II) detection and poisoning. <i>Chinese Chemical Letters</i> , 2022, 33, 1861-1864.	4.8	21
9187	Penispidins C, Aromatic Sesquiterpenoids from <i>Penicillium virgatum</i> and Their Inhibitory Effects on Hepatic Lipid Accumulation. <i>Journal of Natural Products</i> , 2021, 84, 2623-2629.	1.5	6
9188	Theoretical Study of a Two-Photon Fluorescent Probe Based on Nile Red Derivatives with Controllable Fluorescence Wavelength and Water Solubility. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5082-5097.	2.5	8
9189	Achieving a Favorable Activation of the C-F Bond over the C-H Bond in Five- and Six-Membered Ring Complexes by a Coordination and Aromaticity Dually Driven Strategy. <i>Organometallics</i> , 2021, 40, 3397-3407.	1.1	11
9190	Hydrogen-Bonding-Mediated Selective Hydrogenation of Aromatic Ketones over Pd/C in Ionic Liquids at Room Temperature. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 14216-14223.	3.2	7
9191	First-principles study of the binding affinity of monolayer BC6N nanosheet: Implications for drug delivery. <i>Materials Chemistry and Physics</i> , 2022, 276, 125375.	2.0	15
9192	Mechanism of ozone adsorption and activation on B-, N-, P-, and Si-doped graphene: A DFT study. <i>Chemical Engineering Journal</i> , 2022, 430, 133114.	6.6	27
9193	Study of weak intermolecular interactions and vibrational modes in hydroxybenzoic acid isomers using terahertz spectroscopy and density functional theory techniques. <i>Infrared Physics and Technology</i> , 2021, 119, 103950.	1.3	3
9194	Amino-modified metal-organic frameworks as peroxymonosulfate catalyst for bisphenol AF decontamination: ROS generation, degradation pathways, and toxicity evaluation. <i>Separation and Purification Technology</i> , 2022, 282, 119967.	3.9	13
9195	Energetic Windmill: Computational insight into guanidine-based nitroazole-substituted compounds as energetic materials. <i>Computational and Theoretical Chemistry</i> , 2021, 1206, 113485.	1.1	1

#	ARTICLE	IF	CITATIONS
9196	Boosting external quantum efficiency to 38.6% of sky-blue delayed fluorescence molecules by optimizing horizontal dipole orientation. <i>Science Advances</i> , 2021, 7, eabj2504.	4.7	58
9197	2-Nitro- and 4-fluorocinnamaldehyde based receptors as naked-eye chemosensors to potential molecular keypad lock. <i>Scientific Reports</i> , 2021, 11, 20847.	1.6	6
9198	Bent and Linear {CoNO} ⁸ Entities: Structure and Bonding in a Prototypic Class of Nitrosyls. <i>Inorganic Chemistry</i> , 2021, 60, 15980-15996.	1.9	12
9199	Validation of crystal structure of 2-acetamidophenyl acetate: an experimental and theoretical study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-13.	2.0	1
9200	Insights into the origin of selectivity for [2+2] cycloaddition step reaction involved in the mechanism of enantioselective reduction of ketones with borane catalyzed by a B-methoxy oxazaborolidine catalyst derived from (â€“)âˆ’-pinene: an HMDFT and combined topological ELF, NCI and QTAIM study. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	1
9201	Molecular engineering of indenoindene-3-ethylrodanine acceptors with A2-A1-D-A1-A2 architecture for promising fullerene-free organic solar cells. <i>Scientific Reports</i> , 2021, 11, 20320.	1.6	39
9202	Microscopic Insights into Charge Formation and Energetics in n-Doped Organic Semiconductors. <i>Journal of Physical Chemistry C</i> , 2021, 125, 21824-21830.	1.5	6
9203	Structural Tuning of Curved TFAQ-AQ as a Redox-Active Supramolecular Partner for C ₇₀ Fullerene. <i>Journal of Organic Chemistry</i> , 2021, 86, 14855-14865.	1.7	4
9204	Single crystal inspection, Hirshfeld surface investigation and DFT study of a novel derivative of 4-fluoroaniline: 4-((4-fluorophenyl)amino)-4-oxobutanoic acid (BFAOB). <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 1953-1961.	1.2	21
9205	Water-Induced Chiral Separation on a Au(111) Surface. <i>ACS Nano</i> , 2021, 15, 16896-16903.	7.3	20
9206	Effective Enhancement of the Second-Order Nonlinear Optical Responses of Graphynes by Introducing Î€-Conjugated Chains with Donor/Acceptor Groups. <i>ChemistrySelect</i> , 2021, 6, 10806-10816.	0.7	7
9207	Computational chemistry methods for modelling non-covalent interactions and chemical reactivityâ€” An overview. <i>Journal of the Indian Chemical Society</i> , 2021, 98, 100208.	1.3	22
9208	Yellowâ€”green luminescence of four-coordinate copper(I) complexes bearing Nâ€”heterocyclic carbene (NHC) ligands: Synthesis, photophysical and computational studies. <i>Polyhedron</i> , 2021, 210, 115500.	1.0	4
9209	Theoretical sight into hydrogen bond interactions between arsenious acid and thiols in aqueous and HEPES solutions. <i>Journal of Molecular Liquids</i> , 2021, 344, 117713.	2.3	9
9210	Theoretical insights and quantitative prediction of the nature of boronâ€”chalcogen (O, S, Se, Te) interactions using the electron density and the electron localisation function (ELF). <i>Polyhedron</i> , 2021, 210, 115495.	1.0	4
9211	Synthesis, computational, spectroscopic, hirshfeld surface, electronic state and molecular docking studies on diethyl-5-amino-3-methylthiophene-2,4-dicarboxylate. <i>Chemical Physics Letters</i> , 2021, 784, 139103.	1.2	20
9212	Computational studies of the encapsulation of ibuprofen and paracetamol into cucurbit[7]uril. <i>Computational and Theoretical Chemistry</i> , 2021, 1206, 113465.	1.1	1
9213	Nano-saturn and ExBox systems: Dominant role of steric, exchange-correlation, and electrostatic effects. <i>Chemical Physics Letters</i> , 2021, 785, 139151.	1.2	1

#	ARTICLE	IF	CITATIONS
9214	Insights on the water effect on deep eutectic solvents properties and structuring: The archetypical case of choline chloride+Ethylene glycol. Journal of Molecular Liquids, 2021, 344, 117717.	2.3	52
9215	Theoretical evaluation of the hydrolysis of conventional nerve agents and novichok agents. Chemical Physics Letters, 2021, 785, 139116.	1.2	12
9216	C10F as a potential anode material for alkali-ion batteries; a quantum chemical approach. Computational and Theoretical Chemistry, 2021, 1206, 113470.	1.1	5
9217	Electronic properties of solvents (Water, Benzene, Ethanol) using IEFPCM model, spectroscopic exploration with drug likeness and assessment of molecular docking on 1-Octanesulfonic Acid Sodium Salt. Journal of Molecular Liquids, 2021, 344, 117719.	2.3	13
9218	Quantum Chemical Study of the Role of the van der Waals Interaction (2). Journal of Advances in Physical Chemistry, 2013, 02, 33-39.	0.1	0
9219	Theoretical Study on the Interaction between the M(II)/Al-LDH(M=Zn, Mg) Layer and the Interlayer Anion 1-Anilinonaphthalene-8-Sulfonate (1,8-ANS). Material Sciences, 2013, 03, 199-205.	0.0	0
9220	Quantum Chemical Study of the Role of the Van Der Waals Interaction (3). Journal of Advances in Physical Chemistry, 2013, 02, 47-53.	0.1	0
9222	Analysis and comparison of several methods for calculation of positron bulk lifetime in perfect crystals. Wuli Xuebao/Acta Physica Sinica, 2014, 63, 217804.	0.2	1
9223	Distinct Diameter Dependence of Redox Property for Armchair, Zigzag Single-walled, and Double-walled Carbon Nanotubes. Challenges and Advances in Computational Chemistry and Physics, 2014, , 31-60.	0.6	1
9224	The Singlet-Triplet Splitting of Ethylene Interacting with the Cu(100) Surface and with Small Copper Clusters. Himia, Fizika Ta Tehnologija Poverhni, 2015, 6, 42-55.	0.2	0
9225	Computational Study of Photooxidation of 1,1-dimethylhydrazine by nitromethane. , 0, , .		0
9226	Theoretical study on the polarizability properties of liquid crystal in the THz range. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 143101.	0.2	1
9227	A Quantum Chemistry Study of Hydroge Bonds (2). Journal of Advances in Physical Chemistry, 2016, 05, 58-74.	0.1	3
9228	ADSORPTION MECHANISM AND STRUCTURAL INVESTIGATION OF DOPED C60 FULLERENES WITH PENTYLAMINE. Anadolu University Journal of Sciences & Technology, 0, , 1-1.	0.2	0
9229	The Key Role of Orbital Interaction in Cooperativity between Bâ...â...N and Hydrogen/Lithium Bonding: An ab initio Study. ChemistrySelect, 2017, 2, 9113-9121.	0.7	1
9230	Modeling the photoreduction of amines by the triplet nitromethane. , 0, , .		1
9231	A Quantum Chemistry Study of the Chemical Bond (1). Journal of Advances in Physical Chemistry, 2018, 07, 9-18.	0.1	0
9232	Molecular structure and properties of salt cross-linked polyethylene under external electric field based on density functional theory. Wuli Xuebao/Acta Physica Sinica, 2018, 67, 183101.	0.2	3

#	ARTICLE	IF	CITATIONS
9233	A Quantum Chemistry Study of the Chemical Bond (3). Journal of Advances in Physical Chemistry, 2018, 07, 121-130.	0.1	0
9234	A Quantum Chemistry Study of the Chemical Bond (2). Journal of Advances in Physical Chemistry, 2018, 07, 95-103.	0.1	0
9236	The Effect of CaBr ₂ on Mercury Speciation in Flue Gas: An Experimental and DFT Study. Open Fuels and Energy Science Journal, 2018, 11, 1-15.	0.2	0
9237	Modelado de interacciones del ADN con fármacos de actividad anti-cancerígena mediante el método ONIOM. Revista Vive, 2018, 1, 103-111.	0.1	0
9238	Theoretical study on the hydrogen storage properties of (MgO) ₄ under external electric field. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 163601.	0.2	0
9239	A Quantum Chemistry Study of the Chemical Bond (4). Journal of Advances in Physical Chemistry, 2019, 08, 1-10.	0.1	0
9240	Theoretical Study of Tetrel-Bonding Interactions between H ₃ XF (X = Ge, Si) and Aromatic Ring Compounds. Journal of Advances in Physical Chemistry, 2019, 08, 47-58.	0.1	0
9242	The formation of interstellar organic molecules: H ₂ C ₃ O A DFT and ELF theoretical study. Mediterranean Journal of Chemistry, 2019, 9, 175-189.	0.3	0
9243	A Novel Collector 5-(Butylthio)-1,3,4-thiadiazole-2-thiol: Synthesis and Improved Flotation of Galena and Sphalerite from Pyrite. Minerals, Metals and Materials Series, 2020, , 633-649.	0.3	1
9244	The structural elucidation of aqueous H ₃ BO ₃ solutions by DFT and neutron scattering studies. Physical Chemistry Chemical Physics, 2020, 22, 17160-17170. Ground state structures and properties of Be atom doped boron clusters BeB _n (n = 1-10). \$Z-20201005111348-1\$	1.3	7
9245	Super alkali (O ₃) doped boron nitride with enhanced nonlinear optical behavior. Journal of Nonlinear Optical Physics and Materials, 2020, 29, 2050004. \$Z-20200756_Z-20201005111348-1\$	0.2	4
9247	Super alkali (O ₃) doped boron nitride with enhanced nonlinear optical behavior. Journal of Nonlinear Optical Physics and Materials, 2020, 29, 2050004.	1.1	23
9248	Synthesis and crystallographic, spectroscopic and computational characterization of 3,3',4,4'-substituted biphenyls: effects of O <i>R</i> substituents on the intra-ring torsion angle. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 366-377.	0.5	0
9249	Electronic structural properties of amino/hydroxyl functionalized imidazolium-based bromide ionic liquids. Open Chemistry, 2020, 18, 576-583.	1.0	2
9250	Experimental and theoretical study on p-chlorofluorobenzene in the S ₀ , S ₁ and D ₀ states. Chinese Journal of Chemical Physics, 2020, 33, 401-410.	0.6	0
9251	Synthesis, spectral characterization (FT-IR, FT-Raman and NMR) and Quantum computational analysis of (E)-1-(4-Bromophenyl)-3-(5-bromothiophen-2-yl)prop-2-en-1-one. Chemical Data Collections, 2020, 28, 100415.	1.1	4
9252	Supramolecular assembly of ionic liquid induced by UO ₂ ²⁺ : a strategy for selective extraction-precipitation. Radiochimica Acta, 2020, 108, 757-767.	0.5	6
9253	Complexes of the noble-gas atoms with unsaturated ions: A theoretical investigation on the exemplary (H ₂ C=NH ₂ ⁺)Ar. Chemical Physics Letters, 2020, 752, 137532.	1.2	1

#	ARTICLE	IF	CITATIONS
9254	Excited States Analysis of Polyethylene Molecule with Carbonyl Defects Based on Time-dependent Density Function Theory. , 2020, , .		0
9255	Indium complex with task-specific ionic liquid ligands: Ligand to ligand charge transfer in the excited state investigation and reliable DFT predictions. <i>Journal of Luminescence</i> , 2020, 225, 117391.	1.5	2
9256	Non-covalent binding interaction and mechanism between polycyclic aromatic hydrocarbons and extracellular DNA. <i>Chinese Science Bulletin</i> , 2022, 67, 74-84.	0.4	4
9257	Î±-Cyclodextrin-Catalyzed Symmetry Breaking and Precise Regulation of Supramolecular Self-Assembly Handedness with Harata's Kodaka's Rule. <i>ACS Nano</i> , 2021, 15, 19621-19628.	7.3	12
9258	Removal of nafcillin sodium monohydrate from aqueous solution by hydrogels containing nanocellulose: An experimental and theoretical study. <i>Journal of Molecular Liquids</i> , 2022, 347, 117946.	2.3	5
9259	Waste eliminated by waste under COVID-19 pandemic: Mixed plastic waste derived N,O-rich porous carbon nano-coral reefs for chlorophenol pollutants efficient capture. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 106700.	3.3	3
9260	Theoretical study on mechanism of decomposition reaction of 1,2,4-triazole derivatives. <i>Molecular Physics</i> , 0, , .	0.8	0
9261	Non-covalent interactions of cysteine onto C60, C59Si, and C59Ge: a DFT study. <i>Journal of Molecular Modeling</i> , 2021, 27, 330.	0.8	20
9262	Energetic and Geometric Characteristics of the Substituents: Part 2: The Case of NO ₂ , Cl, and NH ₂ Groups in Their Mono-Substituted Derivatives of Simple Nitrogen Heterocycles. <i>Molecules</i> , 2021, 26, 6543.	1.7	4
9263	Effect of solvent on absorption and emission spectra of 2,2'-Bipyridine and its inclusion complex into Î²-cyclodextrin: DFT and TD-DFT study. <i>Computational and Theoretical Chemistry</i> , 2021, , 113481.	1.1	6
9264	Non-covalent interactions in hexanuclear polyoxidometalates [VIV6B2O5OH8]8-. An experimental and theoretical approach. <i>Polyhedron</i> , 2021, 211, 115553.	1.0	2
9265	Ru doped graphitic carbon nitride mediated peroxy monosulfate activation for diclofenac degradation via singlet oxygen. <i>Chemical Engineering Journal</i> , 2022, 430, 133174.	6.6	29
9266	Bimetallic Ru-Pd and Trimetallic Ru-Pd-Cu Assemblies on the Carborane Cluster Surface. <i>Inorganic Chemistry</i> , 2021, 60, 16911-16916.	1.9	0
9267	Molecular and Spectroscopic Insights into a Metal Salt-Based Deep Eutectic Solvent: A Combined Quantum Theory of Atoms in Molecules, Noncovalent Interaction, and Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9680-9690.	1.1	10
9268	Chalcogen Bond Involving Zinc(II)/Cadmium(II) Carbonate and Its Enhancement by Spodium Bond. <i>Molecules</i> , 2021, 26, 6443.	1.7	6
9269	Tuning azulene defects and doping of N atoms in graphene nanosheets: Improving nonlinear optical properties of carbon-based nano materials. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 136, 115040.	1.3	7
9270	BAl ₄ Mg ³⁺ /O ⁺ : Global Minima with a Planar Tetracoordinate or Hypercoordinate Boron Atom. <i>Atoms</i> , 2021, 9, 89.	0.7	7
9271	DFT Study on the Interaction of Lenalidomide Anticancer Drug on the Surface of B12N12 Nanocluster. <i>Letters in Organic Chemistry</i> , 2022, 19, 583-595.	0.2	4

#	ARTICLE	IF	CITATIONS
9272	Triptycene-Based Porous Chalcogen-Bonded Organic Frameworks. <i>Crystal Growth and Design</i> , 2021, 21, 6497-6503.	1.4	11
9273	Comparative Study of Antioxidant and Pro-Oxidant Properties of Homoleptic and Heteroleptic Copper Complexes with Amino Acids, Dipeptides and 1,10-Phenanthroline: The Quest for Antitumor Compounds. <i>Molecules</i> , 2021, 26, 6520.	1.7	7
9274	Demonstrating the Potential of Alkali Metal-Doped Cyclic C ₆ O ₆ Li ₆ Organometallics as Electrides and High-Performance NLO Materials. <i>ACS Omega</i> , 2021, 6, 29852-29861.	1.6	26
9275	Deciphering the Carrier Transport Properties in Two-Dimensional Perovskites via Surface-Enhanced Raman Scattering. <i>Small</i> , 2021, 17, e2103756.	5.2	4
9276	Salts of purine alkaloids caffeine and theobromine with 2,6-dihydroxybenzoic acid as cofomer: structural, theoretical, thermal and spectroscopic studies. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 713-724.	0.2	3
9277	Non-enzymatic glucose sensors based on Hexa-peri-hexabenzocoronene: A computational study. <i>Chemical Physics</i> , 2022, 553, 111388.	0.9	3
9278	Molecular, Supramolecular Structures Combined with Hirshfeld and DFT Studies of Centrosymmetric M(II)-azido {M=Ni(II), Fe(II) or Zn(II)} Complexes of 4-Benzoylpyridine. <i>Symmetry</i> , 2021, 13, 2026.	1.1	3
9279	The molecular mechanism of electroporation: changes in the hydrogen bonds. <i>Computational and Theoretical Chemistry</i> , 2021, 1207, 113487.	1.1	2
9280	Molecular docking of the Cardenolides of <i>Asclepias subulata</i> in the human p53 protein reveals an interaction in the cleft of the Y220C mutant. <i>Current Chemical Biology</i> , 2021, 15, .	0.2	0
9281	Tumuc1: A New Accurate DNA Force Field Consistent with High-Level Quantum Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7096-7105.	2.3	21
9282	Schiff Bases from Î±-ionone with Adenine, Cytosine, and l-leucine Biomolecules: Synthesis, Structural Features, Electronic Structure, and Medicinal Activities. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 1-22.	1.0	19
9283	Excited-State Dynamics of a <i>meta</i> -Dimethylamino Locked GFP Chromophore as a Fluorescence Turn-on Water Sensor. <i>Photochemistry and Photobiology</i> , 2022, 98, 311-324.	1.3	4
9284	B-F bonding and reactivity analysis of mono- and perfluoro-substituted derivatives of closo-borate anions (6, 10, 12): A computational study. <i>Polyhedron</i> , 2022, 211, 115559.	1.0	8
9285	Electron beam induced degradation of indomethacin in aqueous solution: kinetics, degradation mechanism, and toxicity assessment. <i>Environmental Science and Pollution Research</i> , 2022, 29, 19283-19294.	2.7	2
9286	Photoinduced electron transfer properties of 4-phenyl-Pyridine-N-Oxide and its coordination compound. <i>Dyes and Pigments</i> , 2022, 197, 109917.	2.0	2
9287	Molecular structure, interactions, and antimicrobial properties of curcumin-PLGA Complexes—a DFT study. <i>Journal of Molecular Modeling</i> , 2021, 27, 329.	0.8	4
9288	Bismuth microsphere for photo-assisted nitrate removal: Experimental and theoretical investigations. <i>Chemical Engineering Journal</i> , 2022, 431, 133239.	6.6	3
9289	Assembling Nitrogen-rich, thermally Stable, and insensitive energetic materials by polycyclization. <i>Chemical Engineering Journal</i> , 2022, 431, 133235.	6.6	25

#	ARTICLE	IF	CITATIONS
9290	The theoretical investigation of monohydroxy flavone: A combined DFT and molecular docking study. <i>Journal of Molecular Structure</i> , 2022, 1250, 131823.	1.8	6
9291	C ₁₉ Benzylisoquinoline Alkaloid with Unprecedented Architecture from <i>Hypocoum erectum</i> . <i>Journal of Organic Chemistry</i> , 2021, 86, 16764-16769.	1.7	4
9292	Anatomy of π -hole bonds: Linear systems. <i>Journal of Chemical Physics</i> , 2021, 155, 174302.	1.2	5
9293	Quantum chemical exploration on charge transfer interactions, vibrational, topological and molecular docking evaluation of the antimicrobial molecule 2,4, 6-triallyloxy-1,3,5-triazine. <i>Journal of Molecular Structure</i> , 2022, 1250, 131846.	1.8	1
9294	The synergistic effects of methanesulfonic acid (MSA) and methanesulfinic acid (MSIA) on marine new particle formation. <i>Atmospheric Environment</i> , 2022, 269, 118826.	1.9	8
9295	Understanding the effect of antisolvent on processing window and efficiency for large-area flexible perovskite solar cells. <i>Materials Today Physics</i> , 2021, 21, 100565.	2.9	9
9296	Exploring the structural evolution and electronic properties of medium-sized barium doped magnesium clusters. <i>Journal of Molecular Structure</i> , 2022, 1250, 131836.	1.8	4
9297	Can water molecules bind by the oxygen oxygen covalent bond? A confinement induced bonding. <i>Computational and Theoretical Chemistry</i> , 2021, 1206, 113493.	1.1	2
9298	Computational probe for the geometrical structure and spectroscopic properties of Ga ₂ Mgn ⁺ (n=11) clusters. <i>Computational and Theoretical Chemistry</i> , 2021, 1206, 113500.	1.1	1
9299	Structure and excitation characteristics of C ₅ F ₁₀ O under external electric field based on density functional theory. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2020, 69, 013101.	0.2	3
9300	Insights into directional movement in molecular machines from free-energy calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7888-7893.	1.3	1
9301	Monolayer goldene intercalated in graphene layers. <i>Applied Physics Letters</i> , 2020, 117, .	1.5	4
9302	Structures and Properties of CoB ₁₉ ⁺ Clusters. <i>ACS Omega</i> , 2021, 6, 912-916.	1.6	0
9303	Structure-Dependent Fenton Reactivity and Degradation Pathway of Methylimidazolium Ionic Liquids. <i>ACS ES&T Water</i> , 2021, 1, 808-814.	2.3	0
9304	Structure-Dependent Photoluminescence of Europium(III) Coordination Oligomeric Silsesquioxane: Synthesis and Mechanism. <i>ACS Omega</i> , 2021, 6, 227-238.	1.6	4
9305	Intermolecular interaction on excited-state properties of fluoro-substituted thermally activated delayed fluorescence molecules with aggregation-induced emission: a theoretical perspective. <i>Molecular Physics</i> , 2021, 119, e1862931.	0.8	3
9306	Assessing electronic properties of desymmetrized heterocyclic patterns: towards tuning small molecules for photovoltaic applications. <i>MRS Advances</i> , 2020, 5, 3171-3184.	0.5	0
9307	Low cost prototype simulation of spectrum analyzer base on GNU radio and RTL-SDR. <i>IOP Conference Series: Materials Science and Engineering</i> , 2020, 909, 012011.	0.3	0

#	ARTICLE	IF	CITATIONS
9308	Supramolecular Gold Stripping from Activated Carbon Using β -Cyclodextrin. <i>Journal of the American Chemical Society</i> , 2021, 143, 1984-1992.	6.6	22
9309	Millisecond Time-scale Photoluminescence of N-doped Tetrathienonaphthalene with Borane/Amine Substituents. <i>Inorganic Chemistry</i> , 2021, 60, 1099-1106.	1.9	9
9310	Cooperative interactions of copper chloride aggregation in 1- and 3-hexanol solutions for multinuclear catalytic oxidation. <i>Chemical Physics Letters</i> , 2020, 760, 138025.	1.2	0
9311	Effects of Secondary Acceptors on Excited-State Properties of Sky-Blue Thermally Activated Delayed Fluorescence Molecules: Luminescence Mechanism and Molecular Design. <i>Journal of Physical Chemistry A</i> , 2021, 125, 175-186.	1.1	12
9312	Group 11 metal complexes of the dinucleating triazole appended bisphosphine 1,4-bis(5-(diisopropylphosphaneyl)-1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)benzene. <i>Dalton Transactions</i> , 2021, 50, 16782-16794.	1.6	3
9313	Electro-Optical, Electronic and Conformational Transitions of Interstellar Alkyl Molecules at Different Temperatures: An Ab-Initio Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
9314	Design, synthesis, structural analysis and quantum chemical insight into the molecular structure of coumarin derivatives. <i>Molecular Systems Design and Engineering</i> , 2022, 7, 132-157.	1.7	20
9315	Adaptive aromaticity in 16-valence-electron metallazapentalenes. <i>Dalton Transactions</i> , 2021, 50, 16842-16848.	1.6	7
9316	A DFT-design of single component bifunctional organocatalysts for the carbon dioxide/propylene oxide coupling reaction. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26919-26930.	1.3	7
9317	Direct metal-carbon bonding in symmetric bis(C-H) agostic nickel complexes. <i>Chemical Science</i> , 2021, 12, 15298-15307.	3.7	5
9318	Interaction of krypton and xenon with sodium and activated charcoal: Identification and modeling using gas chromatography and density functional theory. <i>Journal of Nuclear Materials</i> , 2022, 558, 153326.	1.3	2
9319	Mechanochromic luminescent property and anti-counterfeiting application of AIE-active cyclometalated platinum(II) complexes featuring a fused five-six-membered metallacycle. <i>Dyes and Pigments</i> , 2022, 197, 109857.	2.0	13
9320	Ultrabright AIE of Ir(III) complexes achieving expeditious monitoring of oxygen and high-definition development of latent fingerprints. <i>Sensors and Actuators B: Chemical</i> , 2022, 350, 130894.	4.0	16
9321	A novel phenoxazine-Meldrum's acid D-A fluorescent sensor for α -turn-on-detecting hydrazine and its applications to practical samples analysis, plant and animal imaging. <i>Sensors and Actuators B: Chemical</i> , 2022, 350, 130850.	4.0	13
9322	Convolutional neural networks for the design and analysis of nonfullerene acceptors. , 2022, , 231-256.		25
9323	Zn(II) complexes based on functional organic ligands: Two-photon activity, theoretical calculation and bioimaging. <i>Dyes and Pigments</i> , 2022, 197, 109878.	2.0	1
9324	Polymorphism and light conversion properties of anthracene-based isomers. <i>Dyes and Pigments</i> , 2022, 197, 109888.	2.0	5
9325	Is nitrogen in ammonia an elusive electron accepting nitrogen in a predominantly phosphorus bonded $PCl_3:NH_3$ dimer?. <i>Chemical Physics Letters</i> , 2022, 786, 139192.	1.2	5

#	ARTICLE	IF	CITATIONS
9326	First-principles calculations of nickel, cadmium, and lead nanoclusters adsorption on single-wall (10,0) boron-nitride nanotube. <i>Applied Surface Science</i> , 2022, 573, 151547.	3.1	7
9327	A novel perspective on interfacial interactions between polypyrrole and carbon materials for improving performance of supercapacitors. <i>Applied Surface Science</i> , 2022, 573, 151626.	3.1	13
9328	Prominent dual Z-scheme mechanism on phase junction WO ₃ /CdS for enhanced visible-light-responsive photocatalytic performance on imidacloprid degradation. <i>Separation and Purification Technology</i> , 2022, 281, 119863.	3.9	76
9329	Comparison results of eight oxygenated organic molecules: Unexpected contribution to new particle formation in the atmosphere. <i>Atmospheric Environment</i> , 2022, 268, 118817.	1.9	5
9330	Theoretical comparative survey on the structure and electronic properties of first row transition metal substituted Keggin type polyoxometalates. <i>Journal of Solid State Chemistry</i> , 2022, 305, 122667.	1.4	4
9331	Persulfate activation by novel iron-carbon composites for organic contaminant removal: Performance, mechanism, and DFT calculations. <i>Separation and Purification Technology</i> , 2022, 281, 119962.	3.9	25
9332	New benzyltriethylammonium/urea deep eutectic solvent: Quantum calculation and application to hydroxylethylcellulose modification. <i>Carbohydrate Polymers</i> , 2022, 276, 118737.	5.1	7
9333	The structure and spectroscopic properties of the metallophilic Pt/Pd complexes based on pyridine/pyrazol ligands: A computational investigation. <i>Inorganica Chimica Acta</i> , 2022, 529, 120663.	1.2	0
9334	Unravelling the non-covalent interactions in certain n-propyl amine ether systems through acoustic and DFT studies at 303.15 K. <i>Journal of Molecular Liquids</i> , 2022, 345, 117806.	2.3	7
9335	Polymorphism-dependent fluorescent emission, acid/base response and selective fluorescent sensor for Cu ²⁺ ions based on single-benzene framework. <i>Dyes and Pigments</i> , 2022, 197, 109903.	2.0	13
9336	Analysis of structural conformation and supramolecular self-assembly of novel oxalate-bridged tetranuclear Cu(II) complex by combined crystallographic and computational studies. <i>Journal of Molecular Structure</i> , 2022, 1250, 131658.	1.8	0
9337	Diverse coordination of isoniazid hydrazone Schiff base ligand towards iron(III): Synthesis, characterization, SC-XRD, HSA, QTAIM, MEP, NCI, NBO and DFT study. <i>Journal of Molecular Structure</i> , 2022, 1250, 131691.	1.8	44
9338	Dual-layered composite nanofiber membrane with Cu-BTC-modified electrospun nanofibers and biopolymeric nanofibers for the removal of uremic toxins and its application in hemodialysis. <i>Journal of Membrane Science</i> , 2022, 642, 119964.	4.1	24
9339	DFT assisted study on activation of surface acidic -COOH debris in graphene oxide supported catalyst for benzyl alcohol oxidation. <i>Journal of Molecular Structure</i> , 2022, 1249, 131620.	1.8	7
9340	Analysis of the combustion mechanism of diesel surrogate fuel under CO ₂ /O ₂ atmosphere. <i>Fuel</i> , 2022, 309, 122223.	3.4	5
9341	Baso-chromic spiropyrrolizine: The spiromerocyanine isomerization and alkaline detection. <i>Journal of Molecular Structure</i> , 2022, 1250, 131631.	1.8	3
9342	Theoretical study on the C ₄ alkylation mechanism catalyzed by Cu-containing chloroaluminate ionic liquids. <i>Fuel</i> , 2022, 310, 122379.	3.4	8
9343	Biochar co-doped with nitrogen and boron switching the free radical based peroxydisulfate activation into the electron-transfer dominated nonradical process. <i>Applied Catalysis B: Environmental</i> , 2022, 301, 120832.	10.8	165

#	ARTICLE	IF	CITATIONS
9344	Combined gas-phase electron diffraction and coupled cluster determination of the molecular structure of 3,4-dinitrofurazan - A propellant ingredient. <i>Journal of Molecular Structure</i> , 2022, 1250, 131669.	1.8	2
9345	Schiff base-type copper(I) complexes exhibiting high molar extinction coefficients: Synthesis, characterization and DFT studies. <i>Journal of Molecular Structure</i> , 2022, 1249, 131638.	1.8	5
9346	Structure analysis of aqueous Mg(NO ₃) ₂ solutions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 267, 120478.	2.0	5
9347	Contrasting effects of microplastic aging upon the adsorption of sulfonamides and its mechanism. <i>Chemical Engineering Journal</i> , 2022, 430, 132939.	6.6	55
9348	Micro-phase separation promoted by electrostatic field in electrospinning of alkaline polymer electrolytes: DFT and MD simulations. <i>Chemical Engineering Science</i> , 2022, 248, 117171.	1.9	9
9349	Facile immobilization of ethylenediamine tetramethylene-phosphonic acid into UiO-66 for toxic divalent heavy metal ions removal: An experimental and theoretical exploration. <i>Science of the Total Environment</i> , 2022, 806, 150652.	3.9	43
9350	Supramolecular structure of the product of unusual [2C=C+2C=N] cycloaddition of dicyclohexylcarbodiimide to N-(3-methylbut-2-en-1-ylidene)triflamide. <i>Journal of Molecular Structure</i> , 2022, 1250, 131676.	1.8	4
9351	Study on the reaction mechanism of CH ₂ O+NO ₂ transformed by PbO/SnO in double-base propellants through theoretical calculation and experiment. <i>Combustion and Flame</i> , 2022, 236, 111768.	2.8	4
9352	Structure-property relationship in thioxotriaza-spiro derivative: Crystal structure and molecular docking analysis against SARS-CoV-2 main protease. <i>Journal of Molecular Structure</i> , 2022, 1250, 131746.	1.8	8
9353	Potential optical molecular switch: Lithium@cyclo[18]carbon complex transforming between two stable configurations. <i>Carbon</i> , 2022, 187, 78-85.	5.4	109
9354	Superalkali-based alkalides Li ₃ O@[12-crown-4]M (where M= Li, Na, and K) with remarkable static and dynamic NLO properties; A DFT study. <i>Materials Science in Semiconductor Processing</i> , 2022, 138, 106254.	1.9	35
9355	Experimental and theoretical calculations study on heterogeneous reduction of NO by char/NH ₃ in the reduction zone of ammonia co-firing with pulverized coal: Influence of mineral Fe. <i>Fuel</i> , 2022, 310, 122374.	3.4	31
9356	Tactfully unveiling the effect of solvent polarity on the ESIPT mechanism and photophysical property of the 3-hydroxyflavone derivative. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 267, 120496.	2.0	8
9357	Insights into the mechanism during viscosity reduction process of heavy oil through molecule simulation. <i>Fuel</i> , 2022, 310, 122270.	3.4	27
9358	A novel solid-liquid phase controllable biphasic amine absorbent for CO ₂ capture. <i>Chemical Engineering Journal</i> , 2022, 430, 132932.	6.6	38
9359	Insights into the interaction between NO and char(N) containing different functional forms: Mechanistic, thermodynamic and kinetic studies. <i>Combustion and Flame</i> , 2022, 237, 111823.	2.8	13
9360	Study on simultaneous binding of resveratrol and curcumin to Î²-lactoglobulin: Multi-spectroscopic, molecular docking and molecular dynamics simulation approaches. <i>Food Hydrocolloids</i> , 2022, 124, 107331.	5.6	46
9361	Theoretical and practical aspects of indirect spin-spin couplings. <i>Nuclear Magnetic Resonance</i> , 2020, , 34-75.	0.1	0

#	ARTICLE	IF	CITATIONS
9362	Equilibrium Cd isotopic fractionation between Cd(OH) ₂ (s), apatite, adsorbed Cd ²⁺ , and Cd ²⁺ (aq): Potential application of ¹¹⁴ Cd in evaluating the effectiveness of Cd-contamination remediation. <i>Geochemical Journal</i> , 2020, 54, 289-297.	0.5	1
9363	A new heteroleptic phosphorescent cuprous complex supported by a BINAP ligand: synthesis, structure, luminescence properties and theoretical analyses. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 177-185.	0.2	4
9364	Quantum chemistry calculations of the growth patterns, simulated photoelectron spectra, and electronic properties of LaASi _x (A = Sc, Y, La; x = 10) compounds and their anions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25679-25688.	1.3	2
9365	The sensing mechanism of pristine and transition metals doped ZnO, SnO and NiO nanocages towards NH ₃ and PH ₃ : a DFT study. <i>Journal of Materials Chemistry C</i> , 2021, 9, 17382-17391.	2.7	7
9366	Triel bonds within anion- $\hat{A}\hat{A}$ -anion complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25097-25106.	1.3	6
9367	Planar hexacoordinate gallium. <i>Chemical Science</i> , 2021, 12, 15067-15076.	3.7	15
9368	Thermally activated delayed fluorescence materials with aggregation-induced emission properties: a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25789-25796.	1.3	10
9369	Photoinduced azobenzene-modified DNA dehybridization: insights into local and cooperativity effects from a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25170-25179.	1.3	7
9370	Probing the role of surface acid sites on the photocatalytic degradation of tetracycline hydrochloride over cerium doped CdS <i>via</i> experiments and theoretical calculations. <i>Dalton Transactions</i> , 2021, 50, 16620-16630.	1.6	9
9371	Mechanisms and Origins of Regioselectivities of Nickel-Catalyzed \hat{I}^2, \hat{I} -Vinylarylation of Alkenyl Esters with Vinyl Triflates and Arylzinc Reagents. <i>Organic Chemistry Frontiers</i> , 0, , .	2.3	2
9372	An ionic hydrogel with stimuli-responsive, self-healable and injectable characteristics for the targeted and sustained delivery of doxorubicin in the treatment of breast cancer. <i>Materials Advances</i> , 2022, 3, 632-646.	2.6	13
9373	Highly efficient carbazoylgold(<i>iii</i>) dendrimers based on thermally activated delayed fluorescence and their application in solution-processed organic light-emitting devices. <i>Chemical Science</i> , 2021, 12, 14833-14844.	3.7	14
9374	Distinct binding modes of pesticides affect the phase transition of lysozyme. <i>CrystEngComm</i> , 0, , .	1.3	0
9375	Bridged and fused triazolic energetic frameworks with an azo building block towards thermally stable and applicable propellant ingredients. <i>Journal of Materials Chemistry A</i> , 2021, 9, 24903-24908.	5.2	22
9376	Density Functional Theory Calculation Aided Screening of SARS-CoV-2 RNA Polymerase Inhibitors. <i>Hans Journal of Medicinal Chemistry</i> , 2020, 08, 29-37.	0.0	0
9377	Density functional theory studies on the excited-state properties of Bilirubin molecule. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2020, 69, 163101.	0.2	0
9378	Density functional theory calculation of spectrum and excitation properties of mer-Alq ₃ . <i>Wuli Xuebao/Acta Physica Sinica</i> , 2020, 69, 023101.	0.2	1
9379	Seeing Delocalized $\hat{E}36$ Bond in OX ₂ (X=Halogen) Molecules. <i>Chinese Journal of Chemical Physics</i> , 0, , .	0.6	1

#	ARTICLE	IF	CITATIONS
9380	Axial Strain Tuning of the Electronic and Structural Properties of a (6,0) Silicon Carbide Nanotube Containing an Ionic Si-C Bond: A Quantum Chemical Approach. <i>Journal of Structural Chemistry</i> , 2020, 61, 8-19.	0.3	0
9381	DFT and NBO Studies of Stability, Electronic, and Structural Features of the 2-fluoroacetaldehyde Conformers. <i>Egyptian Journal of Chemistry</i> , 2020, 63, 315-324.	0.1	1
9382	The photoelectron-imaging spectroscopic study and chemical bonding analysis of VO_2^+ , NbO_2^+ and TaO_2^+ . <i>RSC Advances</i> , 2020, 10, 41612-41617.	1.7	1
9383	Structural properties of the chelating agent 2,6-bis(1-(3-hydroxypropyl)-1,2,3-triazol-4-yl)pyridine: a combined XRD and DFT structural study. <i>RSC Advances</i> , 2020, 10, 19629-19635.	1.7	2
9385	A motif for heteronuclear $\text{C}\ddot{\text{E}}\text{E}$ (E = Si, Ge, Sn, Pb) bonding: Lewis acid-base pair strategy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26720-26727.	1.3	1
9387	Exploiting $\ddot{\text{f}}$ -hole interaction to design small uncharged ligand molecules to stabilize G-quadruplex-DNA: a computational study. <i>Journal of Molecular Modeling</i> , 2020, 26, 38.	0.8	1
9388	Aporphinoid Alkaloids Derivatives as Selective Cholinesterases Inhibitors: Biological Evaluation and Docking Study. <i>Molecular Informatics</i> , 2020, 39, e1900125.	1.4	4
9390	Efficiently luminescent heteroleptic neutral platinum(II) complexes based on N^{O} and N^{P} benzimidazole ligands. <i>Dalton Transactions</i> , 2021, 50, 17319-17327.	1.6	5
9391	Diboron-controlled product selectivity switch in copper-catalyzed decarboxylative substitutions of alkynyl cyclic carbonates. <i>Organic Chemistry Frontiers</i> , 2021, 8, 6950-6961.	2.3	3
9392	Cu^{II} ion induced self-polymerization of Cu phthalocyanine to prepare low-cost organic cathode materials for Li-ion batteries with ultra-high voltage and ultra-fast rate capability. <i>Journal of Materials Chemistry A</i> , 2021, 9, 24915-24921.	5.2	5
9393	Screening RAFT agents and photocatalysts to mediate PET-RAFT polymerization using a high throughput approach. <i>Polymer Chemistry</i> , 2021, 12, 6548-6560.	1.9	15
9394	Substituente en isomeriële effekte op die reduksie van oksidasiepotensiaal van tris(I^2 -diketonato) mangaan(III) komplekse: DFT en MESP analises. <i>South African Journal of Science and Technology</i> , 2020, 119-133.	0.1	0
9395	Cis ve Trans Formundaki 5-Floropirimidin-2-Karboksilik Asit Moleküllerinin DFT/TD-DFT ve NBO Analizleri. <i>Bitlis Eren Üniversitesi Fen Bilimleri Dergisi</i> , 2020, 9, 120-129.	0.1	0
9396	Density functional theory study of donor-acceptor conjugated polymers with substituent effect. <i>Journal of Polymer Research</i> , 2021, 28, 1.	1.2	4
9397	Nontraditional Luminescent Molecular Aggregates Encapsulated by Wormlike Silica Nanoparticles for Latent Fingerprint Detection. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 51695-51707.	4.0	10
9398	Experimental Observation and Energy Performance Calculations of Potential Oxidants O_4^+ and O_6^+ Clusters. <i>FirePhysChem</i> , 2021, , .	1.5	1
9399	How do molecular interactions affect fluorescence behavior of AlEgens in solution and aggregate states?. <i>Science China Chemistry</i> , 2022, 65, 135-144.	4.2	31
9400	Efficient naphthenic acid extraction from high acidic oil using novel 1,5-diazabicyclo[4.3.0]non-5-ene based ionic liquids. <i>Journal of Cleaner Production</i> , 2021, 328, 129634.	4.6	8

#	ARTICLE	IF	CITATIONS
9401	A solar-to-chemical conversion efficiency up to 0.26% achieved in ambient conditions. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	37
9402	Flexible Electron-Rich Ion Channels Enable Ultrafast and Stable Aqueous Zinc-Ion Storage. ACS Applied Materials & Interfaces, 2021, 13, 54096-54105.	4.0	10
9403	New Energetic Metal-Organic Framework (E-MOF) based on a sodium(I)-containing energetic metal salt incorporating guanidinium ions. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 0, , .	0.6	0
9404	Solvent-Dependent Photophysical Properties of a Semiconducting One-Dimensional Silver Cluster-Assembled Material. Inorganic Chemistry, 2021, 60, 18234-18241.	1.9	11
9405	Dual optimization approach to Mo single atom dispersed g-C ₃ N ₄ photocatalyst: Morphology and defect evolution. Applied Catalysis B: Environmental, 2022, 303, 120904.	10.8	203
9406	Mercaptopropionic acid-modified oleic imidazoline as a highly efficient corrosion inhibitor for carbon steel in CO ₂ -saturated formation water. Corrosion Science, 2022, 194, 109930.	3.0	42
9407	Color-Tunable Dual Persistent Emission Via a Triplet Exciton Reservoir for Temperature Sensing and Anti-Counterfeiting. Advanced Optical Materials, 2022, 10, 2101773.	3.6	34
9408	Supramolecular tessellations by the exo-wall interactions of pagoda[4]arene. Nature Communications, 2021, 12, 6378.	5.8	32
9409	Degradation of enrofloxacin in aqueous by DBD plasma and UV: Degradation performance, mechanism and toxicity assessment. Chemical Engineering Journal, 2022, 431, 133360.	6.6	29
9410	Synthesis, single crystal, characterization and computational study of 2-amino-N-cyclopropyl-5-ethyl-thiophene-3-carboxamide. Journal of Molecular Structure, 2022, 1250, 131890.	1.8	27
9411	Interaction mechanism of phenolic acids and zein: A spectrofluorometric and molecular dynamics investigation. Journal of Molecular Liquids, 2022, 348, 118032.	2.3	11
9412	The analyses of solvent effects on infrared spectra and thermodynamic parameters, Hirshfeld surface, reduced density gradient and molecular docking of ketoprofen as a member of nonsteroidal anti-inflammatory drugs. Journal of Molecular Structure, 2021, , 131861.	1.8	5
9413	Self-assembled Bi ₂ SeO ₅ /rGO/MIL-88A Z-scheme heterojunction boosting carrier separation for simultaneous removal of Cr (VI) and chloramphenicol. Chemical Engineering Journal, 2022, 431, 133289.	6.6	8
9414	Assessing Effects of Different ĩ bridges on Properties of Random Benzodithiophene-thienothiophene Donor and Non-fullerene Acceptor Based Active Layer. Journal of Physical Chemistry A, 2021, 125, 9852-9864.	1.1	0
9415	Synthesis of azido-dienediols by enzymatic dioxygenation of benzylazides: an experimental and theoretical study. European Journal of Organic Chemistry, 0, , .	1.2	1
9416	Exploring Guest-Host Interactions in Gas Hydrates: Insights from Quantum Mechanics. Energy & Fuels, 2021, 35, 18604-18614.	2.5	5
9417	Brightly Luminescent Platinum Complexes of N ³ C ³ N ³ Ligands Forming Six-Membered Chelate Rings: Offsetting Deleterious Ring Size Effects Using Site-Selective Benzannulation. Inorganic Chemistry, 2021, 60, 16881-16894.	1.9	10
9418	Rational Design and Characterization of Symmetry-Breaking Organic Semiconductors in Polymer Solar Cells: A Theory Insight of the Asymmetric Advantage. Materials, 2021, 14, 6723.	1.3	21

#	ARTICLE	IF	CITATIONS
9419	MOF-derived 3D porous carbon aerogels as an efficient adsorbent for toluene in humid air. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 106722.	3.3	8
9420	Synthesis, Reactivity, and Properties of a Class of π -Extended BODIPY Derivatives. <i>Journal of Organic Chemistry</i> , 2021, 86, 17110-17118.	1.7	11
9421	Structural and Electronic Properties of Single-Atom Transition Metal-Doped Boron Clusters MB ₂₄ (M = Sc, V, and Mn). <i>ACS Omega</i> , 2021, 6, 30442-30450.	1.6	4
9422	Revealing the Photophysical Dynamics of Selected Rigid Donor–Acceptor Systems: From Ligands to Ruthenium(II) Complexes. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 10927-10935.	2.1	3
9423	Exploration of promising optical and electronic properties of (non-polymer) small donor molecules for organic solar cells. <i>Scientific Reports</i> , 2021, 11, 21540.	1.6	46
9424	Interaction between favipiravir and hydroxychloroquine and their combined drug assessment: in silico investigations. <i>Chemical Papers</i> , 2022, 76, 1471-1478.	1.0	13
9425	Azobenzene-Iron(III)porphyrin Hybrid Composite as a Light-Driven Molecular Spin Regulator: Some Promising Insights from DFT. <i>Chemistry of Materials</i> , 2021, 33, 8786-8799.	3.2	4
9426	Experimental and in silico studies of competitive inhibition of family GH10 <i>Aspergillus fumigatus</i> xylanase A by <i>Oryza sativa</i> xylanase inhibitor protein. <i>International Journal of Biological Macromolecules</i> , 2021, 193, 1391-1399.	3.6	5
9427	Photocatalytic application of graphene oxide–ZnO nanocomposite for the reduction of methylene blue dye. <i>Functional Composites and Structures</i> , 2021, 3, 045006.	1.6	1
9428	Theoretical study of cellulose II nanocrystals with different exposed facets. <i>Scientific Reports</i> , 2021, 11, 21871.	1.6	4
9429	Structural, spectroscopic, and in silico studies of 3-(dimethylamino)-1-(thiophen-2-yl)propan-1-ol: A potential antidepressant agent. <i>Journal of Molecular Structure</i> , 2022, 1250, 131859.	1.8	3
9430	Exploring key reaction sites and deep degradation mechanism of perfluorooctane sulfonate via peroxymonosulfate activation under electrocoagulation process. <i>Water Research</i> , 2021, 207, 117849.	5.3	32
9431	A Naphthalimide–Based Fluorescent Probe for the Detection and Imaging of Mercury Ions in Living Cells. <i>ChemistryOpen</i> , 2021, 10, 1116-1122.	0.9	11
9432	Synthesis, biological assay, chemical descriptors, and molecular docking calculations of novel copper(II) mixed-ligand complexes of n-benzoyl-dl-phenylalanine and n-heterocyclic nitrogen bases. <i>Journal of Molecular Structure</i> , 2022, 1250, 131854.	1.8	7
9433	FeN ₄ -doped carbon nanotubes derived from metal organic frameworks for effective degradation of organic dyes by peroxymonosulfate: Impacts of FeN ₄ spin states. <i>Chemical Engineering Journal</i> , 2022, 431, 133339.	6.6	13
9434	Novel Insights into the Self-assembly Behaviors of Cationic Surfactant and Bivalent Acid: Effects of Group Positions in Bivalent Acid. <i>Journal of Molecular Liquids</i> , 2021, , 118012.	2.3	0
9435	Effect of donor and acceptor on optoelectronic properties of benzo[1,2-b:4,5-b']dithiophene. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	4
9436	Tris(6-diphenylphosphinoacenaphth-5-yl)gallium: Z-Type Ligand and Transmetalation Reagent. <i>Organometallics</i> , 2021, 40, 3785-3796.	1.1	3

#	ARTICLE	IF	CITATIONS
9437	Picomolar-sensitive β -amyloid fibril fluorophores by tailoring the hydrophobicity of biannulated β -elongated dioxaborine-dyes. <i>Bioactive Materials</i> , 2022, 13, 239-248.	8.6	15
9438	Extraction separation of aromatic homologues from n-decane using DMSO: Influence of the alkyl side chain length. <i>Journal of Chemical Thermodynamics</i> , 2021, 166, 106673.	1.0	2
9439	XNgNSi (X = HCC, F; Ng = Kr, Xe, Rn): A New Class of Metastable Insertion Compounds Containing Ng σ -C/F and Ng σ -N Bonds and Possible Isomerization therein. <i>Journal of Physical Chemistry A</i> , 2021, , .	1.1	2
9440	Novel microporous B6N6 covalent organic framework (COF) as an electrochemical sensor for the ultra-selective detection of nitroaniline isomers; a DFT outcome. <i>Surfaces and Interfaces</i> , 2021, 27, 101587.	1.5	14
9441	A Localized Planarization Strategy in Hole Mobility Modulation of Disordered Triphenylamine σ -Based Organic Semiconductors. <i>Advanced Theory and Simulations</i> , 2021, 4, 2100236.	1.3	0
9442	Alkaline Earth Cations Binding Mode Tailors Excited-State Charge Transfer Properties of Guanine Quadruplex: A TDDFT Study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, , 120584.	2.0	0
9443	Understanding Hygroscopicity of Theophylline <i>via</i> a Novel Cocrystal Polymorph: A Charge Density Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9736-9756.	1.1	6
9444	The theoretical investigation of the opto-electronic properties of designed molecules having 2-(2-Methylene-3-oxo-indane-1-ylidene)malononitrile as end-capped acceptors. <i>Zeitschrift Fur Physikalische Chemie</i> , 2021, 235, 785-804.	1.4	0
9445	The theoretical investigation of the opto-electronic properties of designed molecules having 2-(2-Methylene-3-oxo-indane-1-ylidene)malononitrile as end-capped acceptors. <i>Zeitschrift Fur Physikalische Chemie</i> , 2020, .	1.4	0
9448	DENSITY FUNCTIONAL THEORY INVESTIGATION OF DOUBLE SILICON DECORATED FULLERENES AND SINGLE WALLED CARBON NANOTUBES FOR THE DETECTION AND ADSORPTION OF IBUPROFEN. <i>EskiÅŸehir Teknik Åœniversitesi Bilim Ve Teknoloji Dergisi B - Teorik Bilimler</i> , 0, , .	0.0	0
9449	Difluorochloronium(III) Fluoridometallates σ from Molecular Building Blocks to (Helical) Chains. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 4483-4496.	1.0	2
9450	Ionization and dissociation of benzene and aniline under deep ultraviolet laser irradiation. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 583-589.	0.6	2
9451	Multiphase structural models and hyperpolarizability calculations explain second-order nonlinear optical properties of stilbazolium ions. <i>Physical Review Materials</i> , 2020, 4, .	0.9	4
9452	ANALYSIS OF LOCALIZED ORBITALS IN AZABORA DERIVATIVES OF [8] ANNULENE: IN THE VIEWPOINT OF AROMATICITY AND INDUCED RING CURRENTS. <i>Journal of Structural Chemistry</i> , 2020, 61, 1551-1567.	0.3	3
9453	Die grÅŸenbeschleunigte kinetische Racematspaltung sekundÅœrer Alkohole. <i>Angewandte Chemie</i> , 2021, 133, 786-791.	1.6	4
9454	A theoretical study for the role of complex in hydrogen abstraction of OH. <i>Chemical Physics Letters</i> , 2020, 759, 138035.	1.2	1
9455	Position isomers of Ru(II) polypyridine complexes with tunable photophysical properties, aggregation-induced phosphorescence enhancement and application in triplet-triplet annihilated upconversion. <i>Dyes and Pigments</i> , 2020, 180, 108489.	2.0	4
9456	Non-fullerene electron acceptors constructed by four strong electron-withdrawing end groups: Potential to improve the photoelectric performance of organic solar cells by theoretical investigations. <i>Dyes and Pigments</i> , 2020, 181, 108542.	2.0	7

#	ARTICLE	IF	CITATIONS
9457	The structures and nonlinear optical responses of superalkali-doped graphyne and boron-doped graphyne: A density functional study. <i>Optik</i> , 2020, 220, 164947.	1.4	4
9458	Vibrational (FT-IR, FT Raman), electronic and docking studies and wave function analysis with quantum chemical computation on 3-Bromophenyl acetic acid: A potential amidase inhibitor. <i>Materials Today: Proceedings</i> , 2022, 50, 2853-2864.	0.9	1
9459	Screening and Analysis of Hypolipidemic Components from Shuangdan Capsule Based on Pancreatic Lipase. <i>Current Bioinformatics</i> , 2020, 15, 478-492.	0.7	3
9460	Synthesis and photophysical properties of linear gold(^I) complexes based on a CCC carbene. <i>Dalton Transactions</i> , 2021, 50, 17156-17164.	1.6	7
9461	New perspective on the laser initiation for metal tetrazine complexes: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2021, , .	1.3	1
9462	Unusual chalcogen-chalcogen interactions in like-like and unlike Y ₂ Y ₂ complexes (Y = O, S, and Se). <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3386-3399.	1.3	11
9463	Appraising the Potency of Small Molecule Inhibitors and Their Graphene Surface-Mediated Organizational Attributes on Uric Acid-Melamine Clusters. <i>Physical Chemistry Chemical Physics</i> , 2021, , .	1.3	1
9464	The reactivity of Nb _n ⁺ clusters with acetylene and ethylene to produce a cubic aromatic metal carbide Nb ₄ C ₄ ⁺ . <i>New Journal of Chemistry</i> , 2021, 45, 21844-21851.	1.4	3
9465	Theoretical probing of twenty-coordinate actinide-centered boron molecular drums. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26967-26973.	1.3	8
9466	Unveiling the mechanisms of organic room-temperature phosphorescence in various surrounding environments: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26813-26821.	1.3	6
9467	Low efficiency roll-off blue TADF OLEDs employing a novel acridine-pyrimidine based high triplet energy host. <i>Journal of Materials Chemistry C</i> , 2021, 9, 17471-17482.	2.7	14
9468	A new sterically hindered asymmetric zinc phthalocyanine as an efficient sensitizer for dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2022, 46, 714-725.	1.4	16
9469	Luminescent 2-phenylbenzothiazole cyclometalated Pt ^{II} and Ir ^{III} complexes with chelating P ⁺ O ligands. <i>Dalton Transactions</i> , 2021, 51, 274-285.	1.6	7
9470	Highly efficient blue electroluminescence based on TADF emitters with spiroacridine donors: methyl group effect on photophysical properties. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4614-4619.	2.7	7
9471	Understanding gas absorption in multivalent ionic liquids via solute-solvent interaction analyses. <i>Chemical Physics Letters</i> , 2022, 786, 139204.	1.2	7
9472	Organic microporous crystals driven by pure C-H...I interactions with vapor-induced crystal-to-crystal transformations. <i>Materials Horizons</i> , 2022, 9, 731-739.	6.4	14
9473	Identification of raloxifene as a novel α -glucosidase inhibitor using a systematic drug repurposing approach in combination with cross molecular docking-based virtual screening and experimental verification. <i>Carbohydrate Research</i> , 2022, 511, 108478.	1.1	4
9474	Study on thermodynamic property of pyrrolylaldiminato dialkyl-aluminum (Methyl- and Ethyl-) Tj ETQq1 1 0.784314 _{rgBT} /Overlock 10	0.8	3

#	ARTICLE	IF	CITATIONS
9475	A mechanistic study on the regioselective Ni-catalyzed methylation-alkenylation of alkyne with AlMe ₃ and allylic alcohol. <i>Organic Chemistry Frontiers</i> , 2021, 9, 163-172.	2.3	9
9476	Determination of dopamine based on a temperature-sensitive PMEO ₂ MA and Au@rGO-MWCNT nanocomposite-modified electrode. <i>Analyst</i> , 2022, 147, 303-311.	1.7	6
9477	Mechanisms of asymmetric sulfa-Michael additions between phenylacetylene and thioacetic acid: A DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2022, 1207, 113523.	1.1	3
9478	DFT study of interaction of Palladium Pd _n (n = 1-6) nanoparticles with deep eutectic solvents. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 110, 108072.	1.3	3
9479	Molecular insight into the fluidity of cement pastes: Nano-boundary lubrication of cementitious materials. <i>Construction and Building Materials</i> , 2022, 316, 125800.	3.2	37
9480	Theoretical studies on dicopper(II) complexes of phenoxido-bridged ligands: Magneto-structural correlations. <i>Computational and Theoretical Chemistry</i> , 2022, 1207, 113524.	1.1	6
9481	Theoretical investigations of the interaction between B ₉ N ₉ ring and nine adamantane derivatives. <i>Computational and Theoretical Chemistry</i> , 2022, 1207, 113512.	1.1	7
9482	Role of Iodo-Substituted Subphthalocyanine (Subpcs) π -conjugated aromatic N-fused di-iminoisoidole units on the performance of non-fullerene small organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2022, 1207, 113508.	1.1	18
9483	Jellynolide A, pokepola esters, and sponalisolides from the aquaculture sponge <i>Spongia officinalis</i> L. <i>Phytochemistry</i> , 2022, 194, 113006.	1.4	3
9484	Synthesis and enhanced nonlinear optical performance of phthalocyanine indium polymers with electron-donating group porphyrin by efficient energy transfer. <i>Dyes and Pigments</i> , 2022, 198, 109985.	2.0	11
9485	Fabrication of novel anti-fouling poly(m-phenylene isophthalamide) ultrafiltration membrane modified with Pluronic F127 via coupling phase inversion and surface segregation. <i>Separation and Purification Technology</i> , 2022, 282, 120106.	3.9	20
9486	Two-photon excited fluorescence from ground-state charge-transfer cocrystals of acridine and 1,2,4,5-tetracyano-benzene. <i>Dyes and Pigments</i> , 2022, 198, 109965.	2.0	6
9487	Molecular design for organic luminogens with efficient emission in solution and solid-state. <i>Dyes and Pigments</i> , 2022, 198, 109958.	2.0	31
9488	Removal of impurities from bismuth pickling solution using solvent extraction with TBP. <i>Hydrometallurgy</i> , 2022, 207, 105779.	1.8	4
9489	Molecular insights into the uptake of SiO ₂ nanoparticles on phospholipid membrane: Effect of surface properties and particle size. <i>Colloids and Surfaces B: Biointerfaces</i> , 2022, 210, 112250.	2.5	10
9490	Pt(II) diimine complexes bearing varied alkyl chains: Synthesis, tunable photophysical properties and aggregation-induced optical power limiting enhancement. <i>Inorganica Chimica Acta</i> , 2022, 531, 120714.	1.2	0
9491	Quantitative structure-retention relationship for reliable metabolite identification and quantification in metabolomics using ion-pair reversed-phase chromatography coupled with tandem mass spectrometry. <i>Talanta</i> , 2022, 238, 123059.	2.9	11
9492	A comparative study on the autoignition characteristics of cyclopropane and propane at high temperatures. <i>Combustion and Flame</i> , 2022, 237, 111881.	2.8	9

#	ARTICLE	IF	CITATIONS
9493	Revealing the dissolution behavior of trans-p-methoxycinnamic acid in 12 organic solvents by parametric model and molecular simulation. <i>Journal of Chemical Thermodynamics</i> , 2022, 166, 106683.	1.0	5
9494	Degradation of diclofenac sodium by the UV/chlorine process: Reaction mechanism, influencing factors and toxicity evaluation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 425, 113667.	2.0	9
9495	The role of H ₂ O in NO formation and reduction during oxy-steam combustion of bituminous coal char. <i>Combustion and Flame</i> , 2022, 237, 111883.	2.8	14
9496	A fully integrated graphene-polymer field-effect transistor biosensing device for on-site detection of glucose in human urine. <i>Materials Today Chemistry</i> , 2022, 23, 100635.	1.7	8
9497	Nano-porous C ₄ N as a toxic pesticide's scavenger: A quantum chemical approach. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 111, 108078.	1.3	24
9498	Acridin-9(10H)-one-based blue thermally activated delayed fluorescence materials: improvement of color purity and efficiency stability. <i>Materials Today Chemistry</i> , 2022, 23, 100645.	1.7	5
9499	A systematic investigation of structural growth patterns and electronic properties of [LuGe] _n + ₀ and [Ge+1] _n + ₀ (n=17) nanoalloy clusters. <i>Materials Today Communications</i> , 2022, 30, 103018.	0.9	3
9500	A novel mechanism of intramolecular proton transfer in the excited state of 3-hydroxy-4H-benzochromone derivatives: A new explanation at the theoretical level. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 425, 113690.	2.0	7
9501	Theoretical insights into the excited state processes of a novel fluorescent probe for thiophenol with large Stokes shift. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 425, 113691.	2.0	3
9502	SUBSTITUENT EFFECT IN [2+4] DIELS-ALDER CYCLOADDITION REACTIONS OF ANTHRACENE WITH C ₂ X ₂ (X=H, Cl, Br, I). <i>Journal of Physical Chemistry A</i> , 2022, 126, 10784.	0.3	1
9503	The role of center-N-doping in non-radiative recombination loss of nitrogen-doped graphene quantum dots. <i>Materials Science in Semiconductor Processing</i> , 2022, 139, 106323.	1.9	12
9504	Mononuclear Copper(I) 3-(2-pyridyl)pyrazole Complexes: The Crucial Role of Phosphine on Photoluminescence. <i>Molecules</i> , 2021, 26, 6869.	1.7	8
9505	Comparison of Deep Eutectic Solvents and Organic Solvent Effects on the Separation of Ternary Azeotropes by the Experimental Study and Molecular Simulation. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 16424-16436.	3.2	15
9506	Dispersion-corrected DFT investigations on the interaction of glycine amino acid with metal organic framework MOF-5. <i>Physica B: Condensed Matter</i> , 2022, 626, 413446.	1.3	36
9507	A novel induced zero-valent iron electrode for in-situ slow release of Fe ²⁺ to effectively trigger electro-Fenton oxidation under neutral pH condition: Advantages and mechanisms. <i>Separation and Purification Technology</i> , 2022, 283, 120160.	3.9	13
9508	Quantitative tuning of ionic metal species for ultra-selective metal solvent extraction toward high-purity vanadium products. <i>Journal of Hazardous Materials</i> , 2022, 425, 127756.	6.5	9
9509	Preparation of group 3 metal sulfur monoxide complexes via oxidation of metal atoms by SOF ₂ in cryogenic matrixes. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	2
9510	Efficient removal of ciprofloxacin by heterogeneous electro-Fenton using natural air-cathode. <i>Chemical Engineering Journal</i> , 2022, 433, 133767.	6.6	29

#	ARTICLE	IF	CITATIONS
9511	Solvent Co-adsorption Changing the Type of Halogen-Based Bonds Associated with the Position of Bromine Substituents Revealed by Scanning Tunneling Microscopy. <i>Journal of Physical Chemistry C</i> , 2021, 125, 26847-26856.	1.5	1
9512	Absorption Features of CdTe Nanoclusters: Aspect Ratio Dependency of the Singlet/Doublet from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2021, 125, 25660-25669.	1.5	3
9513	Experimental and theoretical analysis of simultaneous removal of methylene blue and tetracycline using boron nitride nanosheets as adsorbent. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 634, 127943.	2.3	32
9514	Discovery of a Novel MyD88 Inhibitor M20 and Its Protection Against Sepsis-Mediated Acute Lung Injury. <i>Frontiers in Pharmacology</i> , 2021, 12, 775117.	1.6	7
9515	Analysis of SO ₂ Physisorption by Edge-Functionalized Nanoporous Carbons Using Grand Canonical Monte Carlo Methods and Density Functional Theory: Implications for SO ₂ Removal. <i>ACS Omega</i> , 2021, 6, 33735-33746.	1.6	4
9516	London Dispersion Helps Refine Steric A-Values: Dispersion Energy Donor Scales. <i>Journal of the American Chemical Society</i> , 2021, 143, 20837-20848.	6.6	35
9517	Synthesis, X-ray crystal structure, Hirshfeld surface analysis, DFT, AIM, ELF, RDG and molecular docking studies of bis[4-(dimethylamino)pyridinium]di-μ-chlorido-bis[dichloridomercurate(II)]. <i>Journal of Coordination Chemistry</i> , 2021, 74, 2927-2946.	0.8	6
9518	9,10-Phenanthrenequinone: A Promising Kernel to Develop Multifunctional Antitumor Systems for Efficient Type I Photodynamic and Photothermal Synergistic Therapy. <i>ACS Nano</i> , 2021, 15, 20042-20055.	7.3	61
9519	On the Ability of Nitrogen to Serve as an Electron Acceptor in a Pnictogen Bond. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10419-10427.	1.1	14
9520	Tuning the properties of ionic liquids by mixing with organic solvents: The case of 1-butyl-3-methylimidazolium glutamate with alkanols. <i>Journal of Molecular Liquids</i> , 2022, 347, 117953.	2.3	4
9521	Probing into the Outcome of Charge Transfer Interactions and Hyperconjugative Effect on the Antibacterial Molecule 4-dimethylaminopyridine using Spectroscopic Elucidations and DFT Calculations. <i>Journal of Molecular Structure</i> , 2022, 1251, 132059.	1.8	6
9522	Being positive is not everything – experimental and computational studies on the selectivity of a self-assembled, multiple redox state, receptor that binds anions with up to picomolar affinities. <i>Chemistry - A European Journal</i> , 2021, , .	1.7	1
9523	Design and selection of pyrazolo[3,4-d][1,2,3]triazole-based high-energy materials. <i>Structural Chemistry</i> , 2022, 33, 421-431.	1.0	1
9524	Nanoscope study on carvone-terpene based natural deep eutectic solvents. <i>Journal of Chemical Physics</i> , 2021, 155, 224702.	1.2	11
9525	Theoretical insights into the degradation of swep by hydroxyl radicals in atmosphere and water environment: Mechanisms, kinetics and toxicity. <i>Science of the Total Environment</i> , 2022, 816, 151651.	3.9	3
9526	Insight into SERS Chemical Enhancement Mechanism of Fungicide Thiram Adsorbed on Silver Nanoparticles. <i>Journal of Cluster Science</i> , 2022, 33, 1-15.	1.7	7
9527	Do non-thermal effects exist in microwave heating of glucose aqueous solutions? Evidence from molecular dynamics simulations. <i>Food Chemistry</i> , 2022, 375, 131677.	4.2	9
9528	Intermolecular Interaction and Extraction Explorations for Separation of High-Boiling Neutral Nitrogen Compounds Using Biodegradable Ionic Liquids. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 15839-15848.	3.2	14

#	ARTICLE	IF	CITATIONS
9529	Facile Nâ%o;N Bond Cleavage by Anionic Trimetallic Clusters V_{3â~}TaC₄^{â~} (<i>x= </i>0â€“3): A DFT Study. ChemPhysChem, 2022, 23, .	1.0	10
9530	Long-bonding and bonding nature in noble gas insertion compounds MNgBY of transition metal-boron bond. Journal of Molecular Modeling, 2021, 27, 360.	0.8	0
9531	A DFT and MP2 mechanistic and kinetic study on hypohalogenation reaction of cysteine and N-acetylcysteine in aqueous solution. Journal of Molecular Liquids, 2022, 349, 118191.	2.3	1
9532	Experimental proof for ĩf and ĩ€-hole driven dual pnicoen bonding in phosphoryl chloride-nitromethane heterodimers: A combined matrix isolation infrared and ab initio computational studies. Journal of Molecular Structure, 2022, 1251, 132045.	1.8	6
9533	New preparation protocols for coumarin-thiosemicarbazone hybrids: Solid state characterization, and in silico/NMR studies of the Z/E isomerization equilibria in solution. Journal of Molecular Structure, 2022, 1251, 131980.	1.8	5
9534	A Persistent Phosphanylâ€“Substituted Thioketyl Radical Anion. Angewandte Chemie - International Edition, 2021, , .	7.2	5
9535	Theoretical treatment of interaction of pyrazinamide with graphene and h-SiC monolayer: A DFT-D3 study. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 138, 115077.	1.3	13
9536	Tailormade Nonradiative Rotation Tuning of the Near-Infrared Photothermal Conversion in Donorâ€“Acceptor Cocrystals. Journal of Physical Chemistry C, 2021, 125, 25462-25469.	1.5	22
9537	Bridge-Length- and Solvent-Dependent Charge Separation and Recombination Processes in Donorâ€“Bridgeâ€“Acceptor Molecules. Journal of Physical Chemistry B, 2021, 125, 13279-13290.	1.2	5
9538	Adducts of 2-Pyridylselenenyl Halides and Nitriles as Novel Supramolecular Building Blocks: Four-Center SeÂ-Â-Â-N Chalcogen Bonding versus Other Weak Interactions. Crystal Growth and Design, 2022, 22, 313-322.	1.4	11
9539	Improved anti-inflammatory and anticancer properties of celecoxib loaded zinc oxide and magnesium oxide nanoclusters: A molecular docking and density functional theory simulation. Arabian Journal of Chemistry, 2022, 15, 103568.	2.3	11
9541	Evidences for sulfur centered hydrogen bond with sulfur atoms as a donor in aromatic thiols and aliphatic thiols in aqueous solution. Journal of Molecular Liquids, 2022, 348, 118078.	2.3	13
9542	Coordination and Electrochemical Switching on Paddle-Wheel Complexes Containing an Asâ€“Ru or a Sbâ€“Ru Axis. Inorganic Chemistry, 2021, 60, 18122-18132.	1.9	4
9543	In-situ cation exchange enhances room temperature phosphorescence of a family of metal-organic frameworks. Science China Chemistry, 2022, 65, 128-134.	4.2	16
9544	Role of Basic Surface Groups of Activated Carbon in Chlordecone and Ĩ ² -Hexachlorocyclohexane Adsorption: A Molecular Modelling Study. Molecules, 2021, 26, 6969.	1.7	1
9545	Magnesium dimer entrapped in cyclo[18]carbon: Mg ₂ @C ₁₈ . Chemical Physics Letters, 2022, 787, 139221.	1.2	9
9546	Additive-assisted cobalt electrodeposition as surface magnetic coating to enhance the inductance of spiral copper inductors. Surfaces and Interfaces, 2022, 28, 101603.	1.5	2
9547	Insights into the Formation and Profile of Chlorinated Polycyclic Aromatic Hydrocarbons during Chlorobenzene and Chloroethylene Manufacturing Processes. Environmental Science & Technology, 2021, 55, 15929-15939.	4.6	6

#	ARTICLE	IF	CITATIONS
9548	Two novel mono-hydroxyl pyranoanthocyanidins bearing dimethylamino substituent(s) for dye-sensitized solar cell. <i>Journal of Molecular Structure</i> , 2021, 1252, 132055.	1.8	7
9549	A DFT Study on the Binuclear Copper(I)-Catalyzed Synthesis Mechanism of 1,2,3-Triazolo[1,5-c]Pyrimidines via Interrupted Click and Ketenimine Rearrangement. <i>ChemPhysChem</i> , 2021, 23, e202100751.	1.0	1
9550	Extensive Redox Non-Innocence in Iron Bipyridine-Diimine Complexes: a Combined Spectroscopic and Computational Study. <i>Inorganic Chemistry</i> , 2021, 60, 18296-18306.	1.9	3
9551	Mechanisms of ion transport in lithium salt-doped polymeric ionic liquid electrolytes at higher salt concentrations. <i>Journal of Polymer Science</i> , 2022, 60, 199-213.	2.0	5
9552	The pH-dependent contributions of radical species during the removal of aromatic acids and bases in light/chlorine systems. <i>Chemical Engineering Journal</i> , 2022, 433, 133493.	6.6	7
9553	Insights into N-Coordinated Bimetallic Site Synergy during NO Selective Catalytic Reduction by CO. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 57182-57192.	4.0	15
9554	B(OH) ₂ -functionalized graphene nanoflakes as a promising nanocarrier for letrozole delivery: a density functional theory study. <i>Journal Physics D: Applied Physics</i> , 2022, 55, 115401.	1.3	2
9555	Bipyridine carboxylic acid as a high-performance anode material for lithium- and sodium-ion batteries. <i>Electrochimica Acta</i> , 2022, 405, 139628.	2.6	8
9556	HAB79: A New Molecular Dataset for Benchmarking DFT and DFTB Electronic Couplings Against High-Level Ab-initio Calculations. <i>Journal of Chemical Physics</i> , 2021, 155, 234115.	1.2	14
9557	Comparative Quantum Chemistry Study on the Unimolecular Decomposition Channels of Pyrazole and Imidazole Energetic Materials. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10340-10350.	1.1	0
9558	Role of edge nitrogen doping in nonradiative decay dynamics of graphene quantum dots: a Fermi's golden rule analysis. <i>Applied Nanoscience (Switzerland)</i> , 2021, 11, 2837-2845.	1.6	9
9559	Multistimuli-Responsive Fluorescent Switches Based on Reversible Decomposition and Regeneration of charge-transfer Complexes. <i>Crystal Growth and Design</i> , 0, , .	1.4	2
9560	Relationship between the Molecular Structure and Stacking Mode: Characteristics of the D ₂ h and D ₃ h Molecules in Planar Layer-Stacked Crystals. <i>Crystal Growth and Design</i> , 2021, 21, 6847-6861.	1.4	15
9561	Simulation degradation of bromophenolic compounds in chlorine-based advanced oxidation processes: Mechanism, microscopic and apparent kinetics, and toxicity assessment. <i>Chemosphere</i> , 2022, 291, 133034.	4.2	4
9562	Phenothiazine-based dyes containing imidazole with -linkers of benzene, furan and thiophene: Synthesis, photophysical, electrochemical and computational investigation. <i>Journal of Molecular Structure</i> , 2022, 1251, 131959.	1.8	19
9563	Oxidation of pyrazolone pharmaceuticals by peracetic acid: Kinetics, mechanism and genetic toxicity variations. <i>Chemosphere</i> , 2022, 291, 132947.	4.2	12
9564	Detoxification of the Toxic Sulfur Mustard Simulant by a Supramolecular Antidote in Vitro and in Vivo. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 58291-58300.	4.0	10
9565	Acceleration of biotic decolorization and partial mineralization of methyl orange by a photo-assisted n-type semiconductor. <i>Chemosphere</i> , 2022, 291, 132846.	4.2	3

#	ARTICLE	IF	CITATIONS
9566	Understanding the activity origin of oxygen-doped carbon materials in catalyzing the two-electron oxygen reduction reaction towards hydrogen peroxide generation. <i>Journal of Colloid and Interface Science</i> , 2022, 610, 934-943.	5.0	15
9567	Electro-catazone treatment of ozone-resistant drug ibuprofen: Interfacial reaction kinetics, influencing mechanisms, and degradation sites. <i>Journal of Hazardous Materials Advances</i> , 2021, 4, 100023.	1.2	7
9568	Structures, Multicenter π -Bonding, and Spin Equilibria in the Mixed-Valence Trimers of Tetramethyltetrathiafulvalene Cation-Radicals. <i>Crystal Growth and Design</i> , 2021, 21, 7257-7268.	1.4	6
9569	Non-covalent assembly of $\hat{\nu}^2$ -iminoamine-chlorocobaltate(II) hybrid material: Molecular structure, computational simulations and antimicrobial activity. <i>Journal of Molecular Structure</i> , 2022, 1251, 131967.	1.8	5
9570	Synthesis, spectroscopic (FT-IR, FT-Raman, NMR & UV-Vis), reactive (ELF, LOL, Fukui), drug likeness and molecular docking insights on novel 4-[3-(3-methoxy-phenyl)-3-oxo-propenyl]-benzotrile by experimental and computational methods. <i>Heliyon</i> , 2021, 7, e08429.	1.4	16
9571	Reconsidering the Roles of Noncovalent Intramolecular π -Locks in π -Conjugated Molecules. <i>Chemistry of Materials</i> , 2021, 33, 9139-9151.	3.2	8
9572	Incorporation of Fluorene and Its Heterocyclic Spiro Derivatives To Realize High-Performance and Stable Sky-Blue-Emitting Arylgold(III) Complexes. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 57673-57683.	4.0	3
9573	Graphitic Carbon Nitride Codoped with Sulfur and Yttrium for Efficient Visible-Light Photocatalytic Performance. <i>ACS Applied Energy Materials</i> , 2021, 4, 14390-14399.	2.5	8
9574	Theoretical investigation on the structure of mixed-metal zeolitic imidazolate framework and its interaction with CO ₂ . <i>Computational Materials Science</i> , 2022, 210, 111033.	1.4	3
9575	High-energy materials based on 1H-tetrazole and furoxan: Molecular design and screening. <i>Journal of Molecular Structure</i> , 2022, 1250, 131900.	1.8	12
9576	Effect of mono-vacant defects on the adsorption properties of deep eutectic solvents onto hexagonal boron-nitride nanoflakes. <i>Journal of Molecular Liquids</i> , 2022, 349, 118122.	2.3	2
9577	All are aromatic: A 3D globally aromatic cage containing five types of 2D aromatic macrocycles. <i>Chem</i> , 2021, 7, 3442-3453.	5.8	15
9578	Computational Study of Photochemical Relaxation Pathways of Platinum(II) Complexes. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10144-10154.	1.1	5
9579	Thiophene-Fused 1,4-Diazapentalene: A Stable C=N-Containing π -Conjugated System with Restored Antiaromaticity. <i>Chemistry - A European Journal</i> , 2021, 27, 16061-16061.	1.7	0
9580	π -Hole Interactions of Tetrahedral Group IV-VIII Lewis Acid Centers with Lewis Bases: A Comparative Study. <i>ChemistrySelect</i> , 2021, 6, 11856-11864.	0.7	5
9581	Zinc(II) Iodide-Directed $\hat{\nu}^2$ -Mannosylation: Reaction Selectivity, Mode, and Application. <i>Journal of Organic Chemistry</i> , 2021, 86, 16901-16915.	1.7	8
9582	Porous P, Fe-doped g-C ₃ N ₄ nanostructure with enhanced photo-Fenton activity for removal of tetracycline hydrochloride: Mechanism insight, DFT calculation and degradation pathways. <i>Chemosphere</i> , 2022, 291, 133039.	4.2	50
9583	Multi-Scale Nanoarchitected Fibrous Networks for High-Performance, Self-Sterilization, and Recyclable Face Masks. <i>Small</i> , 2022, 18, e2105570.	5.2	36

#	ARTICLE	IF	CITATIONS
9584	On the surface interaction of C ₆₀ with superalkalis: a computational approach. <i>Molecular Physics</i> , 2022, 120, .	0.8	0
9585	Structures 4-n-propyl Piperazines as Non-Imidazole Histamine H3 Antagonists. <i>Materials</i> , 2021, 14, 7094.	1.3	0
9586	Peroxymonosulfate activation by algal carbocatalyst for organic dye oxidation: Insights into experimental and theoretical. <i>Science of the Total Environment</i> , 2022, 816, 151611.	3.9	19
9587	Hydrogen and Lithium Bonds Lewis Acid Units Possessing Multi-Center Covalent Bonds. <i>Molecules</i> , 2021, 26, 6939.	1.7	7
9588	Electrocatalytic Hydrogen Evolution by Cobalt Complexes with a Redox Non-Innocent Polypyridine Ligand. <i>Inorganic Chemistry</i> , 2021, 60, 17976-17985.	1.9	15
9589	Density, Speed of Sound, and Refractive Index of Binary Mixture Containing Ethyl Isobutyrate with Cyclohexane at Different Temperatures Combined with Experiment and Molecular Simulation. <i>Journal of Chemical & Engineering Data</i> , 2021, 66, 4534-4541.	1.0	1
9590	Computational Study of CO ₂ Reduction Catalyzed by Iron(II) Complex at Different Spin States: Cooperativity of Hydrogen Bonding and Auxiliary Group Effect. <i>ACS Omega</i> , 2021, 6, 31971-31981.	1.6	0
9591	Dynamic Simulation Based on a Simplified Model of 1/3 Coking Coal Molecule and Its Formation Characteristics of Hydration Films. <i>ACS Omega</i> , 2021, 6, 33339-33353.	1.6	9
9592	Theoretical Investigation of the Excited-State Dynamics Mechanism of the Asymmetric Two-Way Proton Transfer Molecule BTHMB. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10280-10290.	1.1	3
9593	Intra-Molecular Electrical Field Regulated Nonlinear Catalyst Charge Transfer in the Organic Conjugated Molecular System. <i>Catalysts</i> , 2021, 11, 1375.	1.6	0
9594	Higher-Energy Hexafluoroisopropanol-Water Isomer and Its Large Amplitude Motions: Rotational Spectra and DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10401-10409.	1.1	4
9595	Conformations and structures of 1,4-pentadien-3-ol and its water complex characterized by rotational spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 267, 120589.	2.0	0
9596	DFT investigation of Percyanation effect of coronene molecule: Comparative study with their Perhalogenated counterparts.. <i>Polymer Bulletin</i> , 2022, 79, 9663-9684.	1.7	5
9597	Enhanced Growth of Broad Beans (<i>Vicia faba</i> L.) through Separating Antagonistic Nutrients Using Nitrogen-Doped Carbon Nanotubes. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 16437-16449.	3.2	4
9598	Electronic properties (in different solvents), spectroscopic progression and evaluation on 4-morpholinepropane sulfonic acid along with molecular docking analysis. <i>Journal of Molecular Liquids</i> , 2022, 349, 118107.	2.3	10
9599	Inter-anion chalcogen bonds: Are they anti-electrostatic in nature?. <i>Journal of Chemical Physics</i> , 2021, 155, 234302.	1.2	8
9600	Energetic features of antiparallel stacking and hydrogen bonding interactions in two coordination complexes bearing 1,10-phenanthroline-2,9-dicarboxylic acid. <i>Journal of Molecular Structure</i> , 2022, 1251, 131963.	1.8	3
9601	Design of a high-performance ternary LDHs containing Ni, Co and Mn for arsenate removal. <i>Journal of Hazardous Materials</i> , 2022, 427, 127865.	6.5	17

#	ARTICLE	IF	CITATIONS
9602	A Persistent Phosphanyl-Substituted Thioketyl Radical Anion. <i>Angewandte Chemie</i> , 0, , .	1.6	0
9603	Dopant Free Triphenylamine-Based Hole Transport Materials with Excellent Photovoltaic Properties for High-Performance Perovskite Solar Cells. <i>Energy Technology</i> , 2022, 10, 2100838.	1.8	34
9604	Quantum chemical study of reaction mechanism between plutonium and nitrogen. <i>Journal of Molecular Modeling</i> , 2021, 27, 363.	0.8	1
9605	Copper-Catalyzed Enantioselective C-H Arylation between 2-Arylindoles and Hypervalent Iodine Reagents. <i>Organic Letters</i> , 2021, 23, 9246-9250.	2.4	11
9606	π -hole interactions of group IV-VII radical-containing molecules: A comparative study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 111, 108097.	1.3	5
9607	A Comprehensive Experimental and Theoretical Study on the $[(\eta^5\text{-C}_5\text{H}_5)_2\text{Zr}[\mu\text{-P}(\text{NEt}_2)_2\text{P}(\text{NEt}_2)_2\text{P}]]_2\text{O}$ Crystalline System. <i>Molecules</i> , 2021, 26, 7282.	1.7	0
9608	Facile fabrication of phenylenediamine residue derived N, O co-doped hierarchical hyperporous carbon for high-efficient chloroxylenol removal. <i>Chemical Engineering Journal</i> , 2022, 433, 133635.	6.6	4
9609	Computational approach in lignin structural models: Influence of non-covalent intramolecular interactions on I^2O_4 bond properties. <i>Journal of Molecular Structure</i> , 2022, 1251, 131938.	1.8	5
9610	Quantum Chemical Calculations of 5-Diethylamino-2-[[4-(3-Methyl-3-Phenyl-Cyclobutyl)-Thiazol-2-yl]-Hydrazonomethyl]-Phenol Single Crystal Containing Heteroatoms. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-24.	1.4	0
9611	Switching Pathways of Triplet State Formation by Twisted Intramolecular Charge Transfer. <i>Journal of Physical Chemistry B</i> , 2021, 125, 12518-12527.	1.2	6
9612	Palladium-Catalyzed Enantioselective C(sp ³)-H/C(sp ³)-H Umpolung Coupling of <i>N</i> -Allylimine and \pm -Aryl Ketones. <i>Journal of the American Chemical Society</i> , 2021, 143, 20454-20461.	6.6	28
9613	Enhanced peroxymonosulfate activation by hierarchical porous Fe ₃ O ₄ /Co ₃ S ₄ nanosheets for efficient elimination of rhodamine B: Mechanisms, degradation pathways and toxicological analysis. <i>Journal of Colloid and Interface Science</i> , 2022, 610, 751-765.	5.0	34
9614	Halogen-Manipulated Interfacial Charge Transport of π -Conjugated Molecule-Lead Halide Hybrids. <i>ACS Applied Energy Materials</i> , 0, , .	2.5	4
9615	Quantum-Mechanical/Molecular-Mechanical (QM/MM) Simulations for Understanding Enzyme Dynamics. <i>Methods in Molecular Biology</i> , 2022, 2397, 227-248.	0.4	2
9616	Structure Set in Stone: Designing Rigid Linkers to Control the Efficiency of Intramolecular Singlet Fission. <i>Journal of Physical Chemistry B</i> , 2021, 125, 13235-13245.	1.2	5
9617	Substituent effect induced the distinctive ESIPT reaction and photophysical property of <i>N</i> -silylidene-5-chloroaminopyridine. <i>Journal of Molecular Structure</i> , 2022, 1250, 131923.	1.8	6
9618	Experimental and theoretical investigation for the cycloaddition of carbon dioxide to epoxides catalyzed by potassium and boron co-doped carbon nitride. <i>Journal of Colloid and Interface Science</i> , 2022, 609, 523-534.	5.0	11
9619	Photodegradation of chloramphenicol in micro-polluted water using a circulatory thin-layer inclined plate reactor. <i>Chemosphere</i> , 2022, 291, 132883.	4.2	7

#	ARTICLE	IF	CITATIONS
9620	Accurate Analysis of Anisotropic Carrier Mobility and Structure-property Relationships in Organic BOXD Crystalline Materials. <i>Frontiers in Chemistry</i> , 2021, 9, 775747.	1.8	2
9621	Application of Imidazolium-based polyionic liquids to separate the 1,3,5-Trioxane-Water/Ethanol-Water system based on experimental verification and molecular mechanism analysis. <i>Journal of Molecular Liquids</i> , 2022, 348, 118079.	2.3	7
9622	A <sc>Blockwallâ€Type</sc> Layered Bis(dithiolato)nickelate Radical Salt Exhibiting Highâ€and <sc>Twoâ€Dimensional</sc> Antiferromagnetic Coupling Feature. <i>Chinese Journal of Chemistry</i> , 2022, 40, 794-800.	2.6	1
9623	Synthesis, in vitro and in silico antitumor evaluation of 3-(2,6-dichlorophenyl)-1,5-diphenylpentane-1,5â€dione: Structure, spectroscopic, RDG, Hirshfeld and DFT based analyses. <i>Journal of Molecular Structure</i> , 2022, 1251, 132002.	1.8	8
9624	Solid-liquid equilibrium of ropivacaine in fourteen organic solvents: An experimental and molecular simulation study. <i>Journal of Molecular Liquids</i> , 2022, 349, 118163.	2.3	12
9625	Photoactive homomolecular bis(n)-Lophine dyads: Multicomponent synthesis, photophysical properties, theoretical investigation, docking and interaction studies with biomacromolecules. <i>Journal of Molecular Liquids</i> , 2022, 349, 118084.	2.3	7
9626	Nitrogen-doped biochar encapsulated Fe/Mn nanoparticles as cost-effective catalysts for heterogeneous activation of peroxymonosulfate towards the degradation of bisphenol-A: Mechanism insight and performance assessment. <i>Separation and Purification Technology</i> , 2022, 283, 120136.	3.9	55
9627	Boron Triel Bonds: A Quantum Chemical Topology Perspective. <i>ChemistrySelect</i> , 2021, 6, 12431-12439.	0.7	1
9628	Theoretical Studies on Bimetallic Salen Complexes Catalyzed Epoxide Hydration: Effects of Metal Centers, Substrates, and Ligands. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10155-10164.	1.1	3
9629	An updated study on NO catalytic oxidation over activated carbon: The effect of pore structure and a dual-site mechanism. <i>Fuel</i> , 2022, 311, 122627.	3.4	9
9630	A Phosphorusâ€Based Pacman Dication Generated by Cooperative Selfâ€Activation of a Pacman Phosphane. <i>Chemistry - A European Journal</i> , 2021, , .	1.7	7
9631	Encapsulate SrCoO ₃ perovskite crystal within molybdenum disulfide layer as core-shell structure to enhance electron transfer for peroxymonosulfate activation. <i>Separation and Purification Technology</i> , 2022, 283, 120199.	3.9	18
9632	Overcrowded Ethylene-Bridged NanoHoop Dimers: Regioselective Synthesis, Multiconfigurational Electronic States, and Global H ^{1/4} ckel/MÃ¶buis Aromaticity. <i>Journal of the American Chemical Society</i> , 2021, 143, 20419-20430.	6.6	35
9633	Graphene-oxide-bacterial-cellulose nanohybrid gives a â€œsubstrate-driven enhancementâ€ effect to catalytic activity of phthalocyanine. <i>Cellulose</i> , 2022, 29, 849-861.	2.4	4
9634	Microwave-assisted synthesis of RuTe ₂ /black TiO ₂ photocatalyst for enhanced diclofenac degradation: Performance, mechanistic investigation and intermediates analysis. <i>Separation and Purification Technology</i> , 2022, 283, 120214.	3.9	19
9635	Highly efficient absorption of methyl tert-butyl ether with ionic liquids. <i>Separation and Purification Technology</i> , 2022, 282, 120108.	3.9	8
9636	How Cationic Metalloligands Affect the Coordination of Lewis Basic Ligands in RhI Complexes. <i>Organometallics</i> , 0, , .	1.1	4
9637	On the Importance of Halogen Bonding Interactions in Two X-ray Structures Containing All Four (F,) TJ ETQq1 1 0.784314 rgBT/Overl	1.0	29

#	ARTICLE	IF	CITATIONS
9638	Biotinylation as a tool to enhance the uptake of small molecules in Gram-negative bacteria. <i>PLoS ONE</i> , 2021, 16, e0260023.	1.1	4
9639	Adsorption of chlorine oxyanions, as water disinfectant by-products, on graphene flakes: A quantum chemical investigation. <i>Surfaces and Interfaces</i> , 2021, 28, 101601.	1.5	1
9640	Competition between the stabilizing effects of saturated alkyl substituents and pi bonds on complexes of silver ion (Ag ⁺) with alkenes. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, e4301.	0.9	3
9641	Helium nanodroplet infrared spectroscopy of oxazole-(water) _n (n = 1,2) clusters. <i>AIP Advances</i> , 2021, 11, 115112.	0.6	0
9642	Carbon Monoxide Binding to the Iron-Molybdenum Cofactor of Nitrogenase: a Detailed Quantum Mechanics/Molecular Mechanics Investigation. <i>Inorganic Chemistry</i> , 2021, 60, 18031-18047.	1.9	15
9643	Accessing Cationic silylated and germylated Phosphorus Ylides. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	5
9644	Structural, spectral elucidation, wavefunctional properties, natural bond orbitals, and molecular docking analysis of synthesized 1-phenyl-3-(4-methoxyphenyl)-2-propenone: protease kinase inhibitor. <i>Spectroscopy Letters</i> , 2021, 54, 773-789.	0.5	2
9645	Improving the freeze-thaw stability of emulsions via combining phosphatidylcholine and modified starch: A combined experimental and computational study. <i>International Journal of Food Science and Technology</i> , 2022, 57, 1050-1060.	1.3	2
9646	Computational Investigations of a pH-Induced Structural Transition in a CTAB Solution with Toluic Acid. <i>Molecules</i> , 2021, 26, 6978.	1.7	0
9647	Unexpected reactions of 7-amino-8-nitrotetrazolo[1,5-c]pyrimidine. <i>Energetic Materials Frontiers</i> , 2021, .	1.3	0
9648	Force-Induced Molecular Isomerization for the Construction of Multicolor Luminescent Segmented Molecular Crystals. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	4
9649	Synthesis of Azepine- or Azocine-Embedded Hexabenzocoronene-Based Nanographenes. <i>Synlett</i> , 0, .	1.0	2
9650	Antiaromatic Dicyclopenta[<i>b,g</i>]/[<i>a,f</i>]naphthalene Isomers Showing an Open-Shell Singlet Ground State with Tunable Diradical Character. <i>Journal of the American Chemical Society</i> , 2021, 143, 20562-20568.	6.6	37
9651	Novel and Polynuclear K- and Na-Based Superalkali Hydroxides as Superbases Better Than Li-Related Species and Their Enhanced Properties: An Ab Initio Exploration. <i>ACS Omega</i> , 2021, 6, 31077-31092.	1.6	9
9652	Synthesis and potential vasorelaxant effect of a novel ruthenium-based nitro complex. <i>Journal of Inorganic Biochemistry</i> , 2021, 228, 111666.	1.5	1
9653	Superalkali-alkalide ion pairs $\hat{I}^+(M-HMHC)-M\hat{A}^{\ominus}$ (M, $M^{\ominus} = Li, Na$ and K) serving as high-performance NLO molecular materials. <i>Journal of Molecular Liquids</i> , 2022, 349, 118101.	2.3	5
9654	Unveiling the influence of atomic electronegativity on the double ESIPT processes of uralenol: A theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 268, 120660.	2.0	9
9655	Comparison of rhodamine 6G, rhodamine B and rhodamine 101 spirolactam based fluorescent probes: A case of pH detection. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 268, 120662.	2.0	17

#	ARTICLE	IF	CITATIONS
9656	Charge delocalization and hyperpolarizability in ionic liquids. <i>Journal of Molecular Liquids</i> , 2022, 349, 118153.	2.3	5
9657	Novel Dâ€“Aâ€“Î€â€“A Organic Dyes with Phenoxazine as a Donor Unit for Dye-Sensitized Solar Cells: The Effect of an Ethynyl Group on Performance. <i>Energy & Fuels</i> , 2021, 35, 19748-19755.	2.5	12
9658	Low-temperature Hg ⁰ abatement by ionic liquid based on weak interaction. <i>Journal of Hazardous Materials</i> , 2022, 426, 127836.	6.5	3
9659	The transformation of Benzophenone-3 in natural waters and AOPs: The roles of reactive oxygen species and potential environmental risks of products. <i>Journal of Hazardous Materials</i> , 2022, 427, 127941.	6.5	8
9660	Fabrication of environmentally-friendly composited sponges for efficient removal of fluoroquinolones antibiotics from water. <i>Journal of Hazardous Materials</i> , 2022, 426, 127796.	6.5	18
9661	Structural and spectroscopic analysis, ADMET study, and anxiolytic-like effect in adult zebrafish (<i>Danio rerio</i>) of 4-[(1E,2E)-1-(2-(2,4-dinitrophenyl)hydrazono-3-(4-methoxyphenyl)allyl)aniline. <i>Journal of Molecular Structure</i> , 2022, 1251, 132064.	1.8	3
9662	In Situ Fabricated Quasi-Solid Polymer Electrolyte for High-Energy-Density Lithium Metal Battery Capable of Subzero Operation. <i>Advanced Energy Materials</i> , 2022, 12, 2102932.	10.2	69
9663	A comprehensive multidisciplinary investigation on CO ₂ capture from diesel engine. <i>Environmental Science and Pollution Research</i> , 2021, , 1.	2.7	4
9664	Investigating the bio-rejuvenator effects on aged asphalt through exploring molecular evolution and chemical transformation of asphalt components during oxidative aging and regeneration. <i>Journal of Cleaner Production</i> , 2021, 329, 129711.	4.6	36
9665	Self-assembled nanoparticles with bilirubin/JPH203 alleviate imiquimod-induced psoriasis by reducing oxidative stress and suppressing Th17 expansion. <i>Chemical Engineering Journal</i> , 2022, 431, 133956.	6.6	17
9666	Stable Long Cycling of Small Molecular Organic Acid Electrode Materials Enabled by Nonflammable Eutectic Electrolyte. <i>Small</i> , 2022, 18, e2104538.	5.2	9
9667	Electrocatalysis degradation of coal tar wastewater using a novel hydrophobic benzalacetone modified lead dioxide electrode. <i>Chemosphere</i> , 2022, 289, 133014.	4.2	11
9668	Novel Third-Order Nonlinear Optical Materials with Craig-MÃ¶bius Aromaticity. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 11784-11789.	2.1	13
9669	The pre-oxidation kinetics and mechanism of sulfapyridine for biodegradability improvement. <i>Journal of Cleaner Production</i> , 2021, 329, 129698.	4.6	4
9670	End-capped modification of dithienosilole based small donor molecules for high performance organic solar cells using DFT approach. <i>Journal of Molecular Liquids</i> , 2022, 345, 118138.	2.3	59
9671	Computational exploration of gallium-doped neutral and anionic magnesium nanocluster materials: Ga ₂ Mgn _q (n=11; q=0, 1) nanoclusterâ€™s properties based on DFT. <i>Materials Today Communications</i> , 2021, 29, 103004.	0.9	3
9672	Maximal occupation by bases of Î€â€“hole bands surrounding linear molecules. <i>Journal of Computational Chemistry</i> , 2021, , .	1.5	2
9673	PDMS with Tunable Side Group Mobility and Its Highly Permeable Membrane for Removal of Aromatic Compounds. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	2

#	ARTICLE	IF	CITATIONS
9674	Phase- and Halogen-Dependent Room-Temperature Phosphorescence Properties of Biphenylnitrile Derivatives. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27489-27496.	1.5	4
9675	Synthesis, structure of 5,7-dimethyl-3-ferrocenyl-2,3-dihydro-1H-pyrazolo- [1,2-a]-pyrazol-4-ium tetrafluoroborate. DFTB calculations of interaction with DNA. <i>Journal of Molecular Structure</i> , 2022, 1251, 132070.	1.8	3
9676	Investigation on the Ionic Composition and Spectroscopic Properties of Molten NaF \cdot AlF $_3$ \cdot Al $_2$ O $_3$ Salts at 1300 K. <i>Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science</i> , 2022, 53, 474-484.	1.0	4
9677	DFT study of the stabilization effect on anthocyanins via secondary interactions. <i>Food Chemistry Molecular Sciences</i> , 2021, 3, 100057.	0.9	1
9678	Deep eutectic solvents for efficient capture of cyclohexane in volatile organic compound: Thermodynamic and molecular mechanism. <i>AIChE Journal</i> , 2022, 68, e17535.	1.8	19
9679	Superatomic Rydberg State Excitation. <i>Journal of Physical Chemistry Letters</i> , 2021, , 11766-11771.	2.1	8
9680	Enzyme-Like Hydroxylation of Aliphatic C-H Bonds From an Isolable Co-Oxo Complex. <i>Journal of the American Chemical Society</i> , 2021, 143, 20849-20862.	6.6	14
9681	Divalent nitrogen-rich cationic salts with great gas production capacities. <i>Defence Technology</i> , 2023, 22, 54-68.	2.1	2
9682	Phase behavior and extraction mechanism of methanol-n-hexane separation using choline-based deep eutectic solvent. <i>Journal of Molecular Liquids</i> , 2022, 345, 118204.	2.3	13
9683	Product distribution and coke formation during catalytic pyrolysis of oil shale with zeolites. <i>Journal of Thermal Analysis and Calorimetry</i> , 2022, 147, 8535-8549.	2.0	5
9684	Photothermal-driven itinerant adsorption to accelerate self-repairing of reactive sites for efficient removal of salicylic acid. <i>Separation and Purification Technology</i> , 2022, 284, 120251.	3.9	4
9685	Deciphering the Backbone Noncovalent Interactions that Stabilize Polyproline II Conformation and Reduce cis Proline Abundance in Polyproline Tracts. <i>Journal of Physical Chemistry B</i> , 2021, , .	1.2	2
9686	Buchwald \cdot Hartwig Amination of Aryl Halides with Heterocyclic Amines in the Synthesis of Highly Fluorescent Benzodifuran-Based Star-Shaped Organic Semiconductors. <i>Journal of Organic Chemistry</i> , 2021, , .	1.7	2
9687	Acceleration of levofloxacin degradation by combination of multiple free radicals via MoS $_2$ anchored in manganese ferrite doped perovskite activated PMS under visible light. <i>Chemical Engineering Journal</i> , 2022, 431, 133933.	6.6	71
9688	Glycerol \cdot derived Solvents Containing Two or Three Distinct Functional Groups Enabled by Trifluoroethyl Glycidyl Ether. <i>AIChE Journal</i> , 0, , e17533.	1.8	8
9689	Tuning the charge transfer and optoelectronic properties of tetrathiafulvalene based organic dye-sensitized solar cells: a theoretical approach. <i>RSC Advances</i> , 2021, 11, 39246-39261.	1.7	10
9690	Synthesis of cationic π -extended imidazolium salts by sequential Cu-catalyzed arylation/annulation and photocyclization. <i>Chemical Communications</i> , 2022, 58, 541-544.	2.2	4
9691	The second-order NLO and TADF properties of a donor \cdot acceptor dihydropyrene \cdot cyclophanediene system: the impact of molecular architecture and polarizable environment. <i>Journal of Materials Chemistry C</i> , 2022, 10, 886-898.	2.7	10

#	ARTICLE	IF	CITATIONS
9692	Harnessing visible-light energy for unbiased organic photoelectrocatalysis: synthesis of <i>N</i> -bearing fused rings. <i>Green Chemistry</i> , 2022, 24, 837-845.	4.6	10
9693	DFT study on the adsorption of 5-fluorouracil on B ₄₀ , B ₃₉ M, and M@B ₄₀ (M = Mg, Al, Si, Mn, Cu, Zn). <i>RSC Advances</i> , 2021, 11, 39508-39517.	1.7	14
9694	Pseudorotaxane formation affected by stereo-electronic effects. A theoretical and experimental study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1654-1665.	1.3	0
9695	One-step functionalization of mildly and strongly reduced graphene oxide with maleimide: an experimental and theoretical investigation of the Diels-Alder [4+2] cycloaddition reaction. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2491-2503.	1.3	1
9696	Structural and Bonding Properties of Al _n C _{4n} /O (n=2-4) Clusters: Anion Photoelectron Spectroscopy and Theoretical Calculations. <i>Chinese Journal of Chemical Physics</i> , 0, , .	0.6	0
9697	Synthesis of asymmetric [bis(imidazolyl)-BH ₂] ⁺ -cation-based ionic liquids as potential rocket fuels. <i>RSC Advances</i> , 2021, 11, 38040-38046.	1.7	4
9698	Speciation analysis the complexation of uranyl nitrate with tri- <i>n</i> -butyl phosphate in supercritical CO ₂ . <i>RSC Advances</i> , 2021, 11, 36391-36397.	1.7	1
9699	Mechanism of Silver-Catalyzed [2+2] Cycloaddition between Siloxy-Alkynes and Carbonyl Compound: A Silylium Ion Migration Approach. <i>Chinese Journal of Organic Chemistry</i> , 2021, 41, 4327.	0.6	1
9700	Effective Isolation of Phenols by Deep Eutectic Solvents from an Acetonitrile-Extractable Portion of Shale Oil: Noncovalent Interaction. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
9701	Photovoltaic performance and power conversion efficiency prediction of double fence porphyrins. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 27042-27058.	1.3	8
9702	Enhancing CH ₄ /N ₂ Separation Performance within Aluminum-Based Metal-Organic Frameworks: Influence of the Pore Structure and Linker Polarity. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
9704	A theoretical study of allopurinol drug sensing by carbon and boron nitride nanostructures: DFT, QTAIM, RDC, NBO and PCM insights. <i>RSC Advances</i> , 2021, 11, 38457-38472.	1.7	23
9705	Coordination complexes of zinc and manganese based on pyridine-2,5-dicarboxylic acid <i>N</i> -oxide: DFT studies and antiproliferative activities consideration. <i>RSC Advances</i> , 2021, 11, 37403-37412.	1.7	7
9706	An all-organic symmetric battery based on a triquinoxalinylene derivative with different redox voltage active sites and a large conjugation system. <i>Journal of Materials Chemistry A</i> , 2021, 9, 26208-26215.	5.2	22
9707	The interesting luminescence behavior and rare nonlinear optical properties of the {Ag ₅₅ Mo ₆ } nanocluster. <i>RSC Advances</i> , 2021, 11, 38814-38819.	1.7	1
9708	Evaluating first-order molecular properties of delocalized ionic or excited states in molecular aggregates by renormalized excitonic method. <i>Chinese Journal of Chemical Physics</i> , 2021, 34, 670-682.	0.6	2
9709	The degradation effect on proton dissociation and transfer in perfluorosulfonic acid membranes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3007-3016.	1.3	3
9710	The Inhibition of <i>p</i> -Hydroxyphenyl OH in Residual Lignin on Enzymatic Hydrolysis of Cellulose and its Underlying Mechanism. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
9711	Anatomies for the thermal decomposition behavior and product rule of 5,5-dinitro-2,2,3,3-tetra-1,2,4-triazole. RSC Advances, 2021, 11, 40182-40192.	1.7	3
9712	A DFT study on the molecular properties of synthetic ester under the electric field. Open Physics, 2021, 19, 647-656.	0.8	5
9713	M ₇ O ₇ (M = Ni, Pd, Pt): aromatic molecular stars with a planar heptacoordinate transition metal. Chemical Communications, 2021, 57, 13716-13719.	2.2	8
9714	Low-Cost Hydrocarbon Membrane Enables Commercial-Scale Alkaline-Based Flow Batteries for Long-Duration Energy Storage. SSRN Electronic Journal, 0, , .	0.4	0
9715	GW/BSE nonadiabatic dynamics simulations on excited-state relaxation processes of zinc phthalocyanine-fullerene dyads: Roles of bridging chemical bonds. Chinese Journal of Chemical Physics, 2021, 34, 704-716.	0.6	5
9716	Electroless deposition of Ni-P/Au coating on Cu substrate with improved corrosion resistance from Au(DMH based cyanide-free plating bath using hypophosphite as a reducing agent. RSC Advances, 2021, 11, 39153-39168.	1.7	4
9717	Identifying the true origins of selectivity in chiral phosphoric acid catalyzed N-acyl-azetidine desymmetrizations. Chemical Science, 2021, 12, 15662-15672.	3.7	7
9718	Separation and Recovery of Iridium(III) from a Simulated Secondary Resource Leachate by Extraction - Electrodeposition. SSRN Electronic Journal, 0, , .	0.4	1
9719	Exploration of Catalytic Species; For; Highly Efficient Preparation Of; Quinazoline-2,4(1H)-one Derivatives Under Pressure: Combination of Experimental And Theoretical Study. SSRN Electronic Journal, 0, , .	0.4	0
9720	Host-guest interaction-directed strategy for managing mechanochromic luminescence behavior by modulating molecular packing and conformation. Journal of Materials Chemistry C, 2021, 9, 17307-17312.	2.7	10
9721	Pseudotetrahedral Zn(II)-(R or S)-dihalogen-salicylaldehyde complexes with β - or γ -chirality induction at-metal. Dalton Transactions, 2022, , .	1.6	4
9722	Design Novel Environmentally-friendly Flame Retardants. Combustion Science and Technology, 2023, 195, 2474-2490.	1.2	0
9723	Second-Order Nonlinear Optics Response of the Boron-Dipyrromethenes-Based Mislinked Expanded Porphyrins: Revealing the Role of the BF ₂ Group. Journal of Physical Chemistry Letters, 2022, 13, 412-418.	2.1	7
9724	Supramolecular Approach to Tuning the Photophysical Properties of Quadrupolar Squaraines. Frontiers in Chemistry, 2021, 9, 800541.	1.8	1
9725	Useless Channels in a Molecular Crystal Formed via F \cdots F and F \cdots Halogen Bonds. Crystal Growth and Design, 0, , .	1.4	4
9726	H ₂ O adsorption and O-H breaking on Co ₅ M (M = Co, Y-Ag) clusters: A DFT study. Journal of Molecular Liquids, 2022, 348, 118469.	2.3	3
9727	Mechanistic insights into the selectivity of norcaradiene oxidation by oxoMn(V) porphyrin complexes. ChemPhysChem, 2022, , .	1.0	1
9728	Oxygen Interactions with Covalently Grafted 2D Nanometric Carboxyphenyl Thin Films: An Experimental and DFT Study. Coatings, 2022, 12, 49.	1.2	7

#	ARTICLE	IF	CITATIONS
9729	Theoretical insights of structural evolution and electronic properties of Ru ₂ Gen (n=1-16) clusters. <i>European Physical Journal Plus</i> , 2022, 137, 1.	1.2	3
9730	Theoretical Approach to Evaluate the Gas-Sensing Performance of Graphene Nanoribbon/Oligothiophene Composites. <i>ACS Omega</i> , 2022, 7, 2260-2274.	1.6	6
9731	Activity origin of boron doped carbon cluster for thermal catalytic oxidation: Coupling effects of dopants and edges. <i>Journal of Colloid and Interface Science</i> , 2022, 613, 47-56.	5.0	11
9732	Theoretical prediction of FN _g M ₃ (Ng=Ar, Kr, Xe, and Rn; M=Cu, Ag and Au; Q=O ²⁻) molecules. <i>Molecular Physics</i> , 0, , .	0.8	4
9733	Graphene Oxide (Ferrocenylmethyl) Dimethylammonium Nitrate Composites as Catalysts for Ammonium Perchlorate Thermolysis. <i>ACS Applied Nano Materials</i> , 2022, 5, 1209-1219.	2.4	9
9734	Theoretical Investigations on the Detecting Mechanism of a Typical 2,4,6-Trinitrophenol Fluorescence Sensor and Its Design Strategy. <i>Journal of Physical Chemistry A</i> , 2022, 126, 230-238.	1.1	1
9735	Theoretical investigation on the effect of the ligand on bis-silylation of C(sp) ² =C(sp) by Ni complexes. <i>RSC Advances</i> , 2021, 12, 1005-1010.	1.7	1
9736	Ligand-to-metal charge transfer driven by excited state antiaromaticity in metallohexaphyrins. <i>Bulletin of the Korean Chemical Society</i> , 2022, 43, 508-513.	1.0	5
9737	Investigation of [CHCl ₃ -CH ₃ OH] complex using matrix-isolation IR spectroscopy and quantum chemical calculation: Evidence of hydrogen- and halogen-bonding interaction. <i>Chemical Physics</i> , 2022, 555, 111451.	0.9	8
9738	<i>In situ</i> gelation regulating micro-electric fields to induce Li deposition in quasi-solid-state lithium metal batteries. <i>Journal of Materials Chemistry A</i> , 2022, 10, 2907-2916.	5.2	11
9739	Two new photochromic supramolecular compositions based on viologen: photocontrolled fluorescence, aniline detection and inkless erasable printing performance. <i>New Journal of Chemistry</i> , 2022, 46, 1905-1911.	1.4	15
9740	Nature of electronic excitations in small non-stoichiometric quantum dots. <i>Journal of Materials Chemistry A</i> , 2022, 10, 5212-5220.	5.2	10
9741	Vibronic Coupling Effect on the Vibrationally Resolved Electronic Spectra and Intersystem Crossing Rates of a TADF Emitter: 7-PhQAD. <i>Journal of Physical Chemistry A</i> , 2022, 126, 239-248.	1.1	25
9742	A mechanistic study on the gold(scp)-catalyzed cyclization of propargylic amide: revealing the impact of expanded-ring N-heterocyclic carbenes. <i>Catalysis Science and Technology</i> , 2022, 12, 674-685.	2.1	7
9743	On the nature of bonding in a new boronyl species Zn ₂ (BO) ₂ : a linear four-center two-electron σ bond. <i>Physical Chemistry Chemical Physics</i> , 2021, 24, 287-294.	1.3	1
9744	CO ₂ capture and separation from H ₂ /CH ₄ /N ₂ gas mixtures by a novel ternary pentagonal monolayer α -Penta-BCN: First principles investigation. <i>Journal of Molecular Liquids</i> , 2022, 348, 118474.	2.3	4
9745	Synergetic effect and mechanism between propylene carbonate and polymer rich in ester and ether groups for CO ₂ physical absorption. <i>Journal of Cleaner Production</i> , 2022, 336, 130389.	4.6	6
9746	Adsorptive removal of uremic toxins using Zr-based MOFs for potential hemodialysis membranes. <i>Journal of Materials Science</i> , 2022, 57, 2909-2923.	1.7	4

#	ARTICLE	IF	CITATIONS
9747	Traditional herbal compounds as candidates to inhibit the SARS-CoV-2 main protease: an in silico study. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-14.	2.0	3
9748	An insight into triel bonds in $\langle i \rangle O \langle /i \rangle, \langle i \rangle O \langle /i \rangle \hat{=}^2$ -diarylphosphorodithioates of thallium($\langle scp \rangle i \langle /scp \rangle$): experimental and theoretical investigations. <i>New Journal of Chemistry</i> , 2022, 46, 832-843.	1.4	7
9749	Effect of intramolecular charge transfer on nonlinear optical properties of chalcone derivatives: a visual description of the charge transfer process. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 955-965.	1.3	21
9750	High Efficiency Non Fullerene Acceptors Developed by Machine Learning and Quantum Chemistry. <i>Advanced Science</i> , 2022, 9, e2104742.	5.6	28
9751	New insight into lignin aggregation guiding efficient synthesis and functionalization of a lignin nanosphere with excellent performance. <i>Green Chemistry</i> , 2022, 24, 285-294.	4.6	36
9752	Effect of operating conditions and water matrix on the performance of UV combined electrochemical process for treating Chloride-containing solution and its reaction mechanism. <i>Separation and Purification Technology</i> , 2022, 286, 120465.	3.9	4
9753	Thermal decomposition of amino acid ionic liquids: Mechanism insight. <i>Journal of Molecular Liquids</i> , 2022, 349, 118486.	2.3	6
9754	Robust Luminescent Molecules with High Level Reverse Intersystem Crossing for Efficient Near Ultraviolet Organic Light Emitting Diodes. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	6
9755	The implication of phenolic acid matrix effect on the volatility of ethyl acetate in alcohol-free wine model: Investigations with experimental and theoretical methods. <i>Food Chemistry</i> , 2022, 378, 132114.	4.2	7
9756	Theoretical investigation of the mechanism of DMAP-promoted [4 + 2]-annulation of prop-2-ynylsulfonium with isatoic anhydride. <i>Canadian Journal of Chemistry</i> , 0, , 1-9.	0.6	0
9757	Degradation of tris(2-chloroethyl) phosphate (TCEP) by thermally activated persulfate: Combination of experimental and theoretical study. <i>Science of the Total Environment</i> , 2022, 809, 152185.	3.9	15
9758	Structural and molecular properties of complexes of biomolecules and metal organic frameworks: dispersion-corrected DFT treatment. <i>Journal of Molecular Modeling</i> , 2022, 28, 32.	0.8	3
9759	Roles of hydrogen bond and ion bridge in adsorption of two bisphenols onto montmorillonite: an experimental and DFT study. <i>Applied Clay Science</i> , 2022, 217, 106406.	2.6	17
9760	Molecular insight into the interaction of fluorometholone and cholesterol molecules with β -cyclodextrin and sulfobutylether- β -cyclodextrin. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113554.	1.1	5
9761	The inhibition of p-hydroxyphenyl hydroxyl group in residual lignin on enzymatic hydrolysis of cellulose and its underlying mechanism. <i>Bioresource Technology</i> , 2022, 346, 126585.	4.8	8
9762	Expanded spherical trihedral metallo-borosphenenes of transition-metal doped boron clusters: TM ₃ B ₁₅ q (TM = Zr, Hf; q = 1, 0, +1). <i>Results in Physics</i> , 2022, 33, 105214.	2.0	4
9763	Theoretical reconsideration of the mechanism of the excited state proton transfer of indigo carmine in water. <i>Journal of Molecular Liquids</i> , 2022, 347, 118365.	2.3	15
9764	Ruthenium complexes bearing N-heterocyclic carbene based CNC and CN ⁺ CHC ⁺ pincer ligands: Photophysics, electrochemistry, and solar energy conversion. <i>Journal of Organometallic Chemistry</i> , 2022, 959, 122203.	0.8	6

#	ARTICLE	IF	CITATIONS
9765	First-principles studies of imidazolium chloroaluminate ionic liquids with different substitutions on the Pt(111) surface. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 635, 128079.	2.3	1
9766	Oxygen-platinum interaction in alcohol-platinum clusters: Substituent effect and implications to reactivity. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113546.	1.1	1
9767	Redistribution mechanism on the preparation of dichlorodimethylsilane by the ZnCl ₂ /MIL-53(Al) catalyst. <i>Chemical Physics Letters</i> , 2022, 788, 139302.	1.2	1
9768	Evidence of cluster formation of pyrrole with mixed silver metal clusters, Ag _x -My (x=4,5, y=1 and) Tj ETQq1 1.10.784314.rgBT / Qv	1.1	28
9769	Screening of benzophenone ultraviolet absorbers with high-efficiency light absorption capacity, low-permeability and low-toxicity by 3D-QSAR model. <i>Journal of Molecular Liquids</i> , 2022, 347, 118364.	2.3	8
9770	First examples of nickel-Aluminum mixed chalcogenides based on the AuCu ₃ -type fragments: Breaking a robust intermetallic bond system in Ni ₃ Al. <i>Journal of Solid State Chemistry</i> , 2022, 306, 122815.	1.4	6
9771	Interaction of halomethane CH ₃ Z (Z=F, Cl, Br) with X ₁₂ Y ₁₂ (X=Al, Ga & Y=N, P, As) nanocages. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113544.	1.1	18
9772	Molecular simulation and optimization of extractive distillation for separation of dimethyl carbonate and methanol. <i>Chemical Engineering Research and Design</i> , 2022, 158, 181-188.	2.7	12
9773	Adsorption and diffusion of O atoms on metallic (1 0 0) surfaces. Cluster and periodic slab approaches. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113556.	1.1	1
9774	In silico modelling of acceptor materials by End-capped and ð-linker modifications for High-Performance organic solar Cells: Estimated PCE>18%. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113555.	1.1	19
9775	Preparation and characterization of polyphosphazene-based flame retardants with different functional groups. <i>Polymer Degradation and Stability</i> , 2022, 196, 109815.	2.7	13
9776	Non-fullerene acceptor IDIC based on indacineodithiophene used as an electron donor for organic solar cells: A computational study. <i>Journal of Molecular Liquids</i> , 2022, 348, 118289.	2.3	14
9777	Is it possible to switch ESIPT-channel of hydroxyanthraquinones with the strategy of modifying electronic groups?. <i>Journal of Molecular Liquids</i> , 2022, 347, 118343.	2.3	14
9778	Extraction and interaction insights for enhanced separation of phenolic compounds from model coal tar using a hydroxyl-functionalized ionic liquid. <i>Chemical Engineering Research and Design</i> , 2022, 178, 567-574.	2.7	17
9779	Salts of 2-hydroxybenzylamine with improvements on solubility and stability: Virtual and experimental screening. <i>European Journal of Pharmaceutical Sciences</i> , 2022, 169, 106091.	1.9	6
9780	Spectroscopic characterization, host-guest charge transfer, Hirshfeld surfaces, AIM-RDG and ELF study of adsorption and chemical sensing of heavy metals with new derivative of Calix [4]quinone: A DFT-D3 computation. <i>Materials Chemistry and Physics</i> , 2022, 278, 125555.	2.0	14
9781	Impacts of key preparation factors on polymerization and flocculation performance of polyferric silicate sulfate (PFSIS). <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 635, 128109.	2.3	10
9782	One-step synergistic optimization of hierarchical pore topology and nitrogen dopants in activated coke for efficient catalytic oxidation of nitric oxide. <i>Journal of Cleaner Production</i> , 2022, 335, 130360.	4.6	8

#	ARTICLE	IF	CITATIONS
9783	Non covalent interactions analysis and spectroscopic characterization combined with molecular docking study of N ^ε -(4-Methoxybenzylidene)-5-phenyl-1H-pyrazole-3-carbohydrazide. <i>Journal of King Saud University - Science</i> , 2022, 34, 101778.	1.6	4
9784	Exploring of antioxidant and antibacterial properties of novel 1,3,4-thiadiazole derivatives: Facile synthesis, structural elucidation and DFT approach to antioxidant characteristics. <i>Computational Biology and Chemistry</i> , 2022, 96, 107618.	1.1	17
9785	The reaction laws and toxicity effects of phthalate acid esters (PAEs) ozonation degradation on the troposphere. <i>Environmental Pollution</i> , 2022, 295, 118692.	3.7	9
9786	Efficiently red emitting cycloplatinated(II) complexes supported by N ^O and N ^P benzimidazole ancillary ligands. <i>Journal of Organometallic Chemistry</i> , 2022, 960, 122237.	0.8	3
9787	Stable alkoxy chain enhanced anion exchange membrane and its fuel cell. <i>Journal of Membrane Science</i> , 2022, 644, 120179.	4.1	13
9788	Tuning interface stability of nickel-rich LiNi _{0.9} Co _{0.05} Mn _{0.05} O ₂ cathode via a novel bis(vinylsulphonyl)methane additive. <i>Journal of Power Sources</i> , 2022, 521, 230917.	4.0	18
9789	Two effective strategies to improve SOCT-ISC type photosensitizers: Triphenylamine BODIPY with A-D-A configuration and AIE effect and its application in A-549 cells and zebrafish. <i>Dyes and Pigments</i> , 2022, 198, 110018.	2.0	11
9790	Spectroscopic and computational studies of erythrosine food dye protonation in aqueous solution. <i>Dyes and Pigments</i> , 2022, 198, 110028.	2.0	12
9791	Computational investigation on potential energy surface evolution: The tautomerization from enediyne to enyne-allene. <i>Chemical Physics Letters</i> , 2022, 789, 139298.	1.2	1
9792	Energy-based fragmentation contribution approach for calculating the fluorescence spectrum of biomacromolecules. <i>Chemical Physics</i> , 2022, 554, 111425.	0.9	3
9793	Kinetics and molecular mechanism of the Schonberg rearrangement. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113585.	1.1	1
9794	A DFT study of carbon dioxide reduction catalyzed by group 3 metal complexes of silylamides. <i>Chemical Physics Letters</i> , 2022, 788, 139291.	1.2	0
9795	Understanding the lithiation mechanisms of pyrenetetrone-based carbonyl compound as cathode material for lithium-ion battery: Insight from first principle density functional theory. <i>Materials Chemistry and Physics</i> , 2022, 278, 125518.	2.0	87
9796	Mechanisms of bromination between thiophenes and NBS: A DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113545.	1.1	1
9797	Feasibility of micropollutants removal by solar-activated persulfate: Reactive oxygen species formation and influence on DBPs. <i>Water Research</i> , 2022, 210, 117981.	5.3	33
9798	Ultrasonic-assisted extraction of zeaxanthin from <i>Lycium barbarum</i> L. with composite solvent containing ionic liquid: Experimental and theoretical research. <i>Journal of Molecular Liquids</i> , 2022, 347, 118265.	2.3	10
9799	Synthesis, molecular modeling, quantum mechanical calculations and ADME estimation studies of benzimidazole-oxadiazole derivatives as potent antifungal agents. <i>Journal of Molecular Structure</i> , 2022, 1252, 132095.	1.8	19
9800	Measurement of Donor-Acceptor Interchange Tunnelling in Ar(H ₂ O) ₂ using Rotational Spectroscopy and a Re-look at Its Structure and Bonding. <i>Journal of Molecular Structure</i> , 2022, 1252, 132094.	1.8	1

#	ARTICLE	IF	CITATIONS
9801	Deciphering the Ligand's geometric effect on the photophysical properties of osmium complex and its application in triplet-triplet annihilation upconversion. <i>Dyes and Pigments</i> , 2022, 199, 110049.	2.0	10
9802	Synthesis, crystal structure, Hirshfeld surface, DFT and docking studies of 4-[(5-hydroxy-3-methyl-1-phenyl-1H-pyrazol-4-yl)(phenyl)methyl]-5-methyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one. <i>Journal of Molecular Structure</i> , 2022, 1252, 132170.	1.8	13
9803	DFT study of 2D graphitic carbon nitride based preferential targeted delivery of levosimendan, a cardiovascular drug. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113584.	1.1	6
9804	The finite-difference time-domain (FDTD) guided preparation of Ag nanostructures on Ti substrate for sensitive SERS detection of small molecules. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 269, 120743.	2.0	13
9805	Spectroscopic profiling and molecular docking of novel chalcone derivative (2E)-1-(3,4-dimethoxyphenyl)-3-(4-n-propyloxyphenyl)-2-propen-1-one- A prospective respiratory drug. <i>Journal of Molecular Structure</i> , 2022, 1252, 132138.	1.8	0
9806	Anchoring Interfacial Nickel Cations by Tunable Coordinative Structure for Highly Stabilized Nickel-Rich Layered Oxide Cathodes. <i>Nano Energy</i> , 2022, 93, 106803.	8.2	18
9807	A near-infrared fluorescent chemosensor with a remarkably large Stokes shift for the ultrasensitive detection of tyrosinase activity and bioimaging in living cells and mouse xenograft model. <i>Sensors and Actuators B: Chemical</i> , 2022, 354, 131211.	4.0	10
9808	Fullerene binding effects in Al(III)/Zn(II) Porphyrin/Phthalocyanine photophysical properties and charge transport. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 269, 120740.	2.0	9
9809	Synthesis, molecular structure, Hirshfeld surface, energy framework and DFT studies of 1,3,4-oxadiazole derivative. <i>Journal of Molecular Structure</i> , 2022, 1252, 132203.	1.8	17
9810	Structural peculiarities of new benzopyrylium dyes: X-ray, FT-IR, and DFT complex study. <i>Journal of Molecular Structure</i> , 2022, 1252, 132178.	1.8	4
9811	Study on the microscopic aggregation behavior of lignite molecules in water. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 637, 128194.	2.3	6
9812	Synthesis, Spectral, Crystal structure, Hirshfeld surface, Computational analysis, and Antimicrobial studies of Ethyl-(E)-4-(2-(2-arylidenehydrazinyl)-2-oxoethyl)piperazine-1-carboxylates. <i>Journal of Molecular Structure</i> , 2022, 1252, 132082.	1.8	17
9813	Efficient detection for Nitrofurazone based on novel Ag ₂ S QDs/g-C ₃ N ₄ fluorescent probe. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 269, 120727.	2.0	13
9814	Simple reaction to prepare a heat-resistant and insensitive explosive (2-nitro-[1,2,4]triazolo[1,5-a][1,3,5]triazine-5,7-diamine) and its derivatives. <i>Chemical Engineering Journal</i> , 2022, 432, 134297.	6.6	13
9815	Oligomer-first mechanism in the transformation of biomass derivatives selectively to produce D-lactic acid. <i>Chemical Engineering Journal</i> , 2022, 432, 134359.	6.6	8
9816	Extremely low efficiency roll-off in vacuum- and solution-processed deep-red/near-infrared OLEDs based on 1,8-naphthalimide TADF emitters. <i>Journal of Luminescence</i> , 2022, 243, 118683.	1.5	6
9817	Maximizing the utilization of photo-generated electrons and holes of g-C ₃ N ₄ photocatalyst for harmful algae inactivation. <i>Chemical Engineering Journal</i> , 2022, 431, 134105.	6.6	59
9818	Synthesis, characterization and properties of amphoteric heat-resistant explosive materials: Fused [1,2,5]oxadiazolo [3,4-d]pyrido[4,3-d][1,2,3]triazines. <i>Chemical Engineering Journal</i> , 2022, 432, 134293.	6.6	14

#	ARTICLE	IF	CITATIONS
9819	Crystal structure elucidation and DFT studies of imidazopyridine-pyrazoline derivative. <i>Journal of Molecular Structure</i> , 2022, 1251, 132063.	1.8	3
9820	Orange-red emissive Cu(I) complexes bearing Schiff base ligands: Synthesis, structures, and photophysical properties. <i>Journal of Molecular Structure</i> , 2022, 1252, 132180.	1.8	3
9821	Hybrid functional/embedded cluster study of uranium and actinide (actinide=U, Pu, Am or Cm) mixed dioxides bulk and {110} surfaces. <i>Journal of Nuclear Materials</i> , 2022, 560, 153490.	1.3	2
9822	Oxidation of tetracycline antibiotics by peracetic acid: Reaction kinetics, mechanism, and antibacterial activity change. <i>Chemical Engineering Journal</i> , 2022, 431, 134190.	6.6	11
9823	Origins of selective differential oxidation of β -lactam antibiotics with different structure in an efficient visible-light driving mesoporous g-C ₃ N ₄ activated persulfate synergistic mechanism. <i>Journal of Hazardous Materials</i> , 2022, 426, 128111.	6.5	10
9824	Role of glycosidic bond in initial cellulose pyrolysis: Investigation by machine learning simulation. <i>Applications in Energy and Combustion Science</i> , 2022, 9, 100055.	0.9	2
9825	Potential application of Al and Si doped carbon nanotubes for metronidazole detection: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113573.	1.1	5
9826	Combination of theoretical calculation and experiment to study the excited state proton transfer behavior of trifluoroacetamidoanthraquinone with different substitution positions. <i>Journal of Molecular Structure</i> , 2022, 1252, 132084.	1.8	11
9827	Degradation of tetracycline by atmospheric-pressure non-thermal plasma: Enhanced performance, degradation mechanism, and toxicity evaluation. <i>Science of the Total Environment</i> , 2022, 812, 152455.	3.9	28
9828	Iron cycle tuned by thiosulfate in Fenton reactions: Kinetic modelling and mechanisms. <i>Chemical Engineering Journal</i> , 2022, 431, 134252.	6.6	19
9829	Turning ON/OFF the fluorescence of the ESIPT state by changing the hydrogen bond distance and orientation in quinoline-pyrazole derivatives. <i>Journal of Molecular Structure</i> , 2022, 1252, 132146.	1.8	9
9830	Aqueous zinc batteries using N-containing organic cathodes with Zn ²⁺ and H ⁺ Co-uptake. <i>Chemical Engineering Journal</i> , 2022, 431, 134253.	6.6	37
9831	Intermolecular (Isocyano group) π - π interactions involving coordinated isocyanides in cyclometalated Pt(II) complexes. <i>Journal of Molecular Structure</i> , 2022, 1253, 132230.	1.8	9
9832	Doped organic charge-transfer cocrystal with tunable fluorescence of wide band emission. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 426, 113727.	2.0	3
9833	First-principles study on structural, electronic, and magnetic properties of 3d transition metal-substituted chiral (6, 3) carbon nanotube. <i>Computational Condensed Matter</i> , 2022, 30, e00621.	0.9	2
9834	Surfactants directly participate in the molecular recognition for visual and sensitive detection of fentanyl. <i>Sensors and Actuators B: Chemical</i> , 2022, 354, 131215.	4.0	2
9835	First principles investigations and Hirshfeld surface analysis of high-energetic and low-sensitive 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105) crystal. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 163, 110550.	1.9	1
9836	Enhancing CH ₄ /N ₂ separation performance within aluminum-based Metal-Organic Frameworks: Influence of the pore structure and linker polarity. <i>Separation and Purification Technology</i> , 2022, 286, 120446.	3.9	24

#	ARTICLE	IF	CITATIONS
9837	New insights into the capture performance and mechanism of hazardous metals Cr ³⁺ and Cd ²⁺ onto an effective layered double hydroxide based material. <i>Journal of Hazardous Materials</i> , 2022, 426, 128062.	6.5	155
9838	Comprehensive understanding on solubility and solvation performance of curcumin (form I) in aqueous co-solvent blends. <i>Journal of Chemical Thermodynamics</i> , 2022, 167, 106718.	1.0	12
9839	pH-dependent structural changes of arsenic oxoacids in solution and solid phase: Raman spectrometry and computational studies. <i>Microchemical Journal</i> , 2022, 175, 107109.	2.3	4
9840	A pore matching amine-functionalized strategy for efficient CO ₂ physisorption with low energy penalty. <i>Chemical Engineering Journal</i> , 2022, 432, 134403.	6.6	21
9841	The "off-on" fluorescent probe based on salicylic acid for rapid and selective detection of 1-hydroxyethane-1,1-diphosphonic acid. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 426, 113740.	2.0	1
9842	Selective and swift-responsive "off-on" rhodamine B based chemosensors: Recognition of multi-metal ions, on-site sensing of Fe(III) in water samples and bioimaging in aqueous media. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 426, 113748.	2.0	9
9843	Quantum chemical, spectroscopic, hirshfeld surface and molecular docking studies on 2-aminobenzothiazole. <i>Journal of Molecular Structure</i> , 2022, 1253, 132254.	1.8	2
9844	Synergistic strongly coupled super-deamidation of wheat gluten by glucose-organic acid natural deep eutectic solvent and the efficaciousness of structure and functionality. <i>Food Hydrocolloids</i> , 2022, 125, 107437.	5.6	10
9845	Synthesis, structural and spectroscopic analysis, and antiproliferative activity of chalcone derivate (E)-1-(4-aminophenyl)-3-(benzo[b]thiophen-2-yl)prop-2-en-1-one in <i>Trypanosoma cruzi</i> . <i>Journal of Molecular Structure</i> , 2022, 1253, 132197.	1.8	6
9846	Crystal structure elucidation, Hirshfeld surface analysis, and DFT studies of a N-benzyl-3-phenylquinoxalin-2-amine. <i>Journal of Molecular Structure</i> , 2022, 1253, 132271.	1.8	5
9847	A computational perspective for tailor-made selective Mcl-1 and Bcl-XL inhibitors. <i>Journal of Molecular Structure</i> , 2022, 1253, 132269.	1.8	1
9848	A priori design of new natural deep eutectic solvent for lutein recovery from microalgae. <i>Food Chemistry</i> , 2022, 376, 131930.	4.2	32
9849	Pilot-scale and mechanistic study of the degradation of typical odors and organic compounds in drinking water by a combined UV/H ₂ O ₂ -BAC process. <i>Chemosphere</i> , 2022, 292, 133419.	4.2	10
9850	Experimental and density functional theory investigation of 1-(4-Bromophenyl)-3-(4-ethoxyphenyl)-prop-2-en-1-one (EBC) single crystals for high second-order nonlinear optical applications. <i>Journal of Molecular Structure</i> , 2022, 1253, 132243.	1.8	4
9851	Insighting the functionally modified C ₆₀ fullerenes as an efficient nonlinear optical materials: A quantum chemical study. <i>Materials Science in Semiconductor Processing</i> , 2022, 141, 106421.	1.9	17
9852	Enhancing catalytic ozonation activity of MCM-41 via one-step incorporating fluorine and iron: The interfacial reaction induced by hydrophobic sites and Lewis acid sites. <i>Chemosphere</i> , 2022, 292, 133544.	4.2	13
9853	The inner oxygen-substituted strategy effects on structure, aromaticity and absorption spectra of corrole isomers: A theoretical study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 112, 108118.	1.3	0
9854	Rotational spectrum of Isochroman. <i>Journal of Molecular Structure</i> , 2022, 1254, 132322.	1.8	0

#	ARTICLE	IF	CITATIONS
9855	Investigation of ultrafast broadband optical nonlinearity and intensity-dependent nonlinear absorption in novel hydrazone derivatives. <i>Optics and Laser Technology</i> , 2022, 149, 107798.	2.2	7
9856	High-valent iron-oxo species mediated cyclic oxidation through single-atom Fe-N6 sites with high peroxymonosulfate utilization rate. <i>Applied Catalysis B: Environmental</i> , 2022, 305, 121049.	10.8	48
9857	One-Step construction of Polyimide/NH ₂ -UiO-66 heterojunction for enhanced photocatalytic degradation of sulfonamides. <i>Journal of Colloid and Interface Science</i> , 2022, 612, 536-549.	5.0	15
9858	Insight into mercury-laden activated carbon adsorbent product bonding nature by DFT calculations. <i>Chemical Engineering Journal</i> , 2022, 433, 134461.	6.6	7
9859	COSMO-RS prediction, liquid-liquid equilibrium experiment and quantum chemistry calculation for the separation of n-butanol and n-heptane system using ionic liquids. <i>Journal of Chemical Thermodynamics</i> , 2022, 167, 106719.	1.0	6
9860	Low-temperature and high-rate Zn metal batteries enabled by mitigating Zn ²⁺ concentration polarization. <i>Chemical Engineering Journal</i> , 2022, 433, 134589.	6.6	35
9861	Enhanced orientation photocatalytic ability of 1D inorganic imprinted oxygen vacancy CdO _{0.5} S _{0.5} by confining the target to the specific reaction sites enriched in electrons. <i>Journal of Alloys and Compounds</i> , 2022, 901, 163708.	2.8	3
9863	Computational Characterization of the Substrate Activation in the Active Site of SARS-CoV-2 Main Protease. <i>Supercomputing Frontiers and Innovations</i> , 2020, 7, .	0.5	1
9864	Quasi-Static Two-Dimensional Infrared Spectra of the Carboxyhemoglobin Subsystem under Electric Fields: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9570-9578.	1.2	3
9867	Influence of Copper(I) Halides on the Reactivity of Aliphatic Carbodiimides. <i>Chemistry Proceedings</i> , 2020, 3, .	0.1	1
9868	Incorporating Amino Acids Functionalized Graphene Oxide Nanosheets into Pebax Membranes for CO ₂ Separation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
9869	Microporous polycarbazole frameworks with large conjugated π systems for cyclohexane separation from cyclohexane-containing mixtures. <i>New Journal of Chemistry</i> , 2021, 45, 22437-22443.	1.4	6
9870	Bio-inspired AIE pillar[5]arene probe with multiple binding sites to discriminate alkanediamines. <i>Chemical Communications</i> , 2021, 57, 13114-13117.	2.2	12
9872	Effect of Operating Conditions and Water Matrix on the Performance of UV Combined Electrochemical Process for Treating Chloride-Containing Solution and its Reaction Mechanism. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
9873	Construction of a Novel Metal-Organic Framework Adenine-UiO-66 Piezocatalyst for Efficient Diclofenac Removal by Harvesting Stirring Energy. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
9874	Degradation of Microcystin-LR with Expanded Graphite Based Photocatalysts: Performance and Mechanism Based on Active Sites-Radicals Interaction. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
9875	Abnormal Molecular Clusters in Pyridine-Ethanol Mixtures under Electric Fields. <i>Russian Journal of Physical Chemistry B</i> , 2021, 15, S81-S91.	0.2	2
9876	EDA, CDA and QAIM Investigations in the (para-C ₅ H ₄ X) Ir(PH ₃) ₃ Iridabenzene Complexes. <i>Russian Journal of Physical Chemistry B</i> , 2021, 15, S6-S13.	0.2	5

#	ARTICLE	IF	CITATIONS
9877	CRYSTAL STRUCTURE AND X-RAY CRYSTALLOGRAPHIC ANALYSIS OF THE BINUCLEAR CLUSTER THIOCYANATE COMPLEX OF NIOBIUM(IV). <i>Journal of Structural Chemistry</i> , 2021, 62, 1531-1542.	0.3	1
9878	Methyl-mercaptane adsorption and sensing on Fe-/Co-graphene structures: A DFT study. <i>Turkish Computational and Theoretical Chemistry</i> , 0, , .	0.5	0
9879	Se-sensitized NIR hot band absorption photosensitizer for anti-Stokes excitation deep photodynamic therapy. <i>Science China Chemistry</i> , 2022, 65, 563-573.	4.2	19
9880	Transport mechanisms and desalination performance of the PSF/UiO-66 thin-film composite membrane: a molecular dynamics study. <i>Molecular Simulation</i> , 2022, 48, 427-437.	0.9	0
9881	Formation mechanism of typical aromatic sulfuric anhydrides and their potential role in atmospheric nucleation process. <i>Journal of Environmental Sciences</i> , 2022, , .	3.2	0
9882	Ambient hydrogenation of carbon dioxide into liquid fuel by a heterogeneous synergetic dual single-atom catalyst. <i>Cell Reports Physical Science</i> , 2022, 3, 100705.	2.8	18
9883	Safe and Stable Lithium Metal Batteries Enabled by an Amide-Based Electrolyte. <i>Nano-Micro Letters</i> , 2022, 14, 44.	14.4	34
9884	Disintegration of wet microalgae biomass with deep-eutectic-solvent-assisted hydrothermal treatment for sustainable lipid extraction. <i>Green Chemistry</i> , 2022, 24, 1615-1626.	4.6	17
9885	Efficient and Stable Methylammonium-Free Tin-Lead Perovskite Solar Cells with Hexaazatrinaphthylene-Based Hole-Transporting Materials. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 6852-6858.	4.0	13
9886	Controlling the Interaction between Fluorescent Gold Nanoclusters and Bionterfaces for Rapid Discrimination of Fungal Pathogens. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 4532-4541.	4.0	11
9887	Excitons in ZnO Quantum Dots: The Role of Dielectric Confinement. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2833-2838.	1.5	9
9888	Mechanistic investigation of zwitterionic MOF-catalyzed enyne annulation using UNLPF-14-MnIII as catalyst. <i>Chinese Chemical Letters</i> , 2022, 33, 4281-4286.	4.8	12
9889	La@[La ₅ B ₃₀ O] ²⁺ : endohedral trihedral metallo-borosphenes with spherical aromaticity. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3918-3923.	1.3	4
9890	12-Membered Ring Carbides with Stabilization of Actinide Atoms. <i>Inorganic Chemistry</i> , 2022, 61, 2119-2128.	1.9	4
9891	Theoretical exploration of diverse electron-deficient core and terminal groups in A _n type non-fullerene acceptors for organic solar cells. <i>New Journal of Chemistry</i> , 2022, 46, 3370-3382.	1.4	12
9892	Spiroarborin, an <i>ent</i> -Clerodane Homodimer from <i>Callicarpa arborea</i> as an Inhibitor of the Eleven-Nineteen Leukemia (ENL) Protein by Targeting the YEATS Domain. <i>Journal of Natural Products</i> , 2022, 85, 317-326.	1.5	10
9893	Synthesis of (Thio)Furan-Fused Phospholes via Phosphonation Cyclization and a Base-Promoted Phospha-Friedel-Crafts Reaction. <i>Journal of Organic Chemistry</i> , 2022, , .	1.7	4
9894	Sensitive sensors based on bilayer organic field-effect transistors for detecting lithium-ion battery electrolyte leakage. <i>Science China Materials</i> , 2022, 65, 1187-1194.	3.5	9

#	ARTICLE	IF	CITATIONS
9895	Structural design and physicochemical specifications exploring of the new di-cationic ionic liquids (D-ILs) composed of para-xylyl linked N-Methylimidazolium cation and various anions: a full M06â€“2X computational study. Theoretical Chemistry Accounts, 2022, 141, 1.	0.5	10
9896	(E)-4-((4-Bromobenzylidene) Amino)-N-(Pyrimidin-2-yl) Benzenesulfonamide from 4-Bromobenzaldehyde and Sulfadiazine, Synthesis, Spectral (FTIR, UVâ€“Vis), Computational (DFT, HOMOâ€“LUMO, MEP, NBO, NPA,) Tj ETQq 1 0184314	1.7	18
9897	Comparative enantioseparation of planar chiral ferrocenes on polysaccharideâ€“based chiral stationary phases. Chirality, 2022, , .	1.3	7
9898	Investigation of the adsorption properties of gemcitabine anticancer drug with metal-doped boron nitride fullerenes as a drug-delivery carrier: a DFT study. RSC Advances, 2022, 12, 2873-2887.	1.7	31
9899	On the Road Toward More Efficient Biocompatible Twoâ€“Photon Excitable Fluorophores. Chemistry - A European Journal, 2022, , .	1.7	3
9900	A deep blue thermally activated delayed fluorescence emitter: balance between charge transfer and color purity. Journal of Materials Chemistry C, 2022, 10, 4886-4893.	2.7	12
9901	Fascinating 3D energetic [Ag₂(N₅)₂(EDA)]_{<i>n</i>}: filling the ethylenediamine molecules into a [Ag(N₅)]_{<i>n</i>} framework. CrystEngComm, 2022, 24, 1900-1906.	1.3	2
9902	Symmetrical <i>cyclo</i>-N₅^{â€“} hydrogen bonds: stabilization mechanism of four non-metallic cyclo-pentazolates energetic salts. Physical Chemistry Chemical Physics, 2022, 24, 3970-3983.	1.3	4
9903	Simple and efficient visualization of aromaticity: bond currents calculated from NICS values. Physical Chemistry Chemical Physics, 2022, 24, 8631-8644.	1.3	26
9904	Charge transfer and polarisability in ionic liquids: a case study. Physical Chemistry Chemical Physics, 2022, 24, 3144-3162.	1.3	11
9905	First-Principles Plane-Wave-Based Exploration of Cathode and Anode Materials for Li- and Na-Ion Batteries Involving Complex Nitrogen-Based Anions. Chemistry of Materials, 2022, 34, 652-668.	3.2	9
9906	Chalcogen Bonding in the Molecular Dimers of WCh ₂ (Ch = S, Se, Te): On the Basic Understanding of the Local Interfacial and Interlayer Bonding Environment in 2D Layered Tungsten Dichalcogenides. International Journal of Molecular Sciences, 2022, 23, 1263.	1.8	12
9907	Synergistic engineering of end-capped acceptor and bridge on arylborane-arylamine macrocycles to boost the photovoltaic properties of organic solar cells. Optical Materials, 2022, 123, 111907.	1.7	48
9908	A supported Crâ€“Cr sextuple bond in an all-metal cluster. Dalton Transactions, 2022, 51, 2664-2668.	1.6	1
9909	Insights into the intermolecular interactions and temperature-concentration dependence of transport in ionic liquid-based EMIâ€“TFSI/LITFSI electrolytes. New Journal of Chemistry, 2022, 46, 3966-3977.	1.4	9
9910	Unveiling the synthesis of spirocyclic, tricyclic, and bicyclic triazolooxazines from intramolecular [3 + 2] azide-alkyne cycloadditions with a molecular electron density theory perspective. Structural Chemistry, 2022, 33, 555-570.	1.0	6
9911	Edge-oxidation induced non-radiative recombination dynamics in graphene quantum dots: a theoretical insight from Fermiâ€“TM's golden rule. Molecular Physics, 2022, 120, .	0.8	5
9912	Nanostructuring and macroscopic behavior of type V deep eutectic solvents based on monoterpenoids. Physical Chemistry Chemical Physics, 2021, 24, 512-531.	1.3	28

#	ARTICLE	IF	CITATIONS
9913	Theoretical Study of the Structural Stability, Chemical Reactivity, and Protein Interaction for NMP Compounds as Modulators of the Endocannabinoid System. <i>Molecules</i> , 2022, 27, 414.	1.7	7
9914	Study on the extraction of lanthanides by isomeric diglycolamide extractants: an experimental and theoretical study. <i>RSC Advances</i> , 2021, 12, 790-797.	1.7	6
9915	A QM/MM study on through space charge transfer-based thermally activated delayed fluorescence molecules in the solid state. <i>Journal of Materials Chemistry C</i> , 2022, 10, 517-531.	2.7	30
9916	Encapsulation of anticancer drug Ibrance into the CNT(8,8-7) nanotube: A study based on DFT method. <i>Main Group Chemistry</i> , 2022, , 1-19.	0.4	2
9917	Narrowband Deep-Blue Multi-Resonance Induced Thermally Activated Delayed Fluorescence: Insights from the Theoretical Molecular Design. <i>Molecules</i> , 2022, 27, 348.	1.7	3
9918	Molecular Mechanism of the Mononuclear Copper Complexâ€Catalyzed Water Oxidation from Clusterâ€Continuum Model Calculations. <i>ChemSusChem</i> , 2022, 15, .	3.6	2
9919	Deep eutectic solvents boosting solubilization and Se-functionalization of heteropolysaccharide: Multiple hydrogen bonds modulation. <i>Carbohydrate Polymers</i> , 2022, 284, 119159.	5.1	12
9920	Excitation induced asymmetric fluorescence emission in 2D-WS ₂ quantum dots. <i>Materials Advances</i> , 2022, 3, 1772-1779.	2.6	2
9921	Heterospin frustration in a metal-fullerene-bonded semiconductive antiferromagnet. <i>Nature Communications</i> , 2022, 13, 495.	5.8	5
9922	Theoretical investigation complexation characteristics and UVâ€Vis absorption spectral properties of CdTe QDs with four capping agents. <i>Journal of Molecular Modeling</i> , 2022, 28, 28.	0.8	2
9923	An encapsulating lithium-polysulfide electrolyte for practical lithiumâ€sulfur batteries. <i>CheM</i> , 2022, 8, 1083-1098.	5.8	77
9924	All-perovskite tandem solar cells with improved grain surface passivation. <i>Nature</i> , 2022, 603, 73-78.	13.7	544
9925	Theoretical mechanistic insights into dinitrogen cleavage by a dititanium hydride complex bearing PNP-pincer ligands. <i>Dalton Transactions</i> , 2022, 51, 918-926.	1.6	2
9926	Halogen bonding in cadmium(<i>II</i>) MOFs: its influence on the structure and on the nitroaldol reaction in aqueous medium. <i>Dalton Transactions</i> , 2022, 51, 1019-1031.	1.6	22
9927	Graphene oxide nanosheets functionalized protected amine for tuning of interlayer d-spacing with DFT studies: A versatile material design. <i>MRS Communications</i> , 2022, 12, 37.	0.8	1
9928	Inhibition Role of Solvation on the Selective Extraction of Co(II): Toward Eco-Friendly Separation of Ni and Co. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 1160-1171.	3.2	4
9929	Energetic and Geometric Characteristics of Substituents, Part 3: The Case of NO ₂ and NH ₂ Groups in Their Mono-Substituted Derivatives of Six-Membered Heterocycles. <i>Symmetry</i> , 2022, 14, 145.	1.1	1
9930	Metallo-boranes: a class of unconventional superhalogens defying electron counting rules. <i>Nanoscale</i> , 2022, 14, 1767-1778.	2.8	3

#	ARTICLE	IF	CITATIONS
9931	Molecular structure spectroscopic Elucidation, IEFPCM solvation (UV-Vis, MEP, FMO, NBO, NLO), molecular docking and biological assessment studies of lepidine (4-Methylquinoline). <i>Journal of Molecular Liquids</i> , 2022, 345, 118249.	2.3	30
9932	Growth direction dependent separate-channel charge transport in the organic weak charge-transfer co-crystal of anthracene-DTTCNQ. <i>Materials Horizons</i> , 2022, , .	6.4	2
9933	Ester-substituted thiophene-fused benzothiadiazole as a strong electron acceptor to build a red emitters for highly efficient solution-processed OLEDs. <i>Journal of Materials Chemistry C</i> , 2022, 10, 1127-1135.	2.7	8
9934	Mechanism of Fuel Gas Denitration on the KOH-Activated Biochar Surface. <i>Journal of Physical Chemistry A</i> , 2022, 126, 296-305.	1.1	6
9935	A machine learning approach for predicting the nucleophilicity of organic molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1821-1829.	1.3	13
9936	J-aggregation enhanced thermally activated delayed fluorescence for amplified spontaneous emission. <i>Cell Reports Physical Science</i> , 2022, 3, 100686.	2.8	6
9937	Achieving two things at one stroke: crystal engineering simultaneously optimizes the emission and mechanical compliance of organic crystals. <i>Journal of Materials Chemistry C</i> , 2022, 10, 3894-3900.	2.7	8
9938	Experimental Spectroscopic, Computational, Hirshfeld Surface, Molecular Docking Investigations on 1H-Indole-3-Carbaldehyde. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 1263-1287.	1.4	11
9939	An Ionic Cluster Strategy for Performance Improvements and Product Morphology Control in Metal-Catalyzed Olefin Polar Monomer Copolymerization. <i>Journal of the American Chemical Society</i> , 2022, 144, 2245-2254.	6.6	65
9940	Formation and stabilization mechanism of mesoscale clusters in solution. <i>IUCr</i> , 2022, 9, 215-222.	1.0	3
9941	Theoretical insights into effects of solvent polarity on excited-state H proton transfer behavior for a new fluorophore of 3-tosylamino-N-cyclohexylphthalimide. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	2
9942	EnzyHTP: A High-Throughput Computational Platform for Enzyme Modeling. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 647-655.	2.5	16
9943	Computational investigation of a covalent triazine framework (CTF-0) as an efficient electrochemical sensor. <i>RSC Advances</i> , 2022, 12, 3909-3923.	1.7	28
9944	The mechanism and origin of selectivities for NHC-catalyzed synthesis of axially chiral benzothiophene/benzofuran-fused biaryls. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 1662-1670.	1.5	11
9945	Novel zinc (II) and nickel (II) complexes of a quinazoline-based ligand with an imidazole ring: Synthesis, spectroscopic property, antibacterial activities, time-dependent density functional theory calculations and Hirshfeld surface analysis. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	1.7	18
9946	Square tetravalent chalcogen bonds in dimeric aggregates: a joint crystallographic survey and theoretical study. <i>CrystEngComm</i> , 2022, 24, 975-986.	1.3	4
9947	Conformational analysis, molecular structure, spectroscopic, NBO, reactivity descriptors, wavefunction and molecular docking investigations of 5,6-dimethoxy-1-indanone: A potential anti Alzheimer's agent. <i>Heliyon</i> , 2022, 8, e08821.	1.4	7
9948	Carbene-Metal Complexes As Molecular Scaffolds for Construction of through-Space Thermally Activated Delayed Fluorescence Emitters. <i>Inorganic Chemistry</i> , 2022, 61, 2174-2185.	1.9	14

#	ARTICLE	IF	CITATIONS
9949	Energy Counterbalance to Harness Photoinduced Structural Planarization of Dibenzob[<i>b,f</i>]azepines toward Thermal Reversibility. <i>Journal of the American Chemical Society</i> , 2022, 144, 1748-1757.	6.6	15
9950	Understanding the mechanism of interfacial interaction enhancing photodegradation rate of pollutants at molecular level: Intermolecular π - π interactions favor electrons delivery. <i>Journal of Hazardous Materials</i> , 2022, 430, 128386.	6.5	39
9951	Asymmetrical π -Dendronized TADF Emitters for Efficient Non-doped Solution-Processed OLEDs by Eliminating Degenerate Excited States and Creating Solely Thermal Equilibrium Routes. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	5
9952	Screening of transition metal single atom catalysts supported on B36 cluster for nitrogen fixation. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 5281-5291.	3.8	4
9953	Investigation on the dehydrofluorination of 2H,3H-decafluoropentane. <i>Journal of Fluorine Chemistry</i> , 2022, 253, 109931.	0.9	0
9954	A simple and highly efficient composite based on g-C ₃ N ₄ for super rapid removal of multiple organic dyes from water under sunlight. <i>Catalysis Science and Technology</i> , 2022, 12, 786-798.	2.1	9
9955	Noble-gas compounds: A general procedure of bonding analysis. <i>Journal of Chemical Physics</i> , 2022, 156, 014104.	1.2	10
9956	Computational insights into different regioselectivities in the Ir-porphyrin-catalyzed C-H insertion reaction of quinoid carbene. <i>Organic Chemistry Frontiers</i> , 2022, 9, 1143-1151.	2.3	2
9957	DFT and TD-DFT study of adsorption behavior of Zejula drug on surface of the B12N12 nanocluster. <i>Main Group Chemistry</i> , 2022, 21, 405-420.	0.4	8
9958	Revealing the reason for the reversal of properties from fullerene to nonfullerene. <i>Physical Chemistry Chemical Physics</i> , 2021, 24, 30-34.	1.3	1
9959	Electro-optical, electronic and conformational transitions of interstellar alkyl molecules at different temperatures: An ab-initio study. <i>Current Research in Green and Sustainable Chemistry</i> , 2022, 5, 100235.	2.9	1
9960	Structure identification and analysis of the suspected chemical precursor of 2-fluorodeschloroketamine and its decomposition products. <i>Drug Testing and Analysis</i> , 2022, 14, 1065-1078.	1.6	2
9961	Theoretical Insights on Improving Amidoxime Selectivity for Potential Uranium Extraction from Seawater. <i>Journal of Physical Chemistry A</i> , 2022, 126, 406-415.	1.1	11
9962	CO self-promoted oxidation by gas-phase cluster anions IrVO ₄ ⁻ . <i>Chemical Physics Letters</i> , 2022, 787, 139276.	1.2	2
9963	Theoretical Study on the Light-Emitting Mechanism of Multifunctional Thermally Activated Delayed Fluorescence Molecules. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2437-2446.	1.5	10
9964	Elucidating the selectivity of dyotropic rearrangements of β^2 -lactones: a computational survey. <i>Organic Chemistry Frontiers</i> , 2022, 9, 329-341.	2.3	6
9965	Improvement the energy conversion efficiency of organic dye-based solar cells by pioneer solvents. <i>Molecular Physics</i> , 2022, 120, .	0.8	0
9966	Theoretical investigation on the intermolecular interactions between 3-nitro-1,2,4-triazol-5-one and 2,6-diamino-3,5-dinitropyrazine-1-oxide using DFT methods. <i>Chemical Papers</i> , 2022, 76, 2747-2758.	1.0	10

#	ARTICLE	IF	CITATIONS
9967	Simple thiazole-centered oligothiophene donor enables 15.4% efficiency all small molecule organic solar cells. <i>Journal of Materials Chemistry A</i> , 2022, 10, 3009-3017.	5.2	28
9968	Rational design of a zwitterionic porous organic framework loaded with Co(II) ions to host sulfur and synergistically boost polysulfide redox kinetics for lithium sulfur batteries. <i>Materials Advances</i> , 2022, 3, 1594-1601.	2.6	4
9969	Novel Star-Shaped Benzotriindole-Based Nonfullerene Donor Materials: Toward the Development of Promising Photovoltaic Compounds for High-Performance Organic Solar Cells. <i>Energy Technology</i> , 2022, 10, .	1.8	18
9970	Hydrogen/Deuterium Transfer from Anisole to Methoxy Radicals: A Theoretical Study of a Deuterium-Labeled Drug Model. <i>Journal of Physical Chemistry A</i> , 2022, 126, 155-163.	1.1	3
9971	Intensifying strategy of ionic liquids for Pd-based catalysts in anthraquinone hydrogenation. <i>Catalysis Science and Technology</i> , 2022, 12, 1766-1776.	2.1	3
9972	Interactions between typical functional groups of soil organic matter and mica (001) surface: A DFT study. <i>Applied Clay Science</i> , 2022, 216, 106374.	2.6	2
9973	Asymmetric synthesis of N-axially chiral compounds via organocatalytic atroposelective N-acylation. <i>Chemical Science</i> , 2021, 13, 141-148.	3.7	53
9974	Machine learning reveals key ion selectivity mechanisms in polymeric membranes with subnanometer pores. <i>Science Advances</i> , 2022, 8, eabl5771.	4.7	45
9975	Enhanced oil recovery: QM/MM based descriptors for anionic surfactant salt-resistance. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 641, 128422.	2.3	6
9976	Theoretical Design of Stable Pentacoordinate Boron Compounds. <i>ACS Omega</i> , 2022, 7, 2391-2397.	1.6	2
9977	Synthesis, characterization, and crystal structure of 2-oxo-5-nitro-3-(5-nitroimino-1,3,4-oxadiazole-2-yl)-pyrazine. <i>Energetic Materials Frontiers</i> , 2022, 3, 32-37.	1.3	1
9978	Influence of Substituents in the Benzene Ring on the Halogen Bond of Iodobenzene with Ammonia. <i>ChemPhysChem</i> , 2022, 23, .	1.0	19
9979	Synthesis of Asymmetric Coupled Polymethines Based on a 7-Chloropyrido[1,2-a]benzimidazole-8,9-dione Core. <i>Journal of Organic Chemistry</i> , 2022, 87, 2345-2355.	1.7	3
9980	A phenanthro[9,10-d]imidazole-based highly selective fluorescence and visual sensor for Cu ²⁺ ion. <i>Optical Materials</i> , 2022, 123, 111834.	1.7	4
9981	Carbon- and Iron Electron Transport Channels in Porphyrin-Graphene Complex for ppb-Level Room Temperature NO Gas Sensing. <i>Small</i> , 2022, 18, e21103259.	5.2	12
9982	Insights into the binding manners of an Fe doped MOF-808 in high-performance adsorption: a case of antimony adsorption. <i>Environmental Science: Nano</i> , 2022, 9, 254-264.	2.2	10
9983	Synthesis, molecular structure and fluxional behavior of the elusive [HRu ₄ (CO) ₁₂] ³⁺ carbonyl anion. <i>Dalton Transactions</i> , 2022, 51, 2250-2261.	1.6	7
9984	Nickel Phthalocyanines as Potential Aggregation-Induced Antibacterial Agents: Fenton-Like Pathways Driven by Near-Infrared Light. <i>ChemPhotoChem</i> , 2022, 6, .	1.5	3

#	ARTICLE	IF	CITATIONS
9985	Revealing the Relationship between Electric Fields and the Conformation of Oxytocin Using Quasi-Static Amide-I Two-Dimensional Infrared Spectra. <i>ACS Omega</i> , 2022, 7, 3758-3767.	1.6	1
9986	Experimental and computational evidence for stabilising parallel, offset π -C(=O)N(H)N π -C(phenyl) interactions in acetohydrazide derivatives. <i>CrystEngComm</i> , 2022, 24, 962-974.	1.3	0
9987	Superradiance and Directional Exciton Migration in Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2022, 144, 1396-1406.	6.6	22
9988	A Second Near-Infrared Ru(II) Polypyridyl Complex for Synergistic Chemo-Photothermal Therapy. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 2225-2237.	2.9	33
9989	Modification of the Second Harmonic Generation and Fluorescence Efficiency of D289 Dye Based on a Donor-Acceptor Structure. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2234-2242.	1.5	6
9990	H π - and Baird-Type Global Aromaticity in a 3D Fully Conjugated Molecular Cage. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	6
9991	Organic Supramolecular Zippers with Ultralong Organic Phosphorescence by a Dexter Energy Transfer Mechanism. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	2
9992	Charge transfer processes via tandem modification of efficient non-fullerene acceptors for organic solar cells. <i>Solar Energy</i> , 2022, 231, 503-515.	2.9	12
9993	Experimental and Theoretical Study of Gamma Radiolysis and Dose Rate Effect of <i>o</i> -Cresol Formaldehyde Epoxy Composites. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 5959-5972.	4.0	4
9994	H π - and Baird-Type Global Aromaticity in a 3D Fully Conjugated Molecular Cage. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	15
9995	The sensing mechanism of a flavone-based ESIPT fluorescent chemodosimeter for selective recognition towards fluoride: a theoretical. <i>RSC Advances</i> , 2022, 12, 2262-2269.	1.7	1
9996	Syntheses, crystal structures and Hirshfeld surface analysis of (<i>Z</i>)-3-[(3-acetyl-2-hydroxyphenyl)amino]-2-bromoprop-2-enal and a novel Zn(II) complex. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 123-130.	0.2	1
9997	Theoretical predictions of nonlinear optical characteristics of Y-type chromophores with quinoxaline moieties in a bridge. <i>Computational and Theoretical Chemistry</i> , 2022, 1207, 113535.	1.1	3
9998	Structure-property relationship study of blue thermally activated delayed fluorescence molecules with different donor and position substitutions: theoretical perspective and molecular design. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4723-4736.	2.7	17
9999	DFT investigation of BN, AlN, and SiC fullerene sensors for arsine gas detection and removal. <i>Main Group Chemistry</i> , 2022, 21, 513-521.	0.4	5
10000	Near-infrared emitting copper(II) complexes with a pyrazolylpyrimidine ligand: exploring relaxation pathways. <i>Dalton Transactions</i> , 2022, 51, 2898-2911.	1.6	7
10001	DFT Study on the Substituent Effect of Anticancer Picoline-Diazido-Pt(IV) Compounds. <i>Frontiers in Oncology</i> , 2021, 11, 749178.	1.3	2
10002	Tuning the properties of truxene by successive substitution of nitrogen and sulphur heteroatoms: a DFT insight. <i>Journal of Molecular Modeling</i> , 2022, 28, 27.	0.8	2

#	ARTICLE	IF	CITATIONS
10003	Predominance of the second cycle in homogeneous Os-catalyzed dihydroxylation: the nature of Os(vi) vs Os(viii) reoxidation and unprecedented roles of amine-N-oxides. <i>Catalysis Science and Technology</i> , 2022, 12, 880-893.	2.1	2
10004	Development of core-shell structured MNP@Au@MIL-100(Fe) substrates for surface-enhanced Raman spectroscopy and their applications in trace level determination of malachite green in prawn. <i>Journal of Raman Spectroscopy</i> , 2022, 53, 682-693.	1.2	22
10005	Facile fabrication of end-functional PLLA with AIEgens via Ugi reaction. <i>Polymer</i> , 2022, 239, 124432.	1.8	1
10006	Exploration of hydrogen-bonded organic framework (HOF) as highly efficient adsorbent for rhodamine B and methyl orange. <i>Microporous and Mesoporous Materials</i> , 2022, 330, 111624.	2.2	8
10007	Theoretical investigation of mechanism and ligand effects on half-sandwich iridium complexes for direct reductive amination. <i>Molecular Catalysis</i> , 2022, 517, 112050.	1.0	4
10008	Viability of half-sandwich complex of heavier group 4 elements ($\text{Sc}^{\text{II}}/\text{Zr}^{\text{II}}/\text{Hf}^{\text{II}}/\text{Ta}^{\text{II}}/\text{Nb}^{\text{II}}/\text{Pb}^{\text{II}}$) with neutral $\text{Be}^{\text{III}}/\text{Mg}^{\text{III}}/\text{Al}^{\text{III}}$ ring and its potential application as H_2 storage material. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	2
10009	Acid-triggered, degradable and high strength-toughness copolyesters: Comprehensive experimental and theoretical study. <i>Journal of Hazardous Materials</i> , 2022, 430, 128392.	6.5	15
10010	Searching new structures of ruthenium-doped in small-sized silicon clusters: RuSi_n ($n=3-13$) clusters. <i>European Physical Journal Plus</i> , 2022, 137, 1.	1.2	1
10011	Predicting Dinitrogen Activation by Five-Electron Boron-Centered Radicals. <i>Inorganic Chemistry</i> , 2022, 61, 2234-2241.	1.9	13
10012	Bipolar 1,8-naphthalimides showing high electron mobility and red AIE-active TADF for OLED applications. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 5070-5082.	1.3	16
10013	TDOS/PDOS/OPDOS, reduced density gradient (RDG) and molecular docking studies of [3-(3-bromophenyl)-cis-4,5-dihydroisoxazole-4,5-diyl]bis(methylene) diacetate. <i>Balikesir Universitesi Fen Bilimleri Enstitüsü Dergisi</i> , 2022, 24, 100-110.	0.2	3
10014	One order of magnitude increase of triplet state lifetime observed in deprotonated form selenium substituted uracil. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 875-882.	1.3	2
10015	Noncovalent interactions of 1,4-dithiafulvene and nitroaromatics: A combined DFT and ab initio molecular dynamics (AIMD) study. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	1
10016	Dehydrogenation of ammonia-borane to functionalize neutral and Li ⁺ -encapsulated C ₆₀ , C ₇₀ and C ₃₆ fullerene cages: a DFT approach. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4022-4041.	1.3	2
10017	Manipulating Förster and Dexter interactions between a thermally activated delayed fluorescence host and a phosphorescent dopant for highly efficient solution-processed red and white OLEDs. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4637-4645.	2.7	20
10018	Size-dependent reactivity of rhodium deuteride cluster anions Rh_3D_n^- ($n=0-3$) toward dinitrogen: The prominent role of σ donation. <i>Journal of Chemical Physics</i> , 2022, 156, 064303.	1.2	10
10019	Stabilisation of Li(O)-Li(O) bond by normal and mesoionic carbenes and electride characteristics of the complexes. <i>Molecular Physics</i> , 2022, 120, .	0.8	4
10020	Understanding the Effect of pH on the Solubility and Aggregation Extent of Humic Acid in Solution by Combining Simulation and the Experiment. <i>Environmental Science & Technology</i> , 2022, 56, 917-927.	4.6	35

#	ARTICLE	IF	CITATIONS
10021	Halogen Bonding in Haspin-Halogenated Tubercidin Complexes: Molecular Dynamics and Quantum Chemical Calculations. <i>Molecules</i> , 2022, 27, 706.	1.7	2
10022	The effects of solvent nature and steric hindrance on the reactivity, mechanism and selectivity of the cationic imino- Δ^2 -Alder cycloaddition reaction between cationic Δ^2 -azadienes and arylpropene. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	4
10023	New Light on an Old Story: Breaking Kasha's Rule in Phosphorescence Mechanism of Organic Boron Compounds and Molecule Design. <i>International Journal of Molecular Sciences</i> , 2022, 23, 876.	1.8	1
10024	Orbital localization and the role of the Fe and As d -orbitals in $BaFe_2As_2$ d -orbitals. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 10024.	1.1	2
10025	Synthesis, Spectral analysis, XRD, Hirshfeld surface analysis, DFT studies and Anticancer activities of di(<i>o</i> -chlorobenzyl)(dichloro)(1,10-phenanthroline)tin(IV) complex. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10026	Super-stretchable and adhesive cellulose Nanofiber-reinforced conductive nanocomposite hydrogel for wearable Motion-monitoring sensor. <i>Journal of Colloid and Interface Science</i> , 2022, 615, 215-226.	5.0	39
10027	Spirobifluorene modified electron transport materials for high efficiency in phosphorescent organic light-emitting diodes. <i>Materials Chemistry Frontiers</i> , 2022, 6, 757-764.	3.2	5
10028	In-Depth Study of Heavy Metal Removal by an Etidronic Acid-Functionalized Layered Double Hydroxide. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 7450-7463.	4.0	107
10029	Structural characterization of benzketozone monohydrate. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2022, , .	0.3	0
10030	Optimization and design for the curing process of solid azide propellant: Influence of typical components on the curing reactions of PBT binders with TDI . <i>Journal of the Chinese Chemical Society</i> , 2022, 69, 419-439.	0.8	1
10031	$C_{1-Symmetrical [Ir(C^N)(C^N)(N^O)]-tris-heteroleptic Ir(III)-complexes with one strong N^O-ancillary \sigma-donor for efficient all-solution-processed near-infrared (NIR) polymer light-emitting diodes (PLEDs). Journal of Materials Chemistry C, 2022, 10, 3178-3187.$	2.7	3
10032	A Molecular Electron Density Theory Study of the Lewis Acid Catalyzed [3+2] Cycloaddition Reactions of Nitrones with Nucleophilic Ethylenes. <i>European Journal of Organic Chemistry</i> , 2022, 2022, , .	1.2	21
10033	Dual-Emission GFP Chromophore-Based Derivative for Imaging and Discriminating Δ^2 Oligomers and Aggregates. <i>Analytical Chemistry</i> , 2022, 94, 1999-2006.	3.2	13
10034	Remarkable mechanochromism and force-induced thermally activated delayed fluorescence enhancement from white-light-emitting organic luminogens with aggregation-induced emission. <i>Chinese Chemical Letters</i> , 2022, 33, 4536-4540.	4.8	16
10035	Theoretical and Structural Understanding of the Different Factors Influencing the Formation of Multicomponent Crystals of 2,4-Dichlorophenoxyacetic Acid with N-heterocyclic Compounds. <i>Crystal Growth and Design</i> , 2022, 22, 1707-1719.	1.4	5
10036	Crystallization induced realignment of carbon fibers in a phase change material to achieve exceptional thermal transportation properties. <i>Journal of Materials Chemistry A</i> , 2022, 10, 593-601.	5.2	29
10037	Theoretical investigations on the nitro-explosive sensing process of a MOF sensor: Roles of hydrogen bond and π - π stacking. <i>Chemical Physics Letters</i> , 2022, 793, 139393.	1.2	8
10038	Dispersion and Steric Effects on Enantio-/Diastereoselectivities in Synergistic Dual Transition-Metal Catalysis. <i>Journal of the American Chemical Society</i> , 2022, 144, 1971-1985.	6.6	80

#	ARTICLE	IF	CITATIONS
10039	Rate Constant of Hydrogen Transfer from H-Donor Solvents to Coal Radicals. SSRN Electronic Journal, 0, , .	0.4	0
10040	Stable copernicium hexafluoride (CnF ₆) with an oxidation state of VI+. Physical Chemistry Chemical Physics, 2021, 24, 321-325.	1.3	3
10041	Kinetics, thermodynamics, equilibrium, surface modelling, and atomic absorption analysis of selective Cu(II) removal from aqueous solutions and rivers water using silica-2-(pyridin-2-ylmethoxy)ethan-1-ol hybrid material. RSC Advances, 2021, 12, 611-625.	1.7	9
10042	Planar pentacoordinate carbon in a sulphur-surrounded boron wheel: the global minimum of CB ₅ S ₅ ⁺ . Chemical Communications, 2022, 58, 2552-2555.	2.2	17
10043	The First Cocrystallization of Milrinone with Nutraceuticals: The Adjusting Effects of Hydrophilicity/Hydrophobicity in Cavities on the In Vitro/In Vivo Properties of the Cocrystals. Crystal Growth and Design, 2022, 22, 1623-1637.	1.4	17
10044	Theoretical Insight into the Mechanism and Selectivity in Manganese-Catalyzed Oxidative C(sp ³)â€”H Methylation. ACS Catalysis, 2022, 12, 2290-2301.	5.5	12
10045	An Overlooked Pathway in 1,3â€”Dipolar Cycloadditions of Diazoalkanes with Enamines. Angewandte Chemie - International Edition, 2022, 61, .	7.2	9
10046	A controllable and defectless cutting postprocess method <i>via</i> cleavage of an elastic cocrystal based on pyrene and tetrachloroterephthalonitrile. CrystEngComm, 2022, 24, 942-946.	1.3	1
10047	A Thermally Robust Cyclic Dialkylsilylene. Bulletin of the Chemical Society of Japan, 2022, 95, 175-177.	2.0	0
10048	Segregated Array Tailoring Chargeâ€”Transfer Degree of Organic Cocrystal for the Efficient Nearâ€”Infrared Emission beyond 760nm. Advanced Materials, 2022, 34, e2107169.	11.1	60
10049	Computational Evaluation of Li-doped g-C ₂ N Monolayer as Advanced Hydrogen Storage Media. International Journal of Hydrogen Energy, 2022, 47, 3625-3632.	3.8	25
10050	Analysis of spectator chemical bonds in SN ₂ @C and @Si reaction mechanisms in the gas phase. Chemical Physics Letters, 2022, 787, 139282.	1.2	3
10051	Deep-red electro-fluorescence based on an excimer emission with hot-exciton channels. Journal of Materials Chemistry C, 2022, 10, 4579-4583.	2.7	14
10052	ZIF-8 metal-organic framework conjugated to pristine and doped B ₁₂ N ₁₂ nanoclusters as a new hybrid nanomaterial for detection of amphetamine. Inorganic Chemistry Communication, 2022, 135, 109119.	1.8	6
10053	Catalytic activity of Ru ₄ -doped vacancy fullerenes (Ru ₄ â€”C ₅₄) Tj ETQq0 0 0 rgBT /Overl theory investigation. Applied Organometallic Chemistry, 2022, 36, .	1.7	2
10054	Unusual fluorescence behaviour of a heteroleptic Cu(I) complex featuring strong electron donating groups on a diimine ligand. New Journal of Chemistry, 2022, 46, 1693-1703.	1.4	4
10055	Environmentally compatible and highly improved hole transport materials (HTMs) based on benzotrithiophene (BTT) skeleton for perovskite as well as narrow bandgap donors for organic solar cells. Solar Energy, 2022, 231, 793-808.	2.9	56
10056	Metal-Involving Halogen Bonding Including Gold(I) as a Nucleophilic Partner. The Case of Isomorphous Dichloroaurate(I)-Halomethane Cocrystals. Inorganic Chemistry, 2022, 61, 2558-2567.	1.9	10

#	ARTICLE	IF	CITATIONS
10057	Influence of edge and center oxidation configurations on non-radiative relaxation in graphene quantum dots. <i>Journal of Materials Science: Materials in Electronics</i> , 2022, 33, 5024-5036.	1.1	3
10058	A Comparison of Partial Atomic Charges for Electronically Excited States. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1061-1071.	2.3	5
10059	Molecular Simulation and Experimental Study on Low-Viscosity Ionic Liquids for High-Efficient Capturing of CO ₂ . <i>Energy & Fuels</i> , 2022, 36, 1604-1613.	2.5	7
10060	Rotational Spectra of 2-Ethynylpyridine and Its Monohydrate: Influence of the Ortho-Substitution on Ring Geometry and Intermolecular Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2022, 126, 623-629.	1.1	1
10061	Exploring the effect of nitrile substituent position on fluorescence quantum yield of ESIPT-based oxazoline derivatives: A TDDFT investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 272, 120953.	2.0	15
10062	A theoretical study on intermolecular hydrogen bonds of isopropanol-water clusters. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1.	0.5	2
10063	Density functional theory investigation of ozone gas uptake by a BeO nanoflake. <i>Main Group Chemistry</i> , 2022, 21, 773-781.	0.4	2
10064	Silver Cluster Interactions with Tyrosine: Towards Amino Acid Detection. <i>International Journal of Molecular Sciences</i> , 2022, 23, 634.	1.8	7
10065	Quasi-solid electrolytes with tailored lithium solvation for fast-charging lithium metal batteries. <i>Cell Reports Physical Science</i> , 2022, 3, 100722.	2.8	15
10066	Modulation of naphthanthryl chalcone derivatives by push-pull electronic substituents: Ultrafast nonlinear absorption and transient dynamics. <i>Optical Materials</i> , 2022, 123, 111898.	1.7	5
10067	Automatic Approach to Explore the Multireaction Mechanism for Medium-Sized Bimolecular Reactions via Collision Dynamics Simulations and Transition State Searches. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 910-924.	2.3	6
10068	Sorption Studies of Tetracycline Antibiotics on Hydroxyapatite (001) Surface—A First-Principles Insight. <i>Materials</i> , 2022, 15, 797.	1.3	8
10069	Molecular simulation of adsorption properties of thiol-functionalized titanium dioxide (TiO ₂) nanostructure for heavy metal ions removal from aqueous solution. <i>Journal of Molecular Liquids</i> , 2022, 346, 118281.	2.3	10
10070	Study of a carbazole—bromobenzothiadiazole derived fluorescent molecular rotor: crystal structure, redox activity, and solvatochromic effects. <i>New Journal of Chemistry</i> , 2022, 46, 572-581.	1.4	4
10071	Development of a glioclazide ionic liquid and its mesoporous silica particles: an effective formulation strategy to improve oral absorption properties. <i>RSC Advances</i> , 2021, 12, 1062-1076.	1.7	3
10072	Unveiling the relationship between structural and polarization effects on the first hyperpolarizability of a merocyanine dye. <i>Journal of Chemical Physics</i> , 2022, 156, 014305.	1.2	7
10073	Revealing the Role of Polaron Distribution on the Performance of n-Type Organic Electrochemical Transistors. <i>Chemistry of Materials</i> , 2022, 34, 864-872.	3.2	23
10074	Computational Exploration of Anomalous Regioselectivities in Cycloadditions of Ketenes to Oxazolines. <i>Journal of Organic Chemistry</i> , 2022, , .	1.7	1

#	ARTICLE	IF	CITATIONS
10093	Oxidative evolution of Z<i>/i>/E<i>/i>-diaminotetraphenylethylene. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1960-1964.	1.3	2
10094	Computational predictions of adaptive aromaticity for the design of singlet fission materials. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 914-924.	3.0	13
10095	The effects of molecular weight and orientation on the membrane permeation and partitioning of polycyclic aromatic hydrocarbons: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2158-2166.	1.3	2
10096	Asymmetricalâ€œdendronized TADF Emitters for Efficient Nonâ€œdoped Solutionâ€œProcessed OLEDs by Eliminating Degenerate Excited States and Creating Solely Thermal Equilibrium Routes. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	36
10097	Carboxylato Bridged Cyclic SBUs as Robust Features in a Series of Cu(II) Coordination Polymers and Halogenâ€œHalogen Interactions in Crystal Packing. <i>Crystal Growth and Design</i> , 2022, 22, 1253-1262.	1.4	7
10098	A Î€-extended triphenylamine based dopant-free hole-transporting material for perovskite solar cells <i>/i> heteroatom substitution. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4635-4643.	1.3	9
10099	Donor moieties with Dâ€œâ€œa framing modulated electronic and nonlinear optical properties for non-fullerene-based chromophores. <i>RSC Advances</i> , 2022, 12, 4209-4223.	1.7	15
10100	Lattice solvent controlled photochromism of tripyridyl-triazine-based zinc bromide complexes. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 879-888.	3.0	12
10101	Robust Luminescent Molecules with Highâ€œLevel Reverse Intersystem Crossing for Efficient Near Ultraviolet Organic Lightâ€œEmitting Diodes. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	34
10102	Nanostructured transition-metal phthalocyanine complexes for catalytic oxygen reduction reaction. <i>Nanotechnology</i> , 2022, 33, 182001.	1.3	7
10103	In silico design of metal-free hydrophosphate catalysts for hydrogenation of CO2 to formate. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2901-2908.	1.3	1
10104	Excited State Properties of Layered Two-Dimensional MSi2N4 (M = Mo, Cr, and W) Materials from First-Principles Calculations. <i>ECS Journal of Solid State Science and Technology</i> , 2022, 11, 016001.	0.9	7
10105	Synthesis, Crystallographic, Quantum Chemical, Antitumor, and Molecular Docking/Dynamic Studies of 4-Hydroxycoumarin-Neurotransmitter Derivatives. <i>International Journal of Molecular Sciences</i> , 2022, 23, 1001.	1.8	31
10106	A theoretical investigation on the hydrodesulphurisation mechanism of hydrogenated thiophene over Cuâ€œMo-modified FAU zeolite. <i>Molecular Simulation</i> , 0, , 1-22.	0.9	0
10107	1-Hydroxy-1,2,3,4-tetrazole and its transition metal complexes: A family of green high-energy catalysts for ammonium perchlorate. <i>Journal of Solid State Chemistry</i> , 2022, 308, 122896.	1.4	9
10108	Elucidating the mechanism and reactivity of the reaction between the donorâ€œacceptorâ€œacceptor 1,3-bisdiazo compound and cinnamyl alcohol catalyzed by Rh2(OAc)4: a DFT study. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
10109	Chalcogenâ€œChalcogen Bonding in Molybdenum Disulfide, Molybdenum Diselenide and Molybdenum Ditelluride Dimers as Prototypes for a Basic Understanding of the Local Interfacial Chemical Bonding Environment in 2D Layered Transition Metal Dichalcogenides. <i>Inorganics</i> , 2022, 10, 11.	1.2	8
10110	Antiaromaticity-promoted radical anion stability in Î±-vinyl heterocyclics. <i>Organic Chemistry Frontiers</i> , 0, , .	2.3	3

#	ARTICLE	IF	CITATIONS
10111	Highly stable actinide(III) complexes supported by doubly aromatic ligands. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	1.3	1
10112	Multi-scale computational screening to accelerate discovery of IL/COF composites for CO ₂ /N ₂ separation. <i>Separation and Purification Technology</i> , 2022, 287, 120578.	3.9	12
10113	Recovery of Titanium from Ilmenite HCl Leachate Using a Hydrophobic Deep Eutectic Solvent. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 2125-2135.	3.2	14
10114	Ionic Liquids for Capturing 1,2-Dimethoxyethane (DMET) in VOCs: Experiment and Mechanism Exploration. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 2257-2267.	1.8	12
10115	Controllability of Graphene Oxide Doxorubicin Loading Capacity Based on Density Functional Theory. <i>Nanomaterials</i> , 2022, 12, 479.	1.9	3
10116	SbCl ₄ : An Exceptional Superhalogen as the Building Block of a Mixed Valence Supercrystal with Unconventional Ferroelectricity. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1049-1056.	2.1	6
10117	Chiral <i>N</i> -triflylphosphoramidate-catalyzed asymmetric hydroamination of unactivated alkenes: a hetero-ene reaction mechanism. <i>Organic Chemistry Frontiers</i> , 2022, 9, 1649-1661.	2.3	4
10118	Controlled preparation of PAMS hollow core microcapsules with high uniformity and its application in the production of GDP fuel capsules for ICF engineering. <i>Fundamental Research</i> , 2023, 3, 602-610.	1.6	3
10119	DFT study of the influence of boron/nitrogen substitution on the electronic and nonlinear optical properties of the benzene-substituted graphdiyne fragment. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113629.	1.1	4
10120	Remote C(sp ³)-H Acylation of Amides and Cascade Cyclization via N-Heterocyclic Carbene Organocatalysis. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	5
10121	Density functional methods study on the structures and spectral characteristics for pharmacophoric conformers, metabolites, and combined fragments of Erlotinib. <i>Chemical Papers</i> , 0, , 1.	1.0	0
10122	Self-assembly of a new cobalt complex, (C ₆ H ₁₄ N ₂) ₃ [CoCl ₄]Cl: Synthesis, empirical and DFT calculations. <i>Journal of King Saud University - Science</i> , 2022, 34, 101807.	1.6	8
10123	X-ray structures, spectroscopic, antimicrobial activity, ESP/HSA and TD/DFT calculations of Bi(III) complex containing imidazole ring. <i>Journal of Molecular Structure</i> , 2022, 1256, 132517.	1.8	23
10124	Molecular Identification of the Transient Species Mediating the Deactivation Dynamics of Solvated Guanosine and Deazaguanosine. <i>Molecules</i> , 2022, 27, 989.	1.7	3
10125	Computational Insights On Charge Transfer and Non-covalent Interactions of Antibacterial Compound 4-dimethylaminopyridinium pyridine-2-carboxylate pentahydrate. <i>Journal of Molecular Structure</i> , 2022, 1256, 132525.	1.8	9
10126	DFT investigation of adsorption of nitro-explosives over C ₂ N surface: Highly selective towards trinitro benzene. <i>Journal of Molecular Liquids</i> , 2022, 352, 118652.	2.3	32
10127	Unraveling the mechanism and substituent effects on the N-heterocyclic carbene-catalyzed transformation reaction of enals and imines. <i>Molecular Catalysis</i> , 2022, 519, 112122.	1.0	8
10128	Amplifying the photovoltaic properties of azaBODIPY core based small molecules by terminal acceptors modification for high performance organic solar cells: A DFT approach. <i>Solar Energy</i> , 2022, 233, 31-45.	2.9	43

#	ARTICLE	IF	CITATIONS
10129	Spodium and tetrel bonds involving Zn(II)/Cd(II) and their interplay. <i>Chemical Physics</i> , 2022, 556, 111470.	0.9	6
10130	Accelerating Radiative Decay in Blue Through Space Charge Transfer Emitters by Minimizing the Donor-Acceptor Distances. <i>Angewandte Chemie</i> , 0, , .	1.6	11
10131	Theoretical Investigation on H-Abstraction Reactions of Silanes with H and CH ₃ Attacking: A Comparative Study with Alkane Counterparts. <i>ACS Omega</i> , 2022, 7, 5558-5569.	1.6	3
10132	Theoretical investigation on the cycloaddition catalyzed by rhodium silylenoid to construct silicon-containing rings. <i>Molecular Catalysis</i> , 2022, 519, 112138.	1.0	1
10133	Preparation of 5-methyl-3,5-dipropyl-2-pyrazoline catalyzed by chloroaluminate ionic liquids. <i>Journal of Molecular Structure</i> , 2022, 1256, 132539.	1.8	4
10134	Partial Double Metal-Carbon Bonding Model in Transition Metal Methyl Compounds. <i>Inorganic Chemistry</i> , 2022, 61, 2892-2902.	1.9	5
10135	Synthesis of 1, 3, 5-trisubstituted-4,5-dihydro-1H-pyrazole catalyzed by vitamin B1 and its fluorescence properties. <i>Research on Chemical Intermediates</i> , 2022, 48, 983-1001.	1.3	3
10136	Effect of the explicit solvation of 2-propanol on the Darzens reaction mechanism: A computational study. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113628.	1.1	0
10137	Anion photoelectron spectroscopy and theoretical calculations of Cu ₄ O _n ⁿ⁻ (n = 1-4): Identification of stable quasi-square structure for Cu ₄ O ₄ ⁴⁻ . <i>Journal of Chemical Physics</i> , 2022, 156, 054304.	1.2	3
10138	Degradation of OBS (Sodium <i>p</i> -Perfluorous Nonenoxybenzenesulfonate) as a Novel Per- and Polyfluoroalkyl Substance by UV/Persulfate and UV/Sulfite: Fluorinated Intermediates and Treatability in Fluoroprotein Foam. <i>Environmental Science & Technology</i> , 2022, 56, 6201-6211.	4.6	22
10139	Structure and electronic properties of neutral and anionic boron clusters doped with two tantalum atoms. <i>Molecular Physics</i> , 2022, 120, .	0.8	6
10140	Independent gradient model based on Hirshfeld partition: A new method for visual study of interactions in chemical systems. <i>Journal of Computational Chemistry</i> , 2022, 43, 539-555.	1.5	794
10141	Remote C(sp ³) ^α -H Acylation of Amides and Cascade Cyclization via N-Heterocyclic Carbene Organocatalysis. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	45
10142	Quantum Chemical Calculation of the Effect of NH ₃ on CO ₂ Adsorption and Storage in Goaf. <i>Energy & Fuels</i> , 2022, 36, 1948-1959.	2.5	1
10143	Room Temperature Phosphorescence Emission From Multi-States. <i>Frontiers in Chemistry</i> , 2021, 9, 810458.	1.8	6
10144	Accelerating Radiative Decay in Blue Through Space Charge Transfer Emitters by Minimizing the Donor-Acceptor Distances. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	56
10145	Benchmarking of density functionals for the description of optical properties of newly synthesized conjugated TADF blue emitters. <i>Chemistry - A European Journal</i> , 2022, , .	1.7	3
10146	Mechanism of heteroatom-doped Cu ₅ catalysis for hydrogen evolution reaction. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 7802-7812.	3.8	4

#	ARTICLE	IF	CITATIONS
10147	Approximate atomic models for fast computation of the Fokker-Planck equation in fusion plasmas with high-Z impurities and suprathermal electrons. <i>Physics of Plasmas</i> , 2022, 29, .	0.7	3
10148	Structural and Electronic Properties of Boranes Containing Boron-Chalcogen Multiple Bonds and Stabilized by Amido Imidazolineimine Ligands. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	8
10149	Synthesis, Characterization, Crystal Structure, Hirshfeld Surface, Electronic Excitation, Molecular Docking, and DFT Studies on 2-Amino Thiophene Derivative. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 1644-1675.	1.4	13
10150	Structural evolution and hydrogen storage performance of Mg ₃ LaH (n = 9-20). <i>International Journal of Hydrogen Energy</i> , 2022, 47, 7884-7891.	3.8	8
10151	Sc(OTf) ₃ -Catalyzed [3+2]-Cycloaddition of Diazoacetate Enones and N-Aryl Nitrones: Diastereoselective Synthesis of Functionalized Isoxazolidines with Three Contiguous Stereogenic Centers. <i>Synthesis</i> , 0, , .	1.2	1
10152	New Role for an <i>N</i> -Alkylidene Bridge: Taming the Hygroscopicity of Acidic Energetic Materials with Enhanced Stability. <i>Crystal Growth and Design</i> , 2022, 22, 1943-1950.	1.4	16
10153	Adsorption dynamics and intrinsic mechanism of POPs on corrole-based COF: A computational study. <i>Journal of Cleaner Production</i> , 2022, 338, 130566.	4.6	11
10154	A theoretical study of the mono-substituent effect of superhalogens on the geometric structure, electronic properties, and hydrolysis of cisplatin. <i>Chemical Physics</i> , 2022, 555, 111447.	0.9	1
10155	Theoretical electron excitation study in liquid phase (protic, aprotic, non-polar) and inter and intra molecular reactivity of 2-hydroxy-5-[1-hydroxy-2-(4-phenylbutan-2-ylamino) ethyl] benzamide. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100372.	1.3	4
10156	Characterization of metal-metal and metal-ligand interactions in binuclear MnPt vinylidene complexes by molecular orbital and charge density analyses. <i>Journal of Organometallic Chemistry</i> , 2022, 961, 122249.	0.8	1
10157	Separation of 1,8-Cineole and terpenes by Liquid-liquid extraction with green alkanediols. <i>Journal of Molecular Liquids</i> , 2022, 350, 118516.	2.3	10
10158	Preparation of functionalized pectin through acylation with alkyl gallates: Experiments coupled with density functional theory. <i>International Journal of Biological Macromolecules</i> , 2022, 202, 278-285.	3.6	14
10159	Strong π -hole triel-bond between C ₅ H ₅ Tr (Tr B, Al, Ga) and N-base (N-base NCH, NH ₃ , NC ⁺): Cooperativity and solvation effects. <i>Chemical Physics Letters</i> , 2022, 791, 139377.	1.2	2
10160	Electrostatic interaction assisted Ca-decorated C ₂₀ fullerene loaded to anti-inflammatory drugs to manage cardiovascular disease risk in rheumatoid arthritis patients. <i>Journal of Molecular Liquids</i> , 2022, 350, 118564.	2.3	18
10161	Structural, thermal, vibrational, solubility and DFT studies of a tolbutamide co-amorphous drug delivery system for treatment of diabetes. <i>International Journal of Pharmaceutics</i> , 2022, 615, 121500.	2.6	7
10162	Simultaneous interaction of graphene nanoflakes with cations and anions: A cooperativity study. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113601.	1.1	4
10163	Sensing of SO ₃ , SO ₂ , H ₂ S, NO ₂ and N ₂ O toxic gases through aza-macrocycle via DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113606.	1.1	25
10164	Computational study of metformin hydrochloride nucleation in hydroxylic solvents: Experimental kinetics and DFT simulation. <i>International Journal of Pharmaceutics</i> , 2022, 616, 121517.	2.6	2

#	ARTICLE	IF	CITATIONS
10165	Density functional theory study of CL-20/Nitroimidazoles energetic cocrystals in an external electric field. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113607.	1.1	8
10166	Co-hydrothermal carbonization of biomass and PVC for clean blast furnace injection fuel production: Experiment and DFT calculation. <i>Renewable Energy</i> , 2022, 187, 156-168.	4.3	16
10167	Enhanced electrochemical removal of sulfadiazine using stainless steel electrode coated with activated algal biochar. <i>Journal of Environmental Management</i> , 2022, 306, 114535.	3.8	13
10168	Aromatic B3 ring stabilized group 2 Dimer, B3-Y-Y-B3 (Y=Be, Mg, Ca). <i>Polyhedron</i> , 2022, 215, 115681.	1.0	4
10169	Molecular-level insights into inherent heterogeneity of maline deep eutectic system. <i>Journal of Molecular Liquids</i> , 2022, 350, 118478.	2.3	4
10170	The simulation study of transport performance of HU drugs on functionalized graphene nanosheets based on the Density Functional Theory. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113604.	1.1	2
10171	Schiff base (Z)-4-((furan-2-ylmethylene)amino) benzenesulfonamide: Synthesis, solvent interactions through hydrogen bond, structural and spectral properties, quantum chemical modeling and biological studies. <i>Journal of Molecular Liquids</i> , 2022, 350, 118531.	2.3	42
10172	Non-covalent binding interaction between phthalic acid esters and DNA. <i>Environment International</i> , 2022, 161, 107095.	4.8	23
10173	Angle-resolved one and Two-Photon absorption spectrum in twisted bilayer graphene quantum dots. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 271, 120894.	2.0	6
10174	Unavoidable failure of point charge descriptions of electronic density changes for out-of-plane distortions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 271, 120891.	2.0	5
10175	Synthesis of ZIF-67 derived honeycomb porous Co/NC catalyst for AO7 degradation via activation of peroxymonosulfate. <i>Separation and Purification Technology</i> , 2022, 286, 120470.	3.9	34
10176	High performance and heat-resistant pyrazole-1,2,4-triazole energetic materials: Tuning the thermal stability by asymmetric framework and azo-bistriazole bridge. <i>Chemical Engineering Journal</i> , 2022, 433, 134480.	6.6	32
10177	Measurement and correlation of the solubility of kojic acid in pure and binary solvents. <i>Journal of Chemical Thermodynamics</i> , 2022, 167, 106712.	1.0	7
10178	Speciation of organoarsenicals in aqueous solutions by Raman spectrometry and quantum chemical calculations. <i>Microchemical Journal</i> , 2022, 175, 107186.	2.3	2
10179	Selective sensing of NH ₃ and CH ₂ O molecules by novel 2D porous hexagonal boron oxide (B ₃ O ₃) monolayer: A DFT approach. <i>Surfaces and Interfaces</i> , 2022, 29, 101767.	1.5	9
10180	Insights into photocatalytic degradation of phthalate esters over MSnO ₃ perovskites (M = Mg, Ca): Experiments and density functional theory. <i>Journal of Environmental Management</i> , 2022, 307, 114511.	3.8	9
10181	Novel benzonitrile- and benzo[d]imidazole-based bipolar hosts for green PhOLEDs with a low turn-on voltage. <i>Dyes and Pigments</i> , 2022, 200, 110041.	2.0	7
10182	Experimental and theoretical investigation on interactions between xylose-containing hemicelluloses and procyanidins. <i>Carbohydrate Polymers</i> , 2022, 281, 119086.	5.1	8

#	ARTICLE	IF	CITATIONS
10183	Hierarchical Bi _{0.5} Fe _{0.5} VO ₄ /honeycomb ceramic plate synergize plasma induce multi-catalysis by constructing a plasma-catalyst system for organic pollutant degradation. <i>Separation and Purification Technology</i> , 2022, 286, 120444.	3.9	7
10184	Quantitative structure-activity relationship study on the degradation of polyhalogenated carbazoles by sulfidated zero-valent iron/peroxymonosulfate system. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 107244.	3.3	4
10185	Highly efficient As(III) removal through simultaneous oxidation and adsorption by N-CQDs modified MIL-53(Fe). <i>Separation and Purification Technology</i> , 2022, 286, 120409.	3.9	26
10186	FeO-loaded superfine powdered activated carbon prepared by ball milling for synergistic adsorption and persulfate activation to remove aqueous carbamazepine. <i>Chemosphere</i> , 2022, 293, 133665.	4.2	9
10187	Effects of hydroxyl group, glycosylation and solvents on the antioxidant activity and mechanism of maclurin and its derivatives: Theoretical insights. <i>Journal of Molecular Liquids</i> , 2022, 351, 118609.	2.3	7
10188	Synthesis, computational, hepatoprotective, antituberculosis and molecular docking studies of some coumarin derivatives. <i>Journal of Molecular Structure</i> , 2022, 1254, 132410.	1.8	7
10189	Dry and hydrated defective molybdenum Disulfide/Graphene bilayer heterojunction under strain for hydrogen evolution from water Splitting: A First-principle study. <i>Computational Materials Science</i> , 2022, 205, 111234.	1.4	4
10190	Ameliorating the performances of 3,4-bis(4-nitrofurazano-3-yl)furoxan (DNFTF) by establishing tannic acid (TA) interface layer on DNFTF surface. <i>Chemical Engineering Journal</i> , 2022, 434, 134513.	6.6	8
10191	Crystal engineering with energetic picric acid halogen-based salts: Promising properties of a new family of insensitive materials. <i>Journal of Molecular Structure</i> , 2022, 1254, 132381.	1.8	6
10192	Synthesis of selective heteroatomic collectors for the improved separation of sulfide minerals. <i>Separation and Purification Technology</i> , 2022, 287, 120563.	3.9	19
10193	Investigation of bond orientational order of new Schiff base and theoretical study on Covid-19 activity: A molecular dynamics based on DFT and molecular docking analysis. <i>Chemical Physics Letters</i> , 2022, 792, 139390.	1.2	2
10194	Low-temperature and high-voltage lithium-ion battery enabled by localized high-concentration carboxylate electrolytes. <i>Chemical Engineering Journal</i> , 2022, 433, 134138.	6.6	33
10195	Green separation and recovery of cobalt and nickel from sulphuric acid achieved by complexation-assisted solvent extraction. <i>Separation and Purification Technology</i> , 2022, 286, 120343.	3.9	4
10196	Comparison of the synergistic inhibition mechanism of two eco-friendly amino acids combined corrosion inhibitors for carbon steel pipelines in oil and gas production. <i>Applied Surface Science</i> , 2022, 583, 152559.	3.1	42
10197	Synergetic mechanism of defective g-C ₃ N ₄ activated persulfate on removal of antibiotics and resistant bacteria: ROSs transformation, electron transfer and noncovalent interaction. <i>Chemosphere</i> , 2022, 294, 133741.	4.2	13
10198	Fluorescent probe for simultaneous detection of human serum albumin and sulfite: A theoretical analysis. <i>Journal of Molecular Structure</i> , 2022, 1255, 132441.	1.8	5
10199	Synthesis and characterization of Zinc(II) complex with ONO donor type new phenylpropanehydrazide based ligand: Crystal structure, Hirshfeld surface analysis, DFT, energy frameworks and molecular docking. <i>Journal of Molecular Structure</i> , 2022, 1255, 132429.	1.8	5
10200	Two Schiff-base fluorescent-colorimetric probes based on naphthaldehyde and aminobenzoic acid for selective detection of Al ³⁺ , Fe ³⁺ and Cu ²⁺ ions. <i>Journal of Molecular Structure</i> , 2022, 1255, 132431.	1.8	10

#	ARTICLE	IF	CITATIONS
10201	Topological description of complex patterns of bonding, charge transference and structural changes in chemical reactions: SN ₂ type reactions, a case study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 112, 108121.	1.3	0
10202	A comparative study of free chlorine and peroxymonosulfate activated by Fe(II) in the degradation of iopamidol: Mechanisms, density functional theory (DFT) calculations and formation of iodinated disinfection by-products. <i>Chemical Engineering Journal</i> , 2022, 435, 134753.	6.6	19
10203	Electrochemical and theoretical investigation on the behavior of the Co ²⁺ ion in three eutectic solvents. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 112, 108137.	1.3	4
10204	Characteristics of coal-oxygen chemisorption at the low-temperature oxidation stage: DFT and experimental study. <i>Fuel</i> , 2022, 315, 123120.	3.4	31
10205	Properties of binary mixtures of a novel natural deep eutectic solvent (glycolic acid+Xylitol) and water at several temperatures. <i>Fluid Phase Equilibria</i> , 2022, 556, 113390.	1.4	4
10206	Sensitivity of family GH11 <i>Bacillus amyloliquefaciens</i> xylanase A (BaxA) and the T331 mutant to <i>Oryza sativa</i> xylanase inhibitor protein (OsXIP): An experimental and computational study. <i>Enzyme and Microbial Technology</i> , 2022, 156, 109998.	1.6	5
10207	Ultrafast spectroscopic studies of the pH responsive 9-acridinecarboxylic acid as a ratiometric and fluorescence lifetime pH indicator. <i>Microchemical Journal</i> , 2022, 176, 107240.	2.3	1
10208	Unraveling excited state dynamics and photophysical properties for a series of phenol-quinoline derivatives by controlling hydrogen bond geometry. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 427, 113799.	2.0	26
10209	Excipient-free prodrug-based three-in-one nanoparticles co-deliver diversified agents to amplify tumor therapy. <i>Chemical Engineering Journal</i> , 2022, 435, 134880.	6.6	9
10210	Comparison of the excited-state proton transfer and single electron transfer mechanisms of the natural antioxidant Juglone and its dimer 3,3'-bifuglone. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 427, 113825.	2.0	6
10211	Two novel cadmium coordination polymers bearing viologen-derived ligand: Structure and photochromism properties. <i>Inorganica Chimica Acta</i> , 2022, 534, 120818.	1.2	4
10212	Insights into reactive behaviors and mechanisms of nickel-based oxygen carriers doped by Fe/Co during chemical looping combustion from multiple-scale molecular modeling combined with experiments. <i>Fuel Processing Technology</i> , 2022, 229, 107181.	3.7	12
10213	Investigation of the efficient adsorption performance and adsorption mechanism of 3D composite structure La nanosphere-coated Mn/Fe layered double hydroxide on phosphate. <i>Journal of Colloid and Interface Science</i> , 2022, 614, 478-488.	5.0	50
10214	Multi-objective optimization and extraction mechanism understanding of ionic liquid assisted in extracting essential oil from <i>Forsythiae fructus</i> . <i>AEJ - Alexandria Engineering Journal</i> , 2022, 61, 6897-6906.	3.4	6
10215	Superalkali (Li ₂ F, Li ₃ F) doped Al ₁₂ N ₁₂ electrides with enhanced static, dynamic nonlinear optical responses and refractive indices. <i>Materials Science in Semiconductor Processing</i> , 2022, 143, 106518.	1.9	23
10216	The role of doped-Mn on enhancing arsenic removal by MgAl-LDHs. <i>Journal of Environmental Sciences</i> , 2022, 120, 125-134.	3.2	4
10217	Construction of Li/K dopants and cyano defects in graphitic carbon nitride for highly efficient peroxymonosulfate activation towards organic contaminants degradation. <i>Chemosphere</i> , 2022, 294, 133700.	4.2	13
10218	Exploring interaction modes between polysaccharide-based selectors and biologically active 4,4'-bipyridines by experimental and computational analysis. <i>Journal of Chromatography Open</i> , 2022, 2, 100030.	0.8	7

#	ARTICLE	IF	CITATIONS
10219	Can a molecular switch exist in both superalkali electride and superalkalide forms?. Physical Chemistry Chemical Physics, 2022, 24, 5690-5699.	1.3	6
10220	Computational investigation into intramolecular hydrogen bonding controlling the isomer formation and p <i>K_a</i> of octahedral nickel(<i>ii</i>) proton reduction catalysts. Dalton Transactions, 2022, 51, 3676-3685.	1.6	4
10221	High-efficiency separation and extraction of naphthenic acid from high acid oils using imidazolium carbonate ionic liquids. Chinese Journal of Chemical Engineering, 2022, 41, 252-259.	1.7	8
10222	Exploring steric and electronic parameters of biaryl phosphacycles. New Journal of Chemistry, 2022, 46, 4677-4686.	1.4	4
10223	Theoretical Investigation on the Mechanism and Selectivity of Catalyst-Free Annulation of Ynediones and (Iso)quinoline N-Oxides. Heterocycles, 2022, 104, 878.	0.4	0
10224	[Co ₂ @(Ge ₁₇ Ni)] ⁴⁺ : the first edge-sharing double-cage endohedral germanide. Chemical Communications, 2022, 58, 3190-3193.	2.2	4
10225	Regioselectivity of Pd-catalyzed o-Carborane Arylation: A Theoretical View. Organic Chemistry Frontiers, 0, , .	2.3	5
10226	Covalency in Actinide(IV) Hexachlorides in Relation to Chlorine K-Edge X-ray Absorption Structure. Chemical Science, 2022, 13, 3194-3207.	3.7	13
10227	Pressure-induced phase transition of a series of energetic pentazolate anion salts: a DFT study. New Journal of Chemistry, 2022, 46, 5653-5662.	1.4	3
10228	Sustainable cyanide-C60 fullerene cathode to suppress the lithium polysulfides in a lithium-sulfur battery. Sustainable Materials and Technologies, 2022, 32, e00403.	1.7	3
10229	DFT Conformational, Wavefunction Based Reactivity Analysis, Docking and MD Simulations of a Carboxamide Derivative with Potential Anticancer Activity. Polycyclic Aromatic Compounds, 2023, 43, 1590-1601.	1.4	2
10230	Principles Guiding the Square Bonding Motif Containing a Pair of Chalcogen Bonds between Chalcogenadiazoles. Journal of Physical Chemistry A, 2022, 126, 1194-1203.	1.1	13
10231	High-Performance Functional Fe-MOF for Removing Aflatoxin B1 and Other Organic Pollutants. Advanced Materials Interfaces, 2022, 9, .	1.9	14
10232	Expanding the Scope of Hydroxyl-pyridine Supramolecular Synthons to Design Molecular Solids. Crystal Growth and Design, 2022, 22, 1972-1983.	1.4	14
10233	Strong dispersion interaction of the carbanionic center in methide anion derivatives with halogen atom of metal halides. Journal of Chemical Sciences, 2022, 134, 1.	0.7	0
10234	A Squaraine-Linked Zwitterionic Covalent Organic Framework Nanosheets Enhanced Poly(ethylene) Terephthalate Membranes for Water Desalination. Journal of Membrane Science, 2022, 648, 119753.	2.5	19
10235	Exploring Supramolecular Assembly Space of Cationic 1,2,4-Selenodiazoles: Effect of the Substituent at the Carbon Atom and Anions. Molecules, 2022, 27, 1029.	1.7	15
10236	Solvation dynamics of tetracyclic irbesartan in water and dichloromethane: Insights from local energy decomposition and ab initio molecular dynamics simulations library of the heterocyclic rings. Journal of Molecular Liquids, 2022, 352, 118709.	2.3	9

#	ARTICLE	IF	CITATIONS
10237	Molecular design of benzo[c][1,2,5]thiadiazole or thieno[3,4-d]pyridazine-based auxiliary acceptors through different anchoring groups in D- π -A-A framework: A DFT/TD-DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 113, 108148.	1.3	6
10238	Weak intermolecular interactions of cysteine on BNNT, BNAINT and BC2NNT: a DFT investigation. <i>Bulletin of Materials Science</i> , 2022, 45, 1.	0.8	29
10239	Dual aggregation in ground state and ground-excited state induced by high concentrations contributes to chlorophyll stability. <i>Food Chemistry</i> , 2022, 383, 132447.	4.2	2
10240	Adsorption mechanism study of multinuclear metal coordination cluster Zn ₅ for anionic dyes congo red and methyl orange: Experiment and molecular simulation. <i>Applied Surface Science</i> , 2022, 586, 152745.	3.1	39
10241	Degradation of potassium alkyl xanthogenate in wet air oxidation: Enhancement method, degradation mechanism and structure impact. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 107349.	3.3	4
10242	Degradation mechanism and eco-toxicity assessment of bisphenol S based on peroxymonosulfate activated with Co ₃ O ₄ surfaces. <i>Journal of Cleaner Production</i> , 2022, 341, 130881.	4.6	16
10243	Photochromic characteristics, photomodulated luminescence and ammonia vapor sensing properties of three D-A supramolecular assemblies. <i>Journal of Molecular Structure</i> , 2022, 1257, 132609.	1.8	6
10244	Progress toward a one-electron model for the non-valence correlation-bound anions of polycyclic aromatic hydrocarbons. <i>Electronic Structure</i> , 2022, 4, 014010.	1.0	1
10245	An NHC-Mediated Metal-Free Approach towards an NHC-Coordinated Endocyclic Disilene. <i>ChemistryOpen</i> , 2022, , e202100240.	0.9	2
10246	An Ultraflexible and Transparent Graphene-Based Wearable Sensor for Biofluid Biomarkers Detection. <i>Advanced Materials Technologies</i> , 2022, 7, .	3.0	9
10247	Phosphorescent Complexes of {Mo ₆ I ₈ } ⁴⁺ and {W ₆ I ₈ } ⁴⁺ with Perfluorinated Aryl Thiolates featuring Unusual Molecular Structures. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	7
10248	Alkynyl Sulfonium Salts Can Be Employed as Chalcogen-Bonding Catalysts and Generate Alkynyl Radicals under Blue-Light Irradiation. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	36
10249	A terminal neptunium(V)-mono(oxo) complex. <i>Nature Chemistry</i> , 2022, 14, 342-349.	6.6	19
10250	Vibrational Spectra and Molecular Vibrational Behaviors of Dibenzyl Disulfide, Dibenzyl Sulphide and Bibenzyl. <i>International Journal of Molecular Sciences</i> , 2022, 23, 1958.	1.8	8
10251	New Cd(II) complex derived from (1-methylimidazol-2-yl) methanol: Synthesis, crystal structure, spectroscopic study, DFT and TD-DFT calculations, antimicrobial activity and free-radical scavenging capacity. <i>Journal of Molecular Structure</i> , 2022, 1257, 132583.	1.8	3
10252	Uncovering the Potential Mechanisms of <i>Coptis chinensis</i> Franch. for Serious Mental Illness by Network Pharmacology and Pharmacology-Based Analysis. <i>Drug Design, Development and Therapy</i> , 2022, Volume 16, 325-342.	2.0	4
10253	The cycloaddition reaction of ethylene and methane mediated by Ir ⁺ to generate a half-sandwich structure IrHCp ⁺ . <i>Chinese Chemical Letters</i> , 2023, 34, 107196.	4.8	1
10254	Capturing VOCs in the pharmaceutical industry with ionic liquids. <i>Chemical Engineering Science</i> , 2022, 252, 117504.	1.9	18

#	ARTICLE	IF	CITATIONS
10255	2H1C Mimicry: Bioinspired Iron and Zinc Complexes Supported by <i>N,N,O</i> Phenolate Ligands. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	1
10256	A peroxy-Mo(VI)/Mo(VI)-mediated redox synthesis of quinazolin-4(3H)-ones and their aggregation-induced emission property and mechanism. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	2
10257	Structural and Energetic Aspects of Entacapone-Theophylline-Water Cocrystal. <i>Solids</i> , 2022, 3, 66-92.	1.1	3
10258	Experimental and computational (DFT) methods: exploration of thermochromism in homophthalic acid and 4-N-alkoxybenzoic acid comprised hydrogen bond liquid crystals. <i>Molecular Crystals and Liquid Crystals</i> , 2022, 740, 85-103.	0.4	2
10259	Novel modified BODIPY-C60 as photosensitizer in photodynamic therapy. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113632.	1.1	2
10260	Face-to-face order-packed mode promotes thermally activated delayed fluorescence to achieve stronger aggregation-induced emission. <i>Journal of Science: Advanced Materials and Devices</i> , 2022, 7, 100432.	1.5	2
10261	Photophysical properties and sensing mechanism of fluorescent coumarin-chalcone hybrid for biothiols: A theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, .	0.9	1
10262	Halogen Bond Catalysis on Carbonyl-Olefin Ring-Closing Metathesis Reaction: Comparison with Lewis Acid Catalysis. <i>Chinese Journal of Chemistry</i> , 2022, 40, 1275-1284.	2.6	4
10263	Polymerization mechanism of polyferric aluminum phosphatic sulfate (PFAPS) and its flocculation effect on simulated dye wastewater. <i>Korean Journal of Chemical Engineering</i> , 0, , 1.	1.2	3
10264	Thermally activated intra-chain charge transport in high charge-carrier mobility copolymers. <i>Journal of Chemical Physics</i> , 2022, 156, 084115.	1.2	4
10265	Molecular dynamics simulations and quantitative calculations on photo-responsive behavior of wormlike micelles constructed by gemini surfactant 12-(3-(12-Br)-2Br) and cinnamates with different ortho-substituents. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 641, 128476.	2.3	4
10266	Steric Shielding Effects Induced by Intramolecular H \cdots O Hydrogen Bonding: Remote Borylation Directed by Bpin Groups. <i>ACS Catalysis</i> , 2022, 12, 2694-2705.	5.5	14
10267	A comparative study on adsorption behavior of iodinated X-ray contrast media iohexol and amidotrizoic acid by magnetic-activated carbon. <i>Environmental Science and Pollution Research</i> , 2022, 29, 45404-45420.	2.7	4
10268	Analeptic activity of 2-Hydroxyl-5-Nitrobenzaldehyde: Experimental, DFT studies, and in silico molecular docking approach. <i>Healthcare Analytics</i> , 2022, 2, 100030.	2.6	22
10269	A DFT approach for finding therapeutic potential of two dimensional (2D) graphitic carbon nitride (GCN) as a drug delivery carrier for curcumin to treat cardiovascular diseases. <i>Journal of Molecular Structure</i> , 2022, 1257, 132547.	1.8	16
10270	How End-Capped Acceptors Regulate the Photovoltaic Performance of the Organic Solar Cells: A Detailed Density Functional Exploration of Their Impact on the D \cdots A Type Small Molecular Electron Donors. <i>Energy & Fuels</i> , 2022, 36, 2095-2107.	2.5	22
10271	Alkynyl Sulfonium Salts Can Be Employed as Chalcogen-Bonding Catalysts and Generate Alkynyl Radicals under Blue-Light Irradiation. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	8
10272	Impact of fullerene on the holographic properties of PQ/PMMA photopolymer. <i>Composites Science and Technology</i> , 2022, 221, 109335.	3.8	14

#	ARTICLE	IF	CITATIONS
10273	M@[12-crown-4] and M@[15-crown-5] where (M=Li, Na, and K); the very first examples of non-conventional one alkali metal-containing alkalides with remarkable static and dynamic NLO response. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 140, 115170.	1.3	13
10274	Novel catalytic ceramic membranes anchored with MnMe oxide and their catalytic ozonation performance towards atrazine degradation. <i>Journal of Membrane Science</i> , 2022, 648, 120362.	4.1	32
10275	Linear and Nonlinear Photon-Induced Cross Bridge/Space Charge Transfer in STC Molecular Crystals. <i>Nanomaterials</i> , 2022, 12, 535.	1.9	7
10276	Theoretical and experimental investigation of a pyrazole derivative- solvation effects, reactivity analysis and MD simulations. <i>Chemical Physics Letters</i> , 2022, 793, 139469.	1.2	7
10277	Computational Modeling of the Interaction of Silver Clusters with Carbohydrates. <i>ACS Omega</i> , 2022, 7, 4750-4756.	1.6	6
10278	Assembling of Perylene, Naphthalene, and Pyromellitic Diimide-Based Materials and Their Third-Order Nonlinear Optical Properties. <i>Journal of Physical Chemistry A</i> , 2022, 126, 870-878.	1.1	8
10279	Formation pathway of disinfection by-products of lignin monomers in raw water during disinfection. <i>Science of the Total Environment</i> , 2022, 825, 153706.	3.9	2
10280	Reducing the Electron Delocalization of FOX-7 toward a Thermally Stable Explosive as a Hexanitrosilbene (HNS) Replacement. <i>Crystal Growth and Design</i> , 2022, 22, 1867-1873.	1.4	4
10281	The merger of vinyl-N-trifosylhydrazones and silver catalysis to enable stereoselective vinylcyclopropanation of alkenes. <i>Chem Catalysis</i> , 2022, 2, 563-577.	2.9	16
10282	2,5-Diiodothiophene: A Versatile Halogen Bonding Synthone for Crystal Engineering. <i>Crystal Growth and Design</i> , 2022, 22, 1906-1913.	1.4	7
10283	O(N) Stochastic Evaluation of Many-Body van der Waals Energies in Large Complex Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1633-1645.	2.3	12
10284	Theoretical study on excited state intramolecular proton transfer mechanism of thiazole complex in different kinds of solvents. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	4
10285	Insight into the Gd ^{III} -Pt Bond: Slow Magnetic Relaxation of a Heterometallic Gd ^{III} -Pt Complex. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 513-521.	2.0	3
10286	Crystal Facet Structure Dependence and Promising Pd-Based Catalytic Materials for Resistance toward Deactivation and Catalytic Performance in Direct Oxidative Esterification. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 9763-9780.	4.0	8
10287	Ultrafast charge transfer dynamics in 2D covalent organic frameworks/Re-complex hybrid photocatalyst. <i>Nature Communications</i> , 2022, 13, 845.	5.8	46
10288	[Cd(Sn9)2]6 ⁺ and [Cd(Ni@Sn9)2]6 ⁺ : Reactivity and coordination chemistry of empty and Ni-centered [Sn9]4 ⁺ Zintl ions. <i>Chinese Chemical Letters</i> , 2023, 34, 107207.	4.8	2
10289	Ultrasound-assisted deep eutectic solvents extraction of glabridin and isoliquiritigenin from <i>Glycyrrhiza glabra</i> : Optimization, extraction mechanism and in vitro bioactivities. <i>Ultrasonics Sonochemistry</i> , 2022, 83, 105946.	3.8	30
10290	Highly accurate DFT investigation for triggering the ultra-strong static and dynamic nonlinear optical properties of superalkali doped aminated graphdiyne (NH ₂ -GDY) donor-acceptor (D-A) quantum dots. <i>Polyhedron</i> , 2022, 215, 115695.	1.0	17

#	ARTICLE	IF	CITATIONS
10291	Synthesis of 3,3,3-trifluoropropyne from chlorotrifluoropropene isomers in liquid phase. <i>Journal of Fluorine Chemistry</i> , 2022, 255-256, 109950.	0.9	1
10292	Uncovering the geometrical aspects of intramolecular hydrogen bond in meta-benziporphodimethenes through molecular tailoring approach. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113631.	1.1	3
10293	Theoretical investigation of Ga-corrole based dyes with different spatial structure for dye-sensitized solar cells. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113633.	1.1	1
10294	Study of the structural features and solvent effects using ab initio molecular dynamics and energy decomposition analysis of atogepant in water and ammonia. <i>Journal of Molecular Liquids</i> , 2022, 352, 118672.	2.3	17
10295	Exploration of experimental, theoretical, Hirshfeld surface, molecular docking and electronic excitation studies of Menadione: A potent anti-cancer agent. <i>Journal of Molecular Liquids</i> , 2022, 351, 118670.	2.3	6
10296	Synthesis, vibrational Depictions, IRI interpretations and docking research on coordination metal complex Diaqua aspartato zinc (II) monohydrate using DFT approach. <i>Journal of Molecular Liquids</i> , 2022, 351, 118687.	2.3	13
10297	Activated carbon adsorption coupled with ozonation regeneration for efficient removal of chlorobenzene. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 107319.	3.3	19
10298	Preparation, antioxidant activity, and theoretical studies on the relationship between antioxidant and electronic properties of bis(thio/carbohydrazone) derivatives. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 164, 110618.	1.9	17
10299	The synergistic effects of central core size and end group engineering on performance of narrow bandgap nonfullerene acceptors. <i>Chemical Engineering Journal</i> , 2022, 435, 135020.	6.6	14
10300	A DFT investigation of hydrogen adsorption and storage properties of Mg decorated IRMOF-16 structure. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 641, 128510.	2.3	11
10301	Influence of periodic heteroatom substitution in the aryl rings on optical properties and thermal stability of diarylethene derivatives. <i>Journal of Molecular Structure</i> , 2022, 1256, 132529.	1.8	1
10302	Study on structures, electronic, spectral and thermodynamic properties of lanthanide-doped boron-based MBn ⁿ⁺ (M=La, Ce, Pr; n=8, 9) clusters. <i>Journal of Molecular Structure</i> , 2022, 1256, 132566.	1.8	3
10303	Retarded transport properties of graphene oxide based chiral separation membranes modified with dipeptide. <i>Separation and Purification Technology</i> , 2022, 288, 120642.	3.9	9
10304	Experimental, theoretical, hirschfeld surface, electronic excitation and molecular docking studies on fomezole(4-Methyl-1H-pyrazole). <i>Journal of Molecular Structure</i> , 2022, 1256, 132549.	1.8	3
10305	Guaianolides and unusual 3-oxa-guaianolides from <i>Artemisia macrocephala</i> . <i>Phytochemistry</i> , 2022, 197, 113108.	1.4	5
10306	Synthesis, structural, computational, and antiproliferative activity studies of new steroidal tetrazole derivatives. <i>Journal of Molecular Structure</i> , 2022, 1256, 132577.	1.8	1
10307	High yield M-BTC type MOFs as precursors to prepare N-doped carbon as peroxymonosulfate activator for removing sulfamethazine: The formation mechanism of surface-bound SO ₄ ²⁻ on Co-N _x site. <i>Chemosphere</i> , 2022, 295, 133946.	4.2	25
10308	Boosting 2e ⁻ oxygen reduction reaction in garland carbon nitride with carbon defects for high-efficient photocatalysis-self-Fenton degradation of 2,4-dichlorophenol. <i>Applied Catalysis B: Environmental</i> , 2022, 307, 121185.	10.8	118

#	ARTICLE	IF	CITATIONS
10309	The assessment of physicochemical properties of Cisplatin complexes with purines and vitamins B group. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 113, 108144.	1.3	3
10310	Charge scaling parameter evaluation for multivalent ionic liquids with fixed point charge force fields. <i>Journal of Ionic Liquids</i> , 2022, 2, 100020.	1.0	8
10311	Highly efficient blue-emissive electroluminescence: nondestructive color regulation effect of orthogonal cyano-substitution in hybrid locally-excited and charge-transfer (HLCT) backbone emitters. <i>Materials Today Chemistry</i> , 2022, 24, 100785.	1.7	11
10312	Theoretical study of new promising conjugated psoralens in psoralen ultraviolet A therapy. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, .	0.9	1
10313	Decoding the Structure of Non-Proteinogenic Amino Acids: The Rotational Spectrum of Jet-Cooled Laser-Ablated Thioproline. <i>Molecules</i> , 2021, 26, 7585.	1.7	3
10314	Synthesis and Computational Characterization of Organic UV-Dyes for Cosensitization of Transparent Dye-Sensitized Solar Cells. <i>Molecules</i> , 2021, 26, 7336.	1.7	4
10315	The reaction path of cyclooctatetraene dimerization revisited. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	1
10316	Tuning the Excited State of Tetradentate Pd(II) and Pt(II) Complexes through Benzannulated N-Heteroaromatic Ring and Central Metal. <i>Chinese Journal of Chemistry</i> , 2022, 40, 223-234.	2.6	8
10317	Stages of Kitaigorodsky Aufbau Principle Detached in the Cocrystals of Cp ₂ MX ₂ (M = Ti, Zr; X = Cl, Br, I) with f- and ĩ-Hole Donors. <i>Crystal Growth and Design</i> , 2022, 22, 1244-1252.	1.4	5
10318	Largely Enhancing the Blocking Energy Barrier and Temperature of a Linear Cobalt(II) Complex through the Structural Distortion: A Theoretical Exploration. <i>Inorganic Chemistry</i> , 2022, 61, 295-301.	1.9	28
10319	Ir-catalyzed enantioselective B-H alkenylation for asymmetric synthesis of chiral-at-cage o-carboranes. <i>Nature Communications</i> , 2021, 12, 7146.	5.8	34
10320	Designing Potential Donor Materials Based on DRCN5T with Halogen Substitutions: A DFT/TDDFT Study. <i>International Journal of Molecular Sciences</i> , 2021, 22, 13498.	1.8	2
10321	2-Pyridylselenenyl versus 2-Pyridyltellurenyl Halides: Symmetrical Chalcogen Bonding in the Solid State and Reactivity towards Nitriles. <i>Symmetry</i> , 2021, 13, 2350.	1.1	14
10322	Biomass-Derived Carbon Quantum Dots Modified Bi ₂ MoO ₆ /Bi ₂ S ₃ Heterojunction for Efficient Photocatalytic Removal of Organic Pollutants and Cr(III). <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10323	Fast Coupling and Detoxification of Aqueous Halobenzoquinones by Extracellular Nucleophiles: The Relationship Among Structures, Pathways and Toxicity. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10324	1-Hydroxy-1,2,3,4-Tetrazole and its Transition Metal Complexes: A Family of Green High-Energy Catalysts for Ammonium Perchlorate. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10325	Computational and Experimental Insights into Carboxylate-Assisted Carboxylation of Thiophene with CO ₂ in the Solvent-Free Carbonate Medium. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10326	Transformation of Amino Acids and Formation of Nitrophenolic Byproducts in Sulfate Radical Oxidation Processes. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
10327	Synergistic Adsorption-Photocatalysis for Dyes Removal by a Novel Biochar-Based Z-Scheme Heterojunction Bc/Zis/Wo3: Mechanistic Investigation and Degradation Pathways. SSRN Electronic Journal, 0, , .	0.4	0
10328	S-Scheme Cs ₂ agbibr ₆ /Ag ₃ po ₄ Heterojunction with Efficient Photocatalysis Performance for H ₂ Production and Organic Pollutants Oxidation: Predicting Reaction Sites and Mechanism. SSRN Electronic Journal, 0, , .	0.4	0
10329	Acid-Triggered, Degradable and High Strength-Toughness Copolyesters: Comprehensive Experimental and Theoretical Study. SSRN Electronic Journal, 0, , .	0.4	0
10330	Conventional and Nonconventional Hydrogen Bonds Origin of the Different Behavior. SSRN Electronic Journal, 0, , .	0.4	0
10331	New Insights into Ferric Iron-Facilitated Uv254 Photolytic Defluorination of Perfluorooctanoic Acid (Pfoa): Combined Experimental and Theoretical Study. SSRN Electronic Journal, 0, , .	0.4	0
10332	Natural Quinone Molecules as Effective Cath Ode Materials for Lithium-Ion Batteries: A First-Principles Study. SSRN Electronic Journal, 0, , .	0.4	0
10333	Electronic Structure and Bonding in N-Hetero Cyclic Carbene Stabilized Naked Group 16 Atoms In-Plane Hyperconjugation and Bond Polarity. SSRN Electronic Journal, 0, , .	0.4	0
10334	Experimental and computational tuning of metalla-N-heterocyclic carbenes at palladium(Pd) and platinum(Pt) centers. Dalton Transactions, 2022, 51, 6718-6734.	1.6	11
10335	A reduced electrophilicity for simple Lewis acids A involved in non-covalent interactions with Lewis bases B. Physical Chemistry Chemical Physics, 2022, 24, 6856-6865.	1.3	4
10336	Carbon skeleton: route to investigate high-performance insensitive energetic materials. New Journal of Chemistry, 2022, 46, 6690-6693.	1.4	0
10337	Theoretical study of a derivative of chlorophosphine with aliphatic and aromatic Grignard reagents: S _N 2@P or the novel S _N 2@Cl followed by S _N 2@C?. RSC Advances, 2022, 12, 9130-9138.	1.7	0
10338	Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585.		0
10339	Site-specific doping of silver atoms into a Au ₂₅ nanocluster as directed by ligand binding preferences. Chemical Science, 2022, 13, 5148-5154.	3.7	11
10340	The Aggregation and Deposition Behavior of Nanoplastics on Al ₂ O ₃ In Aquatic Environments. SSRN Electronic Journal, 0, , .	0.4	0
10341	Exploring the structure and electronic properties of germanium doped boron clusters using density functional theory based global optimization method. New Journal of Chemistry, 2022, 46, 6244-6254.	1.4	1
10342	Synthesis of Au/Ni ₂ p Nanosheet Arrays with Porous Grids as a High-Performance Electrode for the Determination of Hydroquinone in Domestic Sewage. SSRN Electronic Journal, 0, , .	0.4	0
10343	Three-Coordinated Mononuclear Cu(I) Complexes with Crystallization-Enhanced Thermally Activated Delayed Fluorescence Characteristics. SSRN Electronic Journal, 0, , .	0.4	0
10344	Effect of 3-mercapto-1-propane sulfonate sulfonic acid and polyvinylpyrrolidone on the growth of cobalt pillar by electrodeposition. Nanotechnology Reviews, 2022, 11, 1209-1218.	2.6	5

#	ARTICLE	IF	CITATIONS
10345	Supramolecular networks by imine halogen bonding. <i>Chemical Communications</i> , 2022, , .	2.2	5
10346	Hydroxyl-assisted selective epoxidation of perillyl alcohol with hydrogen peroxide by vanadium-substituted phosphotungstic acid hinged on imidazolyl activated carbon. <i>New Journal of Chemistry</i> , 2022, 46, 6636-6645.	1.4	5
10347	Theoretical insights into photo-induced isomerization mechanisms of phenylsulfinyl radical PhSO $\dot{\text{E}}$ TM . <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6266-6273.	1.3	3
10348	Rational Design of Zr-Mofs Pyrolyzed to Pinpoint Rate-Directing Stage and Catalytic Functions of Surface Acidic Species in Homolytic H ₂ O ₂ Scission. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10349	Influence of charge transfer strength on emission bandwidth for multiple-resonance emitters via systematically tuning the acceptor-donor assembly. <i>Journal of Materials Chemistry C</i> , 2022, 10, 7866-7874.	2.7	16
10350	Deep Purification of Copper from Cu(II)-Edta Acidic Wastewater by Fe(III) Replacement/Diethyldithiocarbamate Precipitation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10351	Surface discharge of bulk materials investigated from change of charge trap characteristics of polyimide single molecular chain. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2022, 71, 052101.	0.2	3
10352	Quantum Chemical Studies of the Electronic Structures of Anti-Tumor Agents: Au(III) (L = Porphine,) Tj ETQq1 1 0.784314 rgBT /Over	0.4	0
10353	Phosphine oxides as NMR and IR spectroscopic probes for the estimation of the geometry and energy of PO $\dot{\text{A}}$ -A hydrogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7121-7133.	1.3	2
10354	Terthiophene Based Non-Fused Electron Acceptors for Efficient Organic Solar Cells. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10356	Experimental and theoretical studies of the interaction of Penicillamine with SWCNT (6,0) as a drug delivery system. <i>Inorganic and Nano-Metal Chemistry</i> , 0, , 1-9.	0.9	2
10357	Supramolecular interaction of inositol phosphates with Cu(II): comparative study of InsP ₆ and InsP ₃ . <i>CrystEngComm</i> , 2022, 24, 2126-2137.	1.3	1
10358	A Mussle-Pearl Side Chain Interaction in Mercury(II) and Phenol Removal by Sulfur-Functionalized Covalent Organic Frameworks: A Dft Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10359	Theoretical investigation of the structures, stabilities, and vibrational and rotational spectroscopic parameters of linear HOMgNC and HMgNCO molecules by density functional theory and coupled-cluster method. <i>New Journal of Chemistry</i> , 2022, 46, 7879-7891.	1.4	5
10360	Ultrafast exciton delocalization and localization dynamics of a perylene bisimide quadruple π -stack: a nonadiabatic dynamics simulation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7293-7302.	1.3	6
10361	The Overlooked Role of Co(OH) ₂ in Co ₃ O ₄ Activated Pms System: Suppression of Co ²⁺ Leaching and Enhanced Degradation Performance of Antibiotics. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10362	Theoretical insight into mercury species adsorption on graphene-based Pt single-atom catalysts. <i>RSC Advances</i> , 2022, 12, 5797-5806.	1.7	5
10363	Theoretical design and characterization of new terpolymer donors based on PTB7Ir for high-efficiency triplet-material-based organic photovoltaics. <i>RSC Advances</i> , 2022, 12, 8578-8587.	1.7	1

#	ARTICLE	IF	CITATIONS
10364	Molecular recognition between bacterial phosphorothioate DNA and sulfur-binding domain (SBD): competition between the water cage and chalcogen-hydrophobic packet. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 9176-9187.	1.3	7
10365	Unveiling the intramolecular [3 + 2] cycloaddition reactions of <i>C</i> -, <i>N</i> -disubstituted nitrones from the molecular electron density theory perspective. <i>New Journal of Chemistry</i> , 2022, 46, 7721-7733.	1.4	9
10366	Experimental and theoretical insights into the formation of weak hydrogen bonds and H \cdots H bonding interactions in the solid-state structure of two eucalyptol derivatives. <i>New Journal of Chemistry</i> , 2022, 46, 5690-5704.	1.4	3
10367	Computational and Experimental Study of Different Brines in Temperature Swing Solvent Extraction Desalination with Amine Solvents. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10368	Isolation and structural characterization of stable carbamic \cdots carbonic anhydrides: an experimental and computational study. <i>Organic Chemistry Frontiers</i> , 2022, 9, 2154-2163.	2.3	1
10369	Crystallinity modulation of donors by heteroatom side-chain engineering and solvent additive achieving 14.3% all-small-molecule organic solar cells. <i>Journal of Materials Chemistry A</i> , 2022, 10, 9635-9642.	5.2	15
10370	Theoretical studies of high-Tc Fe-superconductors based on BaFe ₂ As ₂ in presence of dopants Rh and Pd. <i>Materials Today: Proceedings</i> , 2022, 54, 95-100.	0.9	0
10371	Covalent Organic Framework Modified Carbon Nanotubes for Removal of Uranium (VI) from Mining Wastewater. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10372	Photophysical properties and optical nonlinearity of cyclo[18]carbon (C ₁₈) precursors, C ₁₈ \cdots (CO) _n (<i>n</i> = 2, 4, and 6): focusing on the effect of the carbonyl groups. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7466-7473.	1.3	32
10373	Removal of Cationic and Anionic Dyes by Mof-199: Identifying the Adsorption Mechanism. <i>SSRN Electronic Journal</i> , 0, , .	0.4	1
10374	Synthesis and structure of (O \cdots Si)-chelate fluorosilane, a novel complex of pentacoordinate silicon with N-acetylvaline. <i>Mendeleev Communications</i> , 2022, 32, 37-38.	0.6	4
10375	Towards a computational understanding of water oxidation at graphene-bound Mn _x O _y and Mn _x O _y M ₂₊ particles. <i>Sustainable Energy and Fuels</i> , 0, , .	2.5	0
10376	Sp ² - and sp ³ \cdots C \cdots O tetrel bonds in the 3-oxetanone homodimer. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	1.3	5
10377	Self-association of diphenylpnicotinic acids in solution and solid state: covalent <i>vs.</i> hydrogen bonding. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7882-7892.	1.3	4
10378	Computational Investigation on Structural and Reactive Sites (HOMO-LUMO, MEP, NBO, NPA, ELF, LOL,) Tj ETQq0 0 0 rgBT /Overlock 10 (E)-4-((4-chlorobenzylidene) amino) Benzene Sulfonamide Compound. <i>Analytical Chemistry Letters</i> , 2022, 12, 58-76.	0.4	39
10379	Theoretical Study on the Mechanisms and Rate Constants of Oxidation of Methyl Ethyl Ether Induced by \dot{A} -OH in the Atmosphere. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
10380	Search for an exothermic halogen bond between anions. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6964-6972.	1.3	3
10381	Ternary 14-electron XB ₂ Be ₂ (X = Si, Ge, Sn, Pb) clusters: a planar tetracoordinate silicon (ptSi) system and its ptGe/Sn/Pb congeners. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7068-7076.	1.3	3

#	ARTICLE	IF	CITATIONS
10382	Lithium Selectivity of Crown Ethers: The Effect of Heteroatoms and Cavity Size. SSRN Electronic Journal, 0, , .	0.4	0
10383	Implementation of predictive models: Practical aspects. Theoretical and Computational Chemistry, 2022, , 405-433.	0.2	0
10384	New Insights into Ferric Iron-Facilitated Uv254 Photolytic Defluorination of Perfluorooctanoic Acid (Pfoa): Combined Experimental and Theoretical Study. SSRN Electronic Journal, 0, , .	0.4	0
10385	How the substrate affects amination reaction kinetics of nitrochlorobenzene. Reaction Chemistry and Engineering, 2022, 7, 833-838.	1.9	1
10386	Stereodivergent synthesis of enantioenriched azepino[3,4,5- <i>cd</i>]-indoles <i>via</i> cooperative Cu/Ir-catalyzed asymmetric allylic alkylation and intramolecular Friedel-Crafts reaction. Chemical Science, 2022, 13, 4801-4812.	3.7	32
10387	Theoretical study on an intriguing excited-state proton transfer process induced by weakened intramolecular hydrogen bonds. Physical Chemistry Chemical Physics, 2022, 24, 8453-8462.	1.3	20
10388	Theoretical study for evaluating and discovering organic hydride compounds as novel trifluoromethylation reagents. Organic and Biomolecular Chemistry, 2022, 20, 2831-2842.	1.5	5
10389	Weakly-bound clusters of atmospheric molecules: infrared spectra and structural calculations of (CO) ₂ ⁿ (CO) _m ⁿ (N) ₂ ^p , (<i>n</i> , <i>m</i> , <i>p</i>) = (2,1,0), (2,0,1), (1,2,0), (1,0,2), (1,1,1), (1,3,0), (1,0,3), (1,2,1), (1,1,2). Physical Chemistry Chemical Physics, 2022, 24, 7231-7242.	1.3	2
10390	Complexation of uranyl(^{vi}) with succinimidedioxime in comparison with glutarimidedioxime. New Journal of Chemistry, 0, , .	1.4	0
10391	The strong interaction of actinyl ions with fullerene driven by multiple hydrogen bonds. Dalton Transactions, 2022, 51, 5118-5126.	1.6	5
10392	Intermolecular hydrogen bonds induce restriction of access to the dark state for triggering aggregation-induced emission. Journal of Materials Chemistry C, 2022, 10, 5356-5363.	2.7	11
10393	Simultaneous Removal of Tetracycline and Arsenic(III) Using Copper-Manganese Composite Oxide: Competition Behaviors and Removal Mechanisms. SSRN Electronic Journal, 0, , .	0.4	0
10394	Structural diversity and magnetic properties of copper(^{II}) quinaldinate compounds with amino alcohols. New Journal of Chemistry, 2022, 46, 6899-6920.	1.4	3
10395	Insight into the Cation-Regulated Mechanism For the Hydration of Propargyl Alcohols Catalyzed by [Bu ₄ p ⁺][Im ⁻]. SSRN Electronic Journal, 0, , .	0.4	0
10396	Energy decomposition analysis of cationic carbene analogues with group 13 and 16 elements as a central atom: a comparative study. Physical Chemistry Chemical Physics, 2022, 24, 8970-8978.	1.3	1
10397	Simultaneous enhancement of thermally activated delayed fluorescence and photoluminescence quantum yield <i>via</i> homoconjugation. Journal of Materials Chemistry C, 2022, 10, 6306-6313.	2.7	7
10398	Palladium-catalyzed regio- and chemoselective double-alkoxycarbonylation of 1,3-diyne: a computational study. Organic Chemistry Frontiers, 2022, 9, 2697-2707.	2.3	4
10399	Spectroscopic Identification, Structural Features and Molecular Docking Studies on 5-(4-Propoxybenzylidene)-2-[3-(4-chlorophenyl)-5-[4(propan-2-yl) phenyl]-4,5-dihydro-1H-pyrazol-1-yl]-1,3-thiazol-4(5H)-one using Pim-1 Kinase Cancer Protein. Asian Journal of Chemistry, 2022, 34, 857-870.	0.1	1

#	ARTICLE	IF	CITATIONS
10400	Effects of Different Dissolved Organic Matter on Peroxymonosulfate Activation Over Co-Fe Binary Metal: Experiments and Density Functional Theory. SSRN Electronic Journal, 0, , .	0.4	0
10401	$\text{Ln}^{3+} @ \text{C}_{80}^{+}$ (Ln = lanthanide): a new class of stable metallofullerene cations with multicenter metal-metal bonding in the sub-nanometer confined space. Inorganic Chemistry Frontiers, 2022, 9, 2173-2181.	3.0	9
10402	Tropo(thio)ne-embedded homoHPHACs: does the tropylium cation induce global antiaromaticity in expanded hexapyrrolohexaazacoronene?. Chemical Communications, 2022, 58, 3366-3369.	2.2	5
10403	The Structures and Properties of Mon ($\text{N}=2^{1/4}15$) Cluster. SSRN Electronic Journal, 0, , .	0.4	0
10404	Cocrystallization-driven self-assembly with vanillic acid offers a new opportunity for surmounting fast and excessive absorption issues of antifungal drug 5-fluorocytosine: a combined theoretical and experimental research. CrystEngComm, 2022, 24, 2777-2790.	1.3	7
10405	Insight into the New Catalytic Species for the Hydration of Propargyl Alcohols Catalyzed by $[\text{Bu}_4\text{p}^+][\text{Im}^-]$. SSRN Electronic Journal, 0, , .	0.4	0
10406	Luminescence of Fullerene-like Clusters by a first-principles study. Wuli Xuebao/Acta Physica Sinica, 2022, .	0.2	0
10407	DFT insight into asymmetric alkyl-alkyl bond formation via nickel-catalysed enantioconvergent reductive coupling of racemic electrophiles with olefins. Chemical Science, 2022, 13, 3728-3739.	3.7	9
10408	Boron-based non-fullerene small molecule acceptors via nitrogen substitution: a theoretical study. Materials Advances, 2022, 3, 3229-3237.	2.6	4
10409	Mechanism of DOPA radical generation and transfer in metal-free class Ie ribonucleotide reductase based on density functional theory. Computational and Structural Biotechnology Journal, 2022, 20, 1111-1131.	1.9	1
10410	A tricolor-switchable stimuli-responsive luminescent binuclear $\text{Cu}(\text{O})$ complex with switchable NH^+O^- interactions. Inorganic Chemistry Frontiers, 2022, 9, 2305-2314.	3.0	8
10411	Metal-organic framework bearing new viologen ligand for ammonia and Cr^{2+} sensing. RSC Advances, 2022, 12, 6951-6957.	1.7	17
10412	Probing iron adsorption on the internal and external wall of pristine and N-doped carbon nanotube. Australian Journal of Chemistry, 2022, , .	0.5	1
10413	Evaluation of Vibrational, Electronic, Topology, Reactivity, Bioactivity, Bioavailability and Blood-Brain Barrier Score of 1-(2,6-dimethylphenoxy)propan-2-amine-A DFT, Spectroscopic and Molecular Docking Approach. Analytical Chemistry Letters, 2022, 12, 102-118.	0.4	0
10414	Designing Organic/Inorganic Cathodes of MnO_2 Half-Wrapped by Aromatic Polymers for High-Performance Aqueous Zinc-Ion Batteries. SSRN Electronic Journal, 0, , .	0.4	0
10415	Modulating TTA efficiency through control of high energy triplet states. Journal of Materials Chemistry C, 2022, 10, 4923-4928.	2.7	8
10416	High Yield M-Btc Type Mofs as Precursors to Prepare N-Doped Carbon as Peroxymonosulfate Activator for Removing Sulfamethazine: The Formation Mechanism of Surface-Bound SO_4^{2-} on Co-Nx Site. SSRN Electronic Journal, 0, , .	0.4	0
10417	Accelerated discovery of thermostable high-energy materials with intramolecular donor-acceptor building blocks. Chemical Communications, 2022, 58, 4460-4463.	2.2	13

#	ARTICLE	IF	CITATIONS
10418	STRUCTURE AND CATALYTIC PROPERTIES OF PALLADIUM(II) (ACETYLACETONATO-) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 747 Td (îº20, 63, 125-139.	0.3	2
10419	Insights into Cqds-Doped Perylene Diimide Photocatalysts for the Oxidation of Emerging Contaminants. SSRN Electronic Journal, 0, , .	0.4	0
10420	Multi-Armed Imide-Based Molecules Promote Interfacial Charge Transfer for Efficient Organic Solar Cells. SSRN Electronic Journal, 0, , .	0.4	0
10421	Dft Study on the Effect of Na on No Reduction by Nitrogen-Containing Char from Zhundong Coal. SSRN Electronic Journal, 0, , .	0.4	0
10422	Crystalline radical cations of bis-BN-based analogues of Thiele's hydrocarbon. Chemical Communications, 2022, 58, 5391-5394.	2.2	3
10423	Synthesis of distibiranes and azadistibiranes by cycloaddition reactions of distibenes with diazomethanes and azides. Chemical Science, 2022, 13, 3775-3786.	3.7	6
10424	Dearomative [4 + 3] cycloaddition of furans with vinyl-<i>N</i>-triflylhydrazones by silver catalysis: stereoselective access to oxa-bridged seven-membered bicycles. Organic Chemistry Frontiers, 2022, 9, 2444-2452.	2.3	14
10425	Vibrational Spectral Studies, Thermodynamic Investigations and DFT (NLO, NBO, MEP) Computation of Benzene Derivative. Springer Proceedings in Physics, 2022, , 463-485.	0.1	4
10426	Synthesis and computational aspects of Al(<sc>ii</sc>)â€“Al(<sc>ii</sc>) and Ga(<sc>ii</sc>)â€“Ga(<sc>ii</sc>) dihalides based on an amidinate scaffold. Dalton Transactions, 2022, 51, 4898-4902.	1.6	2
10427	Thermodynamic stability of <i>cis</i>-azobenzene containing DNA materials based on van der Waals forces. Chemical Communications, 2022, 58, 3811-3814.	2.2	5
10428	Mechanisms of ÅUranium Immobiliz Ation ÅOn the Interface between Shewanella Putrefaciens ÅAnd Montmorillonite. SSRN Electronic Journal, 0, , .	0.4	0
10429	Portable Visual Assay of Bacillus Anthracis Biomarker Based on Ligand-Functionalized Dual Emission Lanthanide Metal-Organic Frameworks and Smartphone-Integrated Mini-Device. SSRN Electronic Journal, 0, , .	0.4	0
10430	Conformational and structural stability of <i>n</i> and 2-propylthiols: a revisit. RSC Advances, 2022, 12, 10336-10344.	1.7	1
10431	A DFT Study on the Potential Application of Graphene-Like Pure and Doped Boron Phosphide Monolayer in Li- and Na-Ion Batteries. Russian Journal of Physical Chemistry A, 2022, 96, 125-134.	0.1	1
10432	Insight into the dual action mechanism of 3V-PPh₃ polymers as carriers and ligands in the Rh/3V-PPh₃ heterogeneous catalytic hydroformylation of ethylene to propionaldehyde. Physical Chemistry Chemical Physics, 2022, 24, 9673-9684.	1.3	4
10433	Transformation of Amino Acids and Formation of Nitrophenolic Byproducts in Sulfate Radical Oxidation Processes. SSRN Electronic Journal, 0, , .	0.4	0
10434	One-Step Supramolecular Fabrication of Ionic Liquid/Zif-8 Nanocomposites for High-Efficient Capture and Conversion of Co2 from Flue Gas at Discharged Temperatures. SSRN Electronic Journal, 0, , .	0.4	0
10435	Synthesis, spectroscopic findings and crystal engineering of Pb(<sc>ii</sc>)â€“Salen coordination polymers, and supramolecular architectures engineered by ĩf-hole/spodium/tetrel bonds: a combined experimental and theoretical investigation. RSC Advances, 2022, 12, 6352-6363.	1.7	25

#	ARTICLE	IF	CITATIONS
10436	Pure Hydrocarbon Host Materials Based on 9,9'-Spirobifluorene/Naphthalene Hybrid. Chinese Journal of Organic Chemistry, 2022, 42, 572.	0.6	2
10437	Combined virtual and experimental screening of multicomponent crystals of 2,4-dichlorophenoxyacetic acid. New Journal of Chemistry, 0, , .	1.4	6
10438	Theoretical search of a simple characteristic for long-lived organic room-temperature phosphorescence materials with H aggregation. Journal of Materials Chemistry C, 2022, 10, 5425-5432.	2.7	11
10439	Solvent-Free and Catalyst-Free Chemistry Enables Insertion of Alkenes Into ĩf Bonds. SSRN Electronic Journal, 0, , .	0.4	0
10440	Origin of Metabolites Diversity and Selectivity of P450 Catalyzed Benzo[A]Pyrene Metabolic Activation. SSRN Electronic Journal, 0, , .	0.4	0
10441	Synthesis, Spectral analysis, XRD, Hirshfeld surface analysis, DFT studies and Anticancer activities of di(o-chlorobenzyl)(dichloro)(1,10-phenanthroline)tin(IV) complex. SSRN Electronic Journal, 0, , .	0.4	0
10442	A susceptible multifunctional fluorescent probe based on levulinic acid for the practical detection of SO ₂ . Analytical Methods, 2022, 14, 1529-1533.	1.3	2
10443	From weak to strong interactions: structural and electron topology analysis of the continuum from the supramolecular chalcogen bonding to covalent bonds. Physical Chemistry Chemical Physics, 2022, 24, 8251-8259.	1.3	15
10444	Controlled supramolecular interaction to enhance the bioavailability of hesperetin to targeted cancer cells through graphyne: a comprehensive <i>in silico</i> study. RSC Advances, 2022, 12, 6336-6346.	1.7	12
10445	Improvement of the photostability of cycloalkylamine-7-sulfonyl-2,1,3-benzoxadiazole-based fluorescent dyes by replacing the dimethylamino substituent with cyclic amino rings. New Journal of Chemistry, 2022, 46, 7003-7013.	1.4	4
10446	Methyl nitrate energetic compounds based on bicyclic scaffolds of furazanâ€“isofurazan (isoxazole): syntheses, crystal structures and detonation performances. RSC Advances, 2022, 12, 7712-7719.	1.7	3
10447	A theoretical study on the formation mechanism of carboxylic sulfuric anhydride and its potential role in new particle formation. RSC Advances, 2022, 12, 5501-5508.	1.7	4
10448	A combined crystallography and DFT study on ring-shaped Cucurbit[<i>n</i>]urils: structures, surface character, and hostâ€“guest recognition. RSC Advances, 2022, 12, 10014-10019.	1.7	4
10449	Mechanistic exploration of CO ₂ conversion to dimethoxymethane (DMM) using transition metal (Co, Ru) catalysts: an energy span model. Physical Chemistry Chemical Physics, 2022, 24, 8387-8397.	1.3	9
10450	Optimizing Porous Structure of Carbon Electrodes for Temperature-Independent Capacitance to Realize High Energy Storage and Ultrafast Charge/Discharge Process at Sub-Zero Temperatures. SSRN Electronic Journal, 0, , .	0.4	0
10451	Silver cluster doped graphyne (GY) with outstanding non-linear optical properties. RSC Advances, 2022, 12, 5466-5482.	1.7	29
10452	The unique sandwich K ₆ Be ₂ B ₆ H ₆ cluster with a real borozene B ₆ H ₆ core. RSC Advances, 2022, 12, 8617-8623.	1.7	3
10453	Iodine(<i>scpi</i>) complexes incorporating sterically bulky 2-substituted pyridines. RSC Advances, 2022, 12, 8674-8682.	1.7	6

#	ARTICLE	IF	CITATIONS
10472	Morphology prediction of dihydroxylammonium 5,5-bistetrazole-1,1-diolate (TKX-50) crystal in different solvent systems using modified attachment energy model. <i>Chinese Journal of Chemical Engineering</i> , 2023, 53, 181-193.	1.7	4
10473	Lithium-Assisted Dinitrogen Reduction Mediated by Nb ₂ LiNO ₄ Cluster Anions: Electron Donors or Structural Units. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1511-1517.	1.1	14
10474	Highly Stable Neutral Corrole Radical: Amphoteric Aromatic Antiaromatic Switching and Efficient Photothermal Conversion. <i>Journal of the American Chemical Society</i> , 2022, 144, 3458-3467.	6.6	31
10475	Photoelectron Spectroscopy and Density Functional Investigation of the Structural Evolution, Electronic, and Magnetic Properties of CrSi _n (n = 14-18) Clusters. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1329-1335.	1.1	16
10476	Hydrogen Bond and π - π Stacking Interaction: Stabilization Mechanism of Two Metal Cyclo-N ₅ -Containing Energetic Materials. <i>ACS Omega</i> , 2022, 7, 6627-6639.	1.6	3
10477	Gas-phase catalytic hydration of I ₂ O ₅ in the polluted coastal regions: Reaction mechanisms and atmospheric implications. <i>Journal of Environmental Sciences</i> , 2022, 114, 412-421.	3.2	3
10478	1-ä ¹ TMä ³ -3-ç ² ä ³ ä ³ ”ç”~æ ^o é...ç »ä ^{ee} q ² äl/2“ä ^ž æ ^o çš,,ç,ä ^o ä ¹ /2œç”ç”ç©¶. <i>Scientia Sinica Chimica</i> , 2022, , .	0.2	0
10479	Carbon Dioxide Chemically Responsive Switchable Gas Valves with Protonation-Induced Liquid Gating Self-Adaptive Systems. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	11
10480	Ligand-field regulated superalkali behavior of the aluminum-based clusters with distinct shell occupancy. <i>Chinese Chemical Letters</i> , 2022, 33, 5147-5151.	4.8	4
10481	Intriguing Chloride: Involvement of Chloride Ions in Proton Transfers. <i>Molecules</i> , 2022, 27, 1401.	1.7	0
10482	Activating Energy Transfer Tunnels by Tuning Local Electronegativity of Conjugated Polymeric Backbone for High-Efficiency OLEDs with Low Efficiency Roll-Off. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	17
10483	NO adsorption on Ni ₄ M (M = Ni, Mo, Sc, and Y) nanoclusters: a DFT study. <i>Journal of Nanoparticle Research</i> , 2022, 24, 1.	0.8	1
10484	Understanding Contact Electrification at Water/Polymer Interface. <i>Research</i> , 2022, 2022, 9861463.	2.8	30
10485	Theoretical Investigation on the ESIPT Process and Detection Mechanism for Dual-Proton Type Fluorescent Probe. <i>International Journal of Molecular Sciences</i> , 2022, 23, 2132.	1.8	17
10486	Probing effect of solvation on photoexcited quadrupolar donor-acceptor-donor molecule via ultrafast Raman spectroscopy. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 69-76.	0.6	1
10487	<i>i</i> -Nitroacetanilide Solubility in Several Aqueous Solutions and Its Mathematical Correlation. <i>Journal of Chemical & Engineering Data</i> , 2022, 67, 786-796.	1.0	0
10488	From Molecular-Scale Cavities to Nanoscale Dielectric Breakdown in Polydimethylsiloxane Induced by Local Electric Field. <i>Macromolecules</i> , 2022, 55, 1690-1699.	2.2	2
10489	Solvents and Ligands Matter: Structurally Variable Palladium and Nickel Clusters Assembled by Tridentate Selenium- and Tellurium-Containing Schiff Bases. <i>Inorganic Chemistry</i> , 2022, 61, 3785-3800.	1.9	1

#	ARTICLE	IF	CITATIONS
10490	Tuning Photophysical Properties by p-Functional Groups in Zn(II) and Cd(II) Complexes with Piperonylic Acid. <i>Molecules</i> , 2022, 27, 1365.	1.7	10
10491	Highly Efficient and Stable Blue Organic Light-Emitting Diodes based on Thermally Activated Delayed Fluorophor with Donor-Acceptor Motif. <i>Advanced Science</i> , 2022, 9, e2106018.	5.6	40
10492	Insights from Density Functional Theory on the Feasibility of Modified Reactive Dyes as Dye Sensitizers in Dye-Sensitized Solar Cell Applications. <i>Solar</i> , 2022, 2, 12-31.	0.9	16
10493	Shell-Isolated Nanoparticle-Enhanced Raman Spectroscopy for Probing Riboflavin on Graphene. <i>Materials</i> , 2022, 15, 1636.	1.3	5
10494	Highly Fluorescent Dyes Containing Conformationally Restrained Pyrazolylpyrene (Pyrazoolympicene) Chromophore. <i>Molecules</i> , 2022, 27, 1272.	1.7	0
10495	Single-walled silicon nanotube as an exceptional candidate to eliminate SARS-CoV-2: a theoretical study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 3042-3051.	2.0	1
10496	Conformational, Reactivity Analysis, Wavefunction-Based Properties, Molecular Docking and Simulations of a Benzamide Derivative with Potential Antitumor Activity-DFT and MD Simulations. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 2015-2031.	1.4	3
10497	A DFT study of the molecular and electronic structures of cis-dioxidomolybdenum (VI) complex of 8-hydroxyquinoline and 4-benzoyl-3-methyl-1-phenyl-2-pyrazolin-5-one with water. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1.	0.5	1
10498	Biomimetic Nanochannels: From Fabrication Principles to Theoretical Insights. <i>Small Methods</i> , 2022, 6, e2101255.	4.6	18
10499	Covalently tethering disulfonic acid moieties onto polyoxometalate boosts acid strength and catalytic performance for hydroxyalkylation/alkylation reaction. <i>Science China Chemistry</i> , 2022, 65, 699-709.	4.2	2
10500	Carbon Dioxide Chemically Responsive Switchable Gas Valves with Protonation-Induced Liquid Gating Self-Adaptive Systems. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	0
10501	Persistent Planar Tetracoordinate Carbon in Global Minima Structures of Silicon-Carbon Clusters. <i>Atoms</i> , 2022, 10, 27.	0.7	11
10502	Effect of Agricultural Organic Inputs on Nanoplastics Transport in Saturated Goethite-Coated Porous Media: Particle Size Selectivity and Role of Dissolved Organic Matter. <i>Environmental Science & Technology</i> , 2022, 56, 3524-3534.	4.6	44
10503	Theoretical Study of the Chemical Properties and the Reaction Pathway of Decarbonylative Alkylative Esterification of Styrenes with Aliphatic Aldehydes. <i>Journal of Chemistry</i> , 2022, 2022, 1-11.	0.9	1
10504	Single-Component Molecular Dual Persistent Room Temperature Phosphorescence from Low- and High-Lying Triplet States. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	18
10505	Diaryliodoniums as Hybrid Hydrogen- and Halogen-Bond-Donating Organocatalysts for the Groebke-Blackburn-Bienaym Reaction. <i>Journal of Organic Chemistry</i> , 2022, 87, 4569-4579.	1.7	27
10506	Anion photoelectron spectroscopy and density functional theory studies of AuC _n ⁺ (<i>n</i> =3-8): Odd-even alternation in electron binding energies and structures. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 177-184.	0.6	1
10507	Theoretical Calculations and Experiments on the Thermal Properties of Fluorinated Graphene and Its Effects on the Thermal Decomposition of Nitrate Esters. <i>Nanomaterials</i> , 2022, 12, 621.	1.9	8

#	ARTICLE	IF	CITATIONS
10508	Nitrogen-Containing Compounds Enhance Light Absorption of Aromatic-Derived Brown Carbon. <i>Environmental Science & Technology</i> , 2022, 56, 4005-4016.	4.6	19
10509	Binding Energy of Triplet Excitons in Nonfullerene Acceptors: The Effects of Fluorination and Chlorination. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1393-1402.	1.1	6
10510	The Role of Through-Bond Stereoelectronic Effects in the Reactivity of 3-Azabicyclo[3.3.1]nonanes. <i>Journal of Organic Chemistry</i> , 2022, 87, 3378-3388.	1.7	3
10511	Functionalization of Electrodes with Tunable [EMIM] _x [Cl] _{x+1} ⁺ Ionic Liquid Clusters for Electrochemical Separations. <i>Chemistry of Materials</i> , 2022, 34, 2612-2623.	3.2	5
10512	Organic materials repurposing, a data set for theoretical predictions of new applications for existing compounds. <i>Scientific Data</i> , 2022, 9, 54.	2.4	16
10513	Polymorphs of Green Fluorescence Protein Chromophore Analogue: Fluorescence Switching with Thermal Stimuli. <i>Crystal Growth and Design</i> , 2022, 22, 1892-1905.	1.4	2
10514	A Holstein–Peierls Approach to Excimer Spectra: The Evolution from Vibronically Structured to Unstructured Emission. <i>Journal of Physical Chemistry C</i> , 2022, 126, 4067-4081.	1.5	20
10515	The Phosphorus Bond, or the Phosphorus-Centered Pnictogen Bond: The Covalently Bound Phosphorus Atom in Molecular Entities and Crystals as a Pnictogen Bond Donor. <i>Molecules</i> , 2022, 27, 1487.	1.7	17
10516	Ti ₃ C ₂ T _x MXene–RAN van der Waals Heterostructure–Based Flexible Transparent NIR Photodetector Array for 1024 Pixel Image Sensing Application. <i>Advanced Materials Technologies</i> , 2022, 7, .	3.0	17
10517	Effects of Heterocyclic Ring Fusion and Chain Elongation on Chiroptical Properties of Polyaza[9]helicene: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1412-1421.	1.1	5
10518	LModeA-nano: A PyMOL Plugin for Calculating Bond Strength in Solids, Surfaces, and Molecules via Local Vibrational Mode Analysis. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1821-1837.	2.3	16
10519	C(sp ³)–H Amination Catalyzed by Ir(Me)-Porphyrin: A Computational Study. <i>Organometallics</i> , 2022, 41, 569-580.	1.1	4
10520	Gas-Phase Synthesis of Metal Olefins: Plasma-Assisted Methane Dehydrogenation and C–C Bond Formation. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1123-1131.	1.1	1
10521	Solvent effects on excited-state relaxation dynamics of paddle-wheel BODIPY-Hexaoxatriphenylene conjugates: Insights from non-adiabatic dynamics simulations. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 117-128.	0.6	0
10522	Design of new visible light Pt photocatalyst based on the TDDFT study of properties of transition metal complexes. <i>Applied Organometallic Chemistry</i> , 0, , .	1.7	0
10523	Assembling covalent organic framework membranes with superior ion exchange capacity. <i>Nature Communications</i> , 2022, 13, 1020.	5.8	79
10524	Formation of sulfur oxide groups by SO ₂ and their roles in mercury adsorption on carbon-based materials. <i>Journal of Environmental Sciences</i> , 2022, , .	3.2	1
10525	Machine Learning-Assisted High-Throughput Virtual Screening for On-Demand Customization of Advanced Energetic Materials. <i>Engineering</i> , 2022, 10, 99-109.	3.2	18

#	ARTICLE	IF	CITATIONS
10526	Three-Dimensional Convolutional Neural Networks Utilizing Molecular Topological Features for Accurate Atomization Energy Predictions. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2132-2143.	2.3	4
10527	Electronic structure exploration of the fluxional B ₄ subunit of B ₁₃ ⁺ tri-spoke wheel for understating its rotor action. <i>Materials Today: Proceedings</i> , 2022, , .	0.9	0
10528	Peri- <i>Acenoacene</i> for Solution Processed Distributed Feedback Laser: The Effect of 1,2-Oxaborine Doping. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	9
10529	Quantum Mechanical Investigation into the Adsorption Pattern of Clomipramine and Methotrimeprazine HCl with Graphene and Fullerene. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 2219-2232.	1.4	7
10530	Trihexyl tetradecyl phosphonium bromide as an effective catalyst/extractant in ultrasound-assisted extractive/oxidative desulfurization. <i>Environmental Science and Pollution Research</i> , 2022, 29, 49770-49783.	2.7	3
10531	Vibrational Spectroscopy, Quantum Computational and Molecular Docking Studies on 2-[(1H-Benzimidazol-1-yl)-methyl]benzoic Acid. <i>Crystals</i> , 2022, 12, 337.	1.0	4
10532	Heterogeneous Ti/PbO ₂ -electro-Fenton degradation of aromatic methane dyes using industrial pyrite waste slag as catalyst. <i>Environmental Science and Pollution Research</i> , 2022, 29, 50218-50236.	2.7	12
10533	Integrated Experimental and Computational Studies on the Organocatalytic Kinetic Resolution of <i>l</i> ² -Unfunctionalized Primary Alcohols Using a Chiral 1,2-Diamine: The Importance of Noncovalent Interactions. <i>Journal of Organic Chemistry</i> , 2022, 87, 4468-4475.	1.7	2
10534	Chain Walking as a Strategy for Iridium-Catalyzed Migratory Amidation of Alkenyl Alcohols to Access <i>l</i> -Amino Ketones. <i>Journal of the American Chemical Society</i> , 2022, 144, 4277-4285.	6.6	22
10535	Electronic Structure of Ru ₂ ⁶⁺ Complexes with Electron-Rich Anilinyridinate Ligands. <i>Inorganic Chemistry</i> , 2022, 61, 3443-3457.	1.9	2
10536	Structural Evolution and Bonding Properties of Cr ₂ Si _n (<i>n</i> = 1–12) Clusters: Mass-Selected Anion Photoelectron Spectroscopy and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1182-1193.	1.1	4
10537	Cooperative Activation of CO ₂ and Epoxide by a Heterobinuclear Al ⁺ Fe Complex via Radical Pair Mechanisms. <i>Journal of the American Chemical Society</i> , 2022, 144, 3210-3221.	6.6	36
10538	Multiple locations of boron atoms in the exohedral and endohedral C_{60} fullerene. <i>Physical Review A</i> , 2022, 105, .	1.0	7
10539	Spiral effect of helical carbon nanorods boosting electrocatalysis of oxygen reduction reaction. <i>Science China Materials</i> , 2022, 65, 1531-1538.	3.5	6
10540	Dynamics and mechanism of a light-driven chloride pump. <i>Science</i> , 2022, 375, 845-851.	6.0	43
10541	Computational Investigation of Chemisorption of Thiophosgene on Co@B ₈ . <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 267-272.	0.1	0
10542	Molecular docking/dynamic simulations, MEP, ADME-TOX-based analysis of xanthone derivatives as CHK1 inhibitors. <i>Structural Chemistry</i> , 2022, 33, 833-858.	1.0	4
10543	Design of a D- <i>A-A</i> framework with various auxiliary acceptors on optoelectronic and charge transfer properties for efficient dyes in DSSCs: A DFT/TD-DFT study. <i>Journal of Computational Electronics</i> , 2022, 21, 361-377.	1.3	1

#	ARTICLE	IF	CITATIONS
10544	Molecular Structure, Experimental and Theoretical Vibrational Spectroscopy, (HOMO-LUMO, NBO) Investigation, (RDG, AIM) Analysis, (MEP, NLO) Study and Molecular Docking of Ethyl-2-[[4-Ethyl-5-(Quinolin-8-yloxyMethyl)-4H-1,2,4-Triazol-3-yl] Sulfanyl} Acetate. Polycyclic Aromatic Compounds, 2023, 43, 2152-2176.	1.4	14
10545	Spectroscopic, Solvation Effects and MD Simulation of an Adamantane-Carbohydrazide Derivative, a Potential Antiviral Agent. Polycyclic Aromatic Compounds, 2023, 43, 2056-2070.	1.4	9
10546	Therapeutic potential of C2N as targeted drug delivery system for fluorouracil and nitrosourea to treat cancer: a theoretical study. Journal of Nanostructure in Chemistry, 2023, 13, 89-102.	5.3	16
10547	Investigation of interactions of doxorubicin with purine nucleobases by molecular modeling. Journal of Molecular Modeling, 2022, 28, 69.	0.8	0
10548	Optimized nonlinear optical (NLO) response of silicon carbide nanosheet by alkali metals doping: a DFT insight. European Physical Journal Plus, 2022, 137, 1.	1.2	23
10549	Multivariate Linear Regression Models to Predict Monomer Poisoning Effect in Ethylene/Polar Monomer Copolymerization Catalyzed by Late Transition Metals. Inorganics, 2022, 10, 26.	1.2	3
10550	Removal and Recovery of Gaseous Elemental Mercury Using a Cl-Doped Protonated Polypyrrole@MWCNTs Composite Membrane. Environmental Science & Technology, 2022, 56, 3689-3698.	4.6	23
10551	Thermally Activated Delayed Fluorescence Mechanism of a Bicyclic α -Carbene β -Metal β -Amide β -Copper Compound: DFT/MRCI Studies and Roles of Excited-State Structure Relaxation. Inorganic Chemistry, 2022, 61, 7673-7681.	1.9	13
10552	Construction of Confined Bifunctional 2D Material for Efficient Sulfur Resource Recovery and Hg ²⁺ Adsorption in Desulfurization. Environmental Science & Technology, 2022, 56, 4531-4541.	4.6	13
10553	Phlegmacaritones A and B, a Pair of Serratane-Related Triterpenoid Epimers with an Unprecedented Carbon Skeleton from <i>Phlegmariusus carinatus</i> . Journal of Natural Products, 2022, 85, 899-909.	1.5	6
10554	Effect of Additives on Preferential Crystallization for the Chiral Resolution of Citrulline: Experimental, Statistical, and Molecular Dynamics Simulation Studies. Crystal Growth and Design, 2022, 22, 2392-2406.	1.4	11
10555	A Water-Stable Lanthanide-Based MOF as a Highly Sensitive Sensor for the Selective Detection of Paraquat in Agricultural Products. ACS Sustainable Chemistry and Engineering, 2022, 10, 2761-2771.	3.2	40
10556	Spatial and Electronic Structures of BeB ₈ and MgB ₈ : How far Does the Analogy Go?. ChemPhysChem, 2022, , .	1.0	2
10557	Gallic acid enhanced bisphenol A degradation through Fe ³⁺ /peroxymonosulfate process. Water Science and Technology: Water Supply, 2022, 22, 4852-4863.	1.0	3
10558	Covalent organic framework wrapped by graphene oxide as an efficient sulfur host for high performance lithium β -sulfur batteries. Nanotechnology, 2022, 33, 225402.	1.3	7
10559	Synthesis of a Novel and More Sustainable Cationic Bleach Activator, α -[4-(α -Triethylammoniumchloride-butanoyl)] Butyrolactam, for Cotton: Optimization and Theoretical Limitations. ACS Sustainable Chemistry and Engineering, 2022, 10, 4415-4424.	3.2	1
10560	Cyclohexanone-Based Chalcones as Alternatives for Fuel Additives. ACS Omega, 2022, 7, 11871-11886.	1.6	6
10561	Controllable synthesis of Co β -Al layered double hydroxides with different anionic intercalation layers for the efficient removal of methyl orange. Environmental Technology (United Kingdom), 2023, 44, 3004-3017.	1.2	2

#	ARTICLE	IF	CITATIONS
10562	Excited State Dynamics of Methylated Guanosine Derivatives Revealed by Femtosecond Time-resolved Spectroscopy. <i>Photochemistry and Photobiology</i> , 2022, 98, 1008-1016.	1.3	2
10563	Nonfused Ring Electron Acceptors for Efficient Organic Solar Cells Enabled by Multiple Intramolecular Conformational Locks. <i>ACS Applied Energy Materials</i> , 2022, 5, 5136-5145.	2.5	16
10564	Diaryliodonium Tetracyanidometallates Self-Assemble into Halogen-Bonded Square-Like Arrays. <i>Crystal Growth and Design</i> , 2022, 22, 2749-2758.	1.4	5
10565	Halogen-Free Electrolytes Based on Modified Boranes for Alkali-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5112-5121.	1.5	2
10566	Rational Design of Caprolactam-Based Deep Eutectic Solvents for Extractive Desulfurization of Diesel Fuel and Mechanism Study. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 4551-4560.	3.2	18
10567	A Novel Strategy toward Thermally Activated Delayed Fluorescence from a Locally Excited State. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2653-2660.	2.1	25
10568	Direct α -difluoroalkenylation of $X-H$ Bonds with Trifluoromethyl Ketone α -triflylhydrazones for Synthesis of Tetrasubstituted Heteroatomic α -difluoroalkenes. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	11
10569	Syntheses of three-dimensional catenanes under kinetic control. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2118573119.	3.3	12
10570	Thermodynamic properties, decomposition kinetics of 2-(5-amino-2H-tetrazol-1-yl)-4-amine-3,5-dinitropyridine. <i>Journal of Molecular Modeling</i> , 2022, 28, 79.	0.8	5
10571	Designing Self-Adaptive Donor-Switch-Acceptor Systems for Molecular Optoelectronic Conversion Based on Dimethyldihydropyrene/Cyclophanediene. <i>Chemistry - an Asian Journal</i> , 2022, , .	1.7	0
10572	Formulating noncovalent interactions to predict structural transition in mixed guest hydrates. <i>AIChE Journal</i> , 2022, 68, .	1.8	3
10573	Reversible and Efficient Absorption of SO_2 with Natural Amino Acid Aqueous Solutions: Performance and Mechanism. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 4451-4461.	3.2	12
10574	Synthesis, theoretical and experimental spectroscopic properties, molecular docking, ADMET, and RDC analysis of copper(II) complex of dichloro(1,10-phenanthroline)(1,2,4-triazole-3-carboxylic acid). <i>Chemical Papers</i> , 2022, 76, 4099-4114.	1.0	1
10575	Mechanisms of Strain-Induced Interfacial Strengthening of Wet-Spun Filaments. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 16809-16819.	4.0	5
10576	Manipulating the Intermolecular Interactions through Side Chain Engineering and Unilateral π - π Bridge Strategy for Efficient Small Molecular Photovoltaic Acceptor. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	35
10577	DFT Study of bis(1,10-phenanthroline)copper complexes: Molecular and electronic structure, redox and spectroscopic properties and application to Solar Cells. <i>Electrochimica Acta</i> , 2022, 418, 140276.	2.6	11
10578	In situ photodeposition of platinum clusters on a covalent organic framework for photocatalytic hydrogen production. <i>Nature Communications</i> , 2022, 13, 1355.	5.8	140
10579	Hetero-octanuclear Au_4Ag_4 Cluster Complexes of 4,5-Diethynylacridin-9-One with Luminescent Mechanochromism. <i>Molecules</i> , 2022, 27, 2127.	1.7	2

#	ARTICLE	IF	CITATIONS
10580	Photophysical and Electrochemical Properties of Push-Pull Oligo(ferrocenyl-phenyleneethynylene)s: Supramolecular Orders in Molecular Films. <i>Langmuir</i> , 2022, 38, 4077-4089.	1.6	1
10581	Electron-Deficient Contorted Polycyclic Aromatic Hydrocarbon via One-Pot Annulative π -Extension of Perylene Diimide. <i>Organic Letters</i> , 2022, 24, 2414-2419.	2.4	8
10582	Selective Nucleation of Polymorphs Induced by Multiple Conformations and Self-Association. <i>Crystal Growth and Design</i> , 2022, 22, 2499-2511.	1.4	7
10583	Noncovalent Interaction- and Steric Effect-Controlled Regiodivergent Selectivity in Dimeric Manganese-Catalyzed Hydroarylation of Internal Alkynes: A Computational Study. <i>Journal of Organic Chemistry</i> , 2022, 87, 4215-4225.	1.7	4
10584	Deep-Red-Emissive Flexible Optical Waveguide with High Elastic Performance Based on an Organic Crystal. <i>ChemPhotoChem</i> , 2022, 6, .	1.5	3
10585	Effects of π -conjugation on the charge-transport properties of hole-transporting materials featuring diphenylamine-quinacridone for perovskite solar cells: A theoretical study. <i>Bulletin of the Korean Chemical Society</i> , 0, , .	1.0	1
10586	Synthesis, solvatochromism and DFT study of pyridine substituted benzanthrone with ICT characteristics. <i>Journal of Molecular Structure</i> , 2022, 1262, 132971.	1.8	7
10587	Chaotropic Effect Stabilized Radical-Containing Supramolecular Organic Frameworks for Photothermal Therapy. <i>Small</i> , 2022, 18, e2108055.	5.2	7
10588	Mobile Phone Flashlight-Excited Red Afterglow Bioimaging. <i>Advanced Materials</i> , 2022, 34, e2201280.	11.1	79
10589	Solid-State Assembly by Chelating Chalcogen Bonding in Quinodimethane Tetraesters Fused with a Chalcogenadiazole. <i>ChemPlusChem</i> , 2022, 87, e202200075.	1.3	4
10590	Resonance signatures in DCS and spin polarization for positron scattering with C_{60} and rare gas endohedrals. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2022, 55, 065201.	0.6	1
10591	Role of functionalized graphene quantum dots in hydrogen evolution reaction: A density functional theory study. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 41748-41758.	3.8	12
10592	Precise recognition of palladium through interlaminar chelation in a covalent organic framework. <i>CheM</i> , 2022, 8, 1442-1459.	5.8	53
10593	Theoretical study on Nitride pentazolate high-energy-density materials: Toward excellent energetic performance and good stability. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, .	0.9	3
10594	Dismantlement of ammonia upon interaction with Be_n ($n < 10$) clusters. <i>Journal of Computational Chemistry</i> , 2023, 44, 159-167.	1.5	3
10595	Crystal Structure, Topology, DFT and Hirshfeld Surface Analysis of a Novel Charge Transfer Complex (L3) of Anthraquinone and 4-[(anthracen-9-yl)methyl] amino-benzoic Acid (L2) Exhibiting Photocatalytic Properties: An Experimental and Theoretical Approach. <i>Molecules</i> , 2022, 27, 1724.	1.7	22
10596	Adenosine Triphosphate Disodium Modified Hole Transport Layer for Efficient Inverted Perovskite Solar Cells. <i>ChemNanoMat</i> , 2022, 8, .	1.5	2
10597	The role of hydrogen-bond in solubilizing drugs by ionic liquids: A molecular dynamics and density functional theory study. <i>AIChE Journal</i> , 2022, 68, .	1.8	14

#	ARTICLE	IF	CITATIONS
10599	Synthesis and Theoretical Study of New Guanlylated Cyclophosphazenes and Their Use in the CO ₂ Fixation into Styrene Carbonate. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2022, 32, 1724-1735.	1.9	1
10600	Towards a comprehensive optimization of dielectric and viscoelastic performance of poly(ethylene-co-methyl acrylate) through chain sequence regulation. <i>Polymer</i> , 2022, 243, 124657.	1.8	2
10601	The sensing mechanism of fluorescent probe for PhSH and the process of ESIPT. <i>Photochemical and Photobiological Sciences</i> , 2022, , 1.	1.6	5
10602	Molecular Structure Analysis and Mercury Adsorption Mechanism of Iron-Based Modified Biochar. <i>Energy & Fuels</i> , 2022, 36, 3184-3200.	2.5	15
10603	Soluble and Perfluorinated Polyelectrolyte for Safe and High-Performance Li ⁺ O ₂ Batteries. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	4
10604	A Water-Soluble Highly Oxidizing Cobalt Molecular Catalyst Designed for Bioinspired Water Oxidation. <i>Angewandte Chemie</i> , 0, , .	1.6	0
10605	Evidence for Participation of 4f and 5d Orbitals in Lanthanide Metal-Ligand Bonding and That Y(III) Has Less of This Complex-Stabilizing Ability. A Thermodynamic, Spectroscopic, and DFT Study of Their Complexation by the Nitrogen Donor Ligand TPEN. <i>Inorganic Chemistry</i> , 2022, 61, 4627-4638.	1.9	11
10606	Cross-Linked Polyphosphazene Nanospheres Boosting Long-Lived Organic Room-Temperature Phosphorescence. <i>Journal of the American Chemical Society</i> , 2022, 144, 6107-6117.	6.6	105
10607	Carbon Material With Ordered Sub-Nanometer Hole Defects. <i>Frontiers in Chemistry</i> , 2022, 10, 858154.	1.8	0
10608	Directional Doping and CocrySTALLizing an Open-Shell Ag ₃₉ Superatom <i>via</i> Precursor Engineering. <i>ACS Nano</i> , 2022, 16, 5507-5514.	7.3	24
10609	Metal-ligand bonding in bispidine chelate complexes for radiopharmaceutical applications. <i>Structural Chemistry</i> , 2023, 34, 5-15.	1.0	3
10610	All-hydrocarbon, all-conjugated cycloparaphenylene-polycyclic aromatic hydrocarbon host-guest complexes stabilized by CH ⁺ ⋯π interactions. <i>Nano Research</i> , 2022, 15, 5545-5555.	5.8	11
10611	Study on Spectral Method and Computational Simulation of Chlorinated Bisphenol Compound and Thyroxine-Binding Globulin. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0
10612	Internal dynamics of methyl <i>p</i> -tolyl sulfoxide in the gas phase: Rotational spectroscopy and theoretical studies. <i>Journal of Chemical Physics</i> , 2022, 156, 154304.	1.2	1
10613	Pattern of covalent and non-covalent interactions within the pentaiodide anion in the structure of (3 ⁺ HOOC ₅ H ₉ NH ₂) ₅ . <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 0, , .	0.6	3
10614	Phenylene-Bridged Perylene Monoimides as Acceptors for Organic Solar Cells: A Study on the Structure-Property Relationship. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	5
10615	Vibrational Characterization and Molecular Electronic Investigations of 2-acetyl-5-methylfuran using FT-IR, FT-Raman, UV-VIS, NMR, and DFT Methods. <i>Journal of Fluorescence</i> , 2022, 32, 1005-1017.	1.3	26
10616	Through-Space Conjugated Electron Transport Materials for Improving Efficiency and Lifetime of Organic Light-Emitting Diodes. <i>Advanced Science</i> , 2022, 9, e2200374.	5.6	27

#	ARTICLE	IF	CITATIONS
10617	Simultaneously enhanced efficiency of eco-friendly structural characterization of the dithienocyclopentacarbazole donor based acceptors with narrow bandgap for high-performance organic solar cells. <i>Journal Physics D: Applied Physics</i> , 2022, 55, 235501.	1.3	26
10618	Geometries, electronic structures, and bonding properties of endohedral Group 14 Zintl clusters $\text{TM}@E_{10}$ ($\text{TM} = \text{Fe, Co, Ni}$; $E = \text{Ge, Sn, Pb}$). <i>Journal of Computational Chemistry</i> , 2022, 43, 828-838.	1.5	3
10619	Molecular simulation study on the protective mechanism of three kinds of HTPB propellant antioxidants. <i>FirePhysChem</i> , 2022, 2, 4-13.	1.5	5
10620	The conformational landscape of myrtenol: The structure of the hydroxymethyl group and its robustness upon hydration. <i>Journal of Chemical Physics</i> , 2022, 156, 124301.	1.2	3
10621	Theoretical study of germanium nanoclusters: significance of surface passivation. <i>European Physical Journal Plus</i> , 2022, 137, 1.	1.2	0
10622	Small symmetry-breaking triggering large chiroptical responses of Ag_7O nanoclusters. <i>Nature Communications</i> , 2022, 13, 1177.	5.8	31
10623	A heat-resistant and insensitive energetic material based on the pyrazolo-triazine framework. <i>Energetic Materials Frontiers</i> , 2022, 3, 26-31.	1.3	14
10624	Novel Thienyl DPP derivatives Functionalized with Terminal Electron-Acceptor Groups: Synthesis, Optical Properties and OFET Performance. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	15
10625	Resonance-Induced Stimuli-Responsive Capacity Modulation of Organic Ultralong Room Temperature Phosphorescence. <i>Journal of the American Chemical Society</i> , 2022, 144, 6946-6953.	6.6	68
10626	Solvent Coadsorption Effect on $\text{I}^{\cdot\cdot}\text{O}$ Halogen-Bonded 2D Self-Assembled Nanostructures. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5777-5783.	1.5	11
10627	Dimensionality Modulates Electrical Conductivity in Compositionally Constant One-, Two-, and Three-Dimensional Frameworks. <i>Journal of the American Chemical Society</i> , 2022, 144, 5583-5593.	6.6	24
10628	Design, Synthesis, and Biological Evaluation of Tetrahydro- β -carbolines as Akt1 Inhibitors That Inhibit Colorectal Cancer Cell Proliferation. <i>ChemMedChem</i> , 2022, 17, .	1.6	2
10629	Enantiomeric Water-Soluble Octopus[3]arenes for Highly Enantioselective Recognition of Chiral Ammonium Salts in Water. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	4
10630	A descriptor for the structural stability of organic-inorganic hybrid perovskites based on binding mechanism in electronic structure. <i>Journal of Molecular Modeling</i> , 2022, 28, 80.	0.8	8
10631	Ab initio study of hydrated cesium iodide dimer $(\text{CsI})_2 \cdot n\text{H}_2\text{O}$ and the cation size effect on $(\text{MI})_2 \cdot n\text{H}_2\text{O}$ ($M = \text{Li, Na, K, Cs}$). <i>Journal of Molecular Modeling</i> , 2022, 28, 95.	0.8	1
10632	Computational Exploration on the Structural and Optical Properties of Gold-Doped Alkaline-Earth Magnesium AuMgn ($n = 2-12$) Nanoclusters: DFT Study. <i>Frontiers in Chemistry</i> , 2022, 10, 870985.	1.8	6
10633	Synthesis of Ideal Energetic Materials with High Density and Performance Based on 5-Aminotetrazole. <i>Crystal Growth and Design</i> , 2022, 22, 2594-2601.	1.4	19
10634	Microscopic Study of Molecular Double Doping. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2075-2081.	1.1	6

#	ARTICLE	IF	CITATIONS
10635	Computational Evaluation and Design of Polyethylene Zirconocene Catalysts with Noncovalent Dispersion Interactions. <i>Organometallics</i> , 2022, 41, 581-593.	1.1	4
10636	Hydrogen Generation from Water Splitting by $3\text{H}_2\text{O} + \text{Pd}_{13} \rightarrow 3\text{H}_2 + \text{Pd}_{13}\text{O}_3$ Reaction. <i>Particle and Particle Systems Characterization</i> , 0, , 2200010.	1.2	1
10637	Intermolecular Vibration Energy Transfer Process in Two CL-20-Based Cocrystals Theoretically Revealed by Two-Dimensional Infrared Spectra. <i>Molecules</i> , 2022, 27, 2153.	1.7	2
10638	The Nitrogen Bond, or the Nitrogen-Centered Pnictogen Bond: The Covalently Bound Nitrogen Atom in Molecular Entities and Crystals as a Pnictogen Bond Donor. <i>Compounds</i> , 2022, 2, 80-110.	1.0	20
10639	$\langle \text{sc} \rangle \text{CSiGaAl}_2 \langle / \text{sc} \rangle \langle \text{sup} \rangle \hat{\sim} / \langle / \text{sup} \rangle$ and $\langle \text{sc} \rangle \text{CGeGaAl}_2 \langle / \text{sc} \rangle \langle \text{sup} \rangle \hat{\sim} / \langle / \text{sup} \rangle$ having planar tetracoordinate carbon atoms in their global minimum energy structures. <i>Journal of Computational Chemistry</i> , 2022, 43, 894-905.	1.5	14
10640	Structure-property relationships in para-substituted nitrobenzofurazans: electrochemical, optical, and theoretical analysis. <i>Chemical Papers</i> , 2022, 76, 4059-4080.	1.0	7
10641	Effective Therapy of Drug-Resistant Bacterial Infection by Killing Planktonic Bacteria and Destructing Biofilms with Cationic Photosensitizer Based on Phosphindole Oxide. <i>Small</i> , 2022, 18, e2200743.	5.2	27
10642	On-surface synthesis of triangulene trimers via dehydration reaction. <i>Nature Communications</i> , 2022, 13, 1705.	5.8	30
10643	Free and open source software for computational chemistry education. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, .	6.2	19
10644	Insights into catalytic behavior of TiMgn ($n=1-12$) nanoclusters in hydrogen storage and dissociation process: A DFT investigation. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 13418-13429.	3.8	15
10645	Zafirlukast inhibits the growth of lung adenocarcinoma via inhibiting TMEM16A channel activity. <i>Journal of Biological Chemistry</i> , 2022, 298, 101731.	1.6	14
10646	The ethanol-metal interaction in bimetallic clusters of Pt and Rh. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1.	0.5	2
10647	σ -Hole and LP-Hole Interactions of Pnictogen- $\hat{\sim}$ -Pnictogen Homodimers under the External Electric Field Effect: A Quantum Mechanical Study. <i>ACS Omega</i> , 2022, 7, 11264-11275.	1.6	2
10648	Interaction of Anagrelide drug molecule on pristine and doped boron nitride nanocages: a DFT, RDG, PCM and QTAIM investigation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 3413-3429.	2.0	8
10649	Full-nitro-nitroamino cooperative action: Climbing the energy peak of benzenes with enhanced chemical stability. <i>Science Advances</i> , 2022, 8, eabn3176.	4.7	41
10650	Ab Initio Study of Two-Dimensional Cross-Shaped Non-Fullerene Acceptors for Efficient Organic Solar Cells. <i>ACS Omega</i> , 2022, 7, 10638-10648.	1.6	30
10651	Autoxidation of 4-Hydrazinylquinolin-2(1H)-one; Synthesis of Pyridazino[4,3-c:5,6-c ²]diquinoline-6,7(5H,8H)-diones. <i>Molecules</i> , 2022, 27, 2125.	1.7	0
10652	Theoretical study on the interaction of flutamide anticancer drug with cucurbit[5]uril. <i>J. ETQq1</i> 1 0.784314 rgBT/Overlock 10	1.0	4

#	ARTICLE	IF	CITATIONS
10653	Evaluation of inhibitive corrosion potential of symmetrical hydrazine derivatives containing nitrophenyl moiety in 1M HCl for C38 steel: experimental and theoretical studies. <i>Heliyon</i> , 2022, 8, e09087.	1.4	7
10654	Theoretical insights into the effects of RE doping on the structural, electronic, and optical properties of magnesium clusters. <i>AIP Advances</i> , 2022, 12, .	0.6	2
10655	Model of B9N9 Response under External Electric Field: Geometry, Electronic Properties, Reaction Activity. <i>Molecules</i> , 2022, 27, 1714.	1.7	7
10656	Deep oxidative desulfurization via rGO-immobilized tin oxide nanocatalyst: Experimental and theoretical perspectives. <i>Advanced Powder Technology</i> , 2022, 33, 103499.	2.0	8
10657	Azaboratrane as an exceptionally potential organocatalyst for the activation of CO ₂ and coupling with epoxide. <i>Molecular Catalysis</i> , 2022, 521, 112201.	1.0	9
10658	Computational Insights into the Multisite Nature of the Phillips CrO _x /SiO ₂ Catalyst for Ethylene Polymerization: The Perspective of Chromasiloxane Ring Size and F Modification. <i>ACS Catalysis</i> , 2022, 12, 3589-3603.	5.5	5
10659	1,4-Phenylene-Incorporated Decaphyrin(1.0.1.0.0.1.0.1.0.0): Synthesis, Structure, and Topological Chirality. <i>Organic Letters</i> , 2022, 24, 2509-2514.	2.4	12
10660	Coveâ€Edged Hexaâ€i>peri</i>â€hexabenoâ€bisâ€i>peri</i>â€octacene: Molecular Conformations and Amplified Spontaneous Emission. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	8
10661	Coveâ€Edged Hexaâ€i>peri</i>â€hexabenoâ€bisâ€i>peri</i>â€octacene: Molecular Conformations and Amplified Spontaneous Emission. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	22
10662	Lowâ€Valent Zirconoceneâ€Mediated Synthesis of Porphyrin(2.1.2.1)s and Its Extension to Synthesis of a Porphyrin(2.1.2.1) Nanobarrel. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	2
10663	Enantiomeric Waterâ€Soluble Octopus[3]arenes for Highly Enantioselective Recognition of Chiral Ammonium Salts in Water. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	32
10664	Exploration of the Intriguing Photovoltaic Behavior for Fused Indacenodithiophene-Based Aâ€Dâ€A Conjugated Systems: A DFT Model Study. <i>ACS Omega</i> , 2022, 7, 11606-11617.	1.6	38
10665	Experimental and theoretical investigation on the thermal isomerization reaction of triazolotriazines. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	1
10666	Mechanistic Investigations of the Synthesis of Lactic Acid from Glycerol Catalyzed by an Iridiumâ€NHC Complex. <i>Processes</i> , 2022, 10, 626.	1.3	4
10667	Thermodynamic and molecular insights into natural gas dehydration using choline chlorideâ€based deep eutectic solvents. <i>AIChE Journal</i> , 2022, 68, .	1.8	22
10668	Development of Strong Visibleâ€Lightâ€Absorbing Cyclometalated Iridium(III) Complexes for Robust and Efficient Lightâ€Driven Hydrogen Production. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	16
10669	Super-Exchange Charge Transfer in One-Photon and Two-Photon Absorption of Multibranched Compounds. <i>ACS Omega</i> , 2022, 7, 9743-9753.	1.6	1
10670	Electronic Structure, Solvation Effects and Wave Function Based Properties of a New Triazole Based Symmetric Chromene Derivative of Apigenin. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 2810-2822.	1.4	1

#	ARTICLE	IF	CITATIONS
10671	Antimicrobial activities of two 1 λ^5 , 2 λ^5 , and 3 λ^5 mononuclear Mn (II) and dinuclear Bi (III) complexes: X-ray structures, spectroscopic, electrostatic potential, Hirshfeld surface analysis, and time-dependent/density functional theory studies. Applied Organometallic Chemistry, 2022, 36, .	1.7	12
10672	Double pentavalent pnictogen-bonding interactions in the homodimers of pnictogenoxide species: CSD search and theoretical study. Computational and Theoretical Chemistry, 2022, 1209, 113636.	1.1	4
10673	Study on geometry and chemical activity of twisted cucurbit[13]uril based on density functional theory. Chemical Papers, 0, , 1.	1.0	0
10674	<i>N,N</i> -dimethylformamide tailors solvent effect to boost Zn anode reversibility in aqueous electrolyte. National Science Review, 2022, 9, .	4.6	53
10675	Substituent Effects of Structures and Bonds of Noble Gas Compounds R ₂ (Rg = Ar, Kr, Xe, and) Tj ETQq0,0 0 rgBT/Overlock	0.1	0
10676	Ionic Rigid Organic Dual-State Emission Compound With Rod-Shaped and Conjugated Structure for Sensitive Al ³⁺ Detection. Frontiers in Chemistry, 2022, 10, 807088.	1.8	7
10677	The quasi-activity coefficients of non-electrolytes in aqueous solution with organic ions and its application on the phase splitting behaviors prediction for CO ₂ absorption. Chinese Journal of Chemical Engineering, 2022, 43, 316-323.	1.7	6
10678	Type IV Halogen-Halogen Interactions: A Comparative Theoretical Study in Halobenzene-Halobenzene Homodimers. International Journal of Molecular Sciences, 2022, 23, 3114.	1.8	21
10679	On the Origins of Stereo- and Regio-Selectivities in the Formation of Fullerene-Fluorene Dyads. Journal of Organic Chemistry, 2022, 87, 4702-4711.	1.7	2
10680	Online Orbital Explorer and BingOrbital Game for Inquiry-Based Activities. Journal of Chemical Education, 2022, 99, 2135-2142.	1.1	5
10681	Investigation on the Lithium Extraction Process with the TBP-FeCl ₃ Solvent System Using Experimental and DFT Methods. Industrial & Engineering Chemistry Research, 2022, 61, 4672-4682.	1.8	18
10682	Extending the Range of Nitrofurantoin Solid Forms: Effect of Molecular and Crystal Structure on Formation Thermodynamics and Physicochemical Properties. Crystal Growth and Design, 2022, 22, 2569-2586.	1.4	12
10683	Halogen Bonds Exist between Noncovalent Ligands and Natural Nucleic Acids. Journal of Medicinal Chemistry, 2022, 65, 4424-4435.	2.9	11
10684	Unique Solvated Electron State and Its Remarkable Enhancement Effect on Internuclear <i>J</i> -Couplings in Fluorocarbon Cage Electron Clathrates. Journal of Physical Chemistry C, 2022, 126, 4965-4974.	1.5	3
10685	PtCu@Ir-PCN-222: Synergistic Catalysis of Bimetallic PtCu Nanowires in Hydrosilane-Concentrated Interspaces of an Iridium(III)-Porphyrin-Based Metal-Organic Framework. ACS Catalysis, 2022, 12, 3604-3614.	5.5	22
10686	Theoretical Probing of Size-Selective Crown Ether Macrocyclic Ligands for Transplutonium Element Separation. Inorganic Chemistry, 2022, 61, 4404-4413.	1.9	15
10687	Light-Induced EPR Study of Polymorphic Acene-Stipulated Transition in P3DDT:PC ₆₁ BM Composite. Journal of Physical Chemistry C, 2022, 126, 4495-4507.	1.5	0
10688	Characterization of Type I and II Interactions between Halogen Atoms. Crystal Growth and Design, 2022, 22, 2692-2702.	1.4	16

#	ARTICLE	IF	CITATIONS
10689	A Water-Soluble Highly Oxidizing Cobalt Molecular Catalyst Designed for Bioinspired Water Oxidation. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	13
10690	Low-cost hydrocarbon membrane enables commercial-scale flow batteries for long-duration energy storage. <i>Joule</i> , 2022, 6, 884-905.	11.7	53
10691	Chalcogen Bond versus Halogen Bond: Changing Contributions in Determining the Crystal Packing of Dihalobenzochalcogenadiazoles. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 522-531.	2.0	12
10692	Low-Valent Zirconocene-Mediated Synthesis of Porphyrin(2.1.2.1)s and Its Extension to Synthesis of a Porphyrin(2.1.2.1) Nanobarrel. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	11
10693	Physical Cross-Linkage Constructed Supramolecular Conductive Hydrogel as Sustainable and Remolded Epidermal Electronics. <i>ACS Applied Polymer Materials</i> , 2022, 4, 2585-2594.	2.0	6
10694	Effect of hydrogen bonds and CF ₃ group on the regioselectivity and mechanism of [3+2] cycloaddition reactions between nitrile oxide and 2,4-disubstituted cyclopentenes. A MEDT study. <i>Journal of Molecular Modeling</i> , 2022, 28, 104.	0.8	4
10695	Soluble and Perfluorinated Polyelectrolyte for Safe and High-Performance Li ⁺ O ₂ Batteries. <i>Angewandte Chemie - International Edition</i> , 2022, 61, e202116635.	7.2	28
10696	Transformation mechanism of carbamic acid elimination and hydrolysis reaction in microbial self-healing concrete. <i>Molecular Simulation</i> , 2022, 48, 719-735.	0.9	5
10697	Discovery, Topo I inhibitory activity and mechanism evaluation of two novel cytosine-type alkaloid dimers from the seeds of <i>Sophora alopecuroides</i> L. <i>Bioorganic and Medicinal Chemistry</i> , 2022, 61, 116723.	1.4	1
10698	Crystal Structure Characterization, Hirshfeld Surface Analysis, and Non-covalent Interactions of 2,5-Bis(4-chlorophenyl)-1,3,4-Oxadiazole. <i>Journal of Chemical Crystallography</i> , 2022, 52, 324-336.	0.5	1
10699	Halogen Bonding and CO-Ligand Blue-Shift in Hybrid Organic-Organometallic Cocrystals [CpFe(CO)2X] (C2I4) (X = Cl, Br). <i>Crystals</i> , 2022, 12, 412.	1.0	1
10700	High-Stability Light-Element Magnetic Superatoms Determined by Hund's Rule. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2632-2637.	2.1	4
10701	Efficient Construction of Elastic and Ion Response Red Fluorophores with Crystallization-Induced Enhanced Emission and Large Stokes Shifts. <i>Crystal Growth and Design</i> , 2022, 22, 3198-3205.	1.4	9
10702	The Tail Wags the Dog: The Far Periphery of the Coordination Environment Manipulates the Photophysical Properties of Heteroleptic Cu(I) Complexes. <i>Molecules</i> , 2022, 27, 2250.	1.7	1
10703	The Role of Hydrogen Bonds in Interactions between [PdCl ₄] ²⁻ Dianions in Crystal. <i>Molecules</i> , 2022, 27, 2144.	1.7	4
10704	Theoretical study of the substituent effect on the C-H insertion reaction of copper carbenoids. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1.	0.5	1
10705	Efficient gaseous iodine capture enhanced by charge-induced effect of covalent organic frameworks with dense tertiary-amine nodes. <i>Chinese Chemical Letters</i> , 2022, 33, 3556-3560.	4.8	17
10706	Insights Into the Properties of Amygdalin Solvatomorphs: X-ray Structures, Intermolecular Interactions, and Transformations. <i>ACS Omega</i> , 2022, 7, 8906-8918.	1.6	3

#	ARTICLE	IF	CITATIONS
10707	Carboxylate-Assisted Carboxylation of Thiophene with CO ₂ in the Solvent-Free Carbonate Medium. <i>Catalysts</i> , 2022, 12, 369.	1.6	1
10708	Spectroscopic and topological analysis and in vitro antimicrobial activity of phenothiazine. <i>Spectroscopy Letters</i> , 2022, 55, 212-228.	0.5	1
10709	Design of a gold clustering site in an engineered apo-ferritin cage. <i>Communications Chemistry</i> , 2022, 5, .	2.0	5
10710	Pyrazolon-dithiocarbonic acid and dibromoalcanes " cyclic keto-dithioacetals formation vs. open chain products: A theoretical study. <i>Molecular Physics</i> , 2022, 120, .	0.8	1
10711	Cocrystals of Praziquantel with Phenolic Acids: Discovery, Characterization, and Evaluation. <i>Molecules</i> , 2022, 27, 2022.	1.7	7
10712	Imidazolium bromide: A tri-functional additive for rechargeable Li-O ₂ batteries. <i>Energy Storage Materials</i> , 2022, 49, 401-408.	9.5	8
10713	Targeting Individual Tautomers in Equilibrium by Resonant Inelastic X-ray Scattering. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2459-2466.	2.1	4
10714	Sodium Ions Affect Pyrroline Formation in the Maillard Reaction With Lys-Containing Dipeptides and Tripeptides. <i>Frontiers in Nutrition</i> , 2022, 9, 874650.	1.6	4
10715	Interplay of Steric Effects and Aromaticity Reversals to Expand the Structural/Electronic Responses of Dihydrophenazines. <i>Journal of the American Chemical Society</i> , 2022, 144, 4883-4896.	6.6	17
10716	Computational assessment of nitrogen-enriched, stable and insensitive tris(1,2,4,5-tetrazin-3-yl)amine building block for energetic applications. <i>Energetic Materials Frontiers</i> , 2022, 3, 47-52.	1.3	5
10717	The Fluorine-Rich Electrolyte as an Interface Modifier to Stabilize Lithium Metal Battery at Ultra-Low Temperature. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	38
10718	Three Rings Schiff Base Ester Liquid Crystals: Experimental and Computational Approaches of Mesogenic Core Orientation Effect, Heterocycle Impact. <i>Molecules</i> , 2022, 27, 2304.	1.7	5
10719	Purification of biflavonoids from <i>Selaginella derleinii</i> Hieron by special covalent organic polymers material. <i>Journal of Chromatography A</i> , 2022, 1668, 462920.	1.8	2
10720	High Fe utilization efficiency and low toxicity of Fe ₃ C@Fe ₀ loaded biochar for removing of tetracycline hydrochloride in wastewater. <i>Journal of Cleaner Production</i> , 2022, 353, 131630.	4.6	18
10721	Deep purification of copper from Cu(II)-EDTA acidic wastewater by Fe(III) replacement/diethyldithiocarbamate precipitation. <i>Chemosphere</i> , 2022, 300, 134546.	4.2	10
10722	Tailoring the D electron-withdrawing core as hole transport materials towards boosting the transport performance of perovskite solar cells. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	0
10723	Chalcogen Bonding with Diaryl Ditellurides: Evidence from Solid State and Solution Studies.. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	9
10724	The synergetic and multifaceted nature of carbon-carbon rotation reveals the origin of conformational barrier heights with bulky alkane groups. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	3

#	ARTICLE	IF	CITATIONS
10725	Investigation the effect of π -bridge and side chain on photovoltaic properties of benzodithiophene and quinoxaline based conjugated polymers. <i>European Polymer Journal</i> , 2022, 169, 111141.	2.6	6
10726	Boron Oxide B ₅ O ₆ ⁺ Cluster as a Boronyl-Based Inorganic Analog of Phenolate Anion. <i>Frontiers in Chemistry</i> , 2022, 10, 868782.	1.8	1
10727	Effects of auxiliary electron-withdrawing moieties on the photovoltaic properties of D- π -A TM - π -A phosphonic acid-based DSSCs. <i>Computational and Theoretical Chemistry</i> , 2022, 1210, 113645.	1.1	6
10728	Multicomponent Quantum Mechanics/Molecular Mechanics Study of Hydrated Positronium. <i>Journal of Physical Chemistry B</i> , 2022, , .	1.2	0
10729	Theoretical Unravelling the Complexation and Separation of Uranyl ^{VI} Ligand Complexes towards Chiral R/S π -Profenofos. <i>Applied Organometallic Chemistry</i> , 0, , .	1.7	5
10730	DFT-based study on the molecular interaction of hydrochloric acid with different extractants. <i>Journal of Molecular Liquids</i> , 2022, 357, 119108.	2.3	3
10731	Roads Not Taken: Mechanism and Origins of Regio- and Chemoselectivity of Directed Co ^{III} -Catalyzed Alkenylation of <i>N</i> -Pyridyl 2-Pyridone. <i>Organometallics</i> , 2022, 41, 937-947.	1.1	2
10732	Overlooked Effects of La-4f Orbitals in Endohedral Metallofullerenes. <i>Inorganic Chemistry</i> , 2022, 61, 5891-5902.	1.9	6
10733	Hofmann-MOF derived nanoball assembled by FeNi alloy confined in carbon nanotubes as a magnetic catalyst for activating peroxydisulfate to degrade an ionic liquid. <i>Separation and Purification Technology</i> , 2022, 295, 120945.	3.9	19
10734	Additive Engineering in Antisolvent for Widening the Processing Window and Promoting Perovskite Seed Formation in Perovskite Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 17348-17357.	4.0	9
10735	Green Phosphorescent Zn(II) Halide Complexes with <i>N,N,N',N'</i> -tetramethyl π -indolylphosphonic Diamide as Ligand. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.2	12
10736	Inclusive DFT insight into sensing mechanism of cyclotetrapyrrole towards lung irritants. <i>Journal of Molecular Modeling</i> , 2022, 28, 110.	0.8	4
10737	Electronic structure and bonding in N-hetero cyclic carbene stabilized naked group 16 atoms π In-plane hyperconjugation and bond polarity. <i>Computational and Theoretical Chemistry</i> , 2022, 1210, 113661.	1.1	0
10738	Nuclearity enlargement from [PW ₉ O ₃₄ @Ag ₅₁] to [(PW ₉ O ₃₄) ₂ @Ag ₇₂] and 2D and 3D network formation driven by bipyridines. <i>Nature Communications</i> , 2022, 13, 1802.	5.8	19
10739	Reconstructed covalent organic frameworks. <i>Nature</i> , 2022, 604, 72-79.	13.7	190
10740	Host-guest interactions between oleic acid and β -cyclodextrin: A combined experimental and theoretical study. <i>Food Chemistry</i> , 2022, 387, 132910.	4.2	6
10741	Base-Tuning HOF-Based Host-Guest Ultralong Organic Phosphorescence Systems with Phosphorescent Thermochromism Using for Information Security and Thermometer. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	19
10742	Insight into the self-aggregation behavior of lignite and anthracite in water: Atomic-level research using experiments and molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , 2022, 357, 119099.	2.3	3

#	ARTICLE	IF	CITATIONS
10743	Electronic Tuning in Reaction-Based Fluorescent Sensing for Instantaneous and Ultrasensitive Visualization of Ethylenediamine. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	31
10744	Controlling Solution-State Aggregation and Solid-State Microstructures of Conjugated Polymers by Tuning Backbone Conformation. <i>Macromolecular Rapid Communications</i> , 2022, , 2200069.	2.0	5
10745	Revealing the Structure-Interaction-Dissolubility Relationships through Computational Investigation Coupled with Solubility Measurement: Toward Solvent Design for Organosulfide Capture. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 7183-7192.	1.8	7
10746	Synthesis, structural, DFT, quantum chemical modeling and molecular docking studies of (E)-4-(((5-methylfuran-2-yl)methylene)amino) benzenesulfonamide from 5-methyl-2-furaldehyde and sulfanilamide. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100418.	1.3	40
10747	Multistimuli responsive supramolecular polymer networks via host-guest complexation of pillararene-containing polymers and sulfonium salts. <i>Chinese Chemical Letters</i> , 2022, 33, 5111-5115.	4.8	16
10748	Ultrafast Photophysics of Multiple-Resonance Ultrapure Blue Emitters. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2729-2739.	1.2	5
10749	Synergistic halogenation of backbone and end group for high-performance non-fused acceptors based organic solar cells. <i>Dyes and Pigments</i> , 2022, 200, 110178.	2.0	7
10750	Quantum study on the optoelectronic properties and chemical reactivity of phenoxazine-based organic photosensitizer for solar cell purposes. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1.	0.5	18
10751	Nucleophilic Ring-Opening of Thiolactones: A Facile Method for Sulfhydrylization of a Carbon Nanotube-Based Cathode toward High-Performance Li-S Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 5005-5014.	3.2	10
10752	Competition between Intra and Intermolecular Pnicogen Bonds. Complexes between Naphthalene Derivatives and Neutral or Anionic Bases. <i>ChemPhysChem</i> , 2022, , .	1.0	4
10753	Theoretical investigation on the fluorescence properties and ESIPT mechanism of the Al ³⁺ ion sensor 1-((2-hydroxynaphthalen-1-yl)methylene)urea(OCN). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 277, 121237.	2.0	3
10754	Computational Study of Aromatic Hydroxylation Catalyzed by the Iron-Dependent Hydroxylase PqqB Involved in the Biosynthesis of Redox Cofactor Pyrroloquinoline Quinone. <i>Inorganic Chemistry</i> , 2022, 61, 5943-5956.	1.9	2
10755	Wheat straw-core hydrogel spheres with polypyrrole nanotubes for the removal of organic dyes. <i>Journal of Cleaner Production</i> , 2022, 344, 131100.	4.6	15
10756	A DFT investigation of CO and NO adsorption on Cu ₅ Sc and Cu ₆ Sc ⁺ metallic clusters. <i>Computational and Theoretical Chemistry</i> , 2022, 1210, 113657.	1.1	1
10757	Imidazolium based superalkalis as building block for Lewis base. <i>Computational and Theoretical Chemistry</i> , 2022, 1210, 113639.	1.1	2
10758	Exploring trimetallic clusters containing alkali and alkaline earth metal atoms with high activity for nitrogen activation. <i>Structural Chemistry</i> , 2023, 34, 87-96.	1.0	4
10759	A High Performance 2-Hydroxynaphthalene Acylhydrazone Fluorescent Chemosensor for Detection of Al ³⁺ Ions Through ESIPT and PET Signalling Mechanism. <i>Journal of Cluster Science</i> , 0, , 1.	1.7	0
10760	A novice cocrystal nanomicelle formulation of 5-fluorouracil with proline: The design, self-assembly and in vitro/vivo biopharmaceutical characteristics. <i>International Journal of Pharmaceutics</i> , 2022, 617, 121635.	2.6	10

#	ARTICLE	IF	CITATIONS
10761	Molecular insights into the encapsulation of fluorouracil molecule inside the single-walled carbon nanotubes. <i>Diamond and Related Materials</i> , 2022, 124, 108900.	1.8	2
10762	Hydrogen adsorption on Ni doped carbon nanocone. <i>Diamond and Related Materials</i> , 2022, 124, 108921.	1.8	9
10763	Effect of external electric field on hexadiene homolog C ₆ H ₆ (SiF) ₂ . <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 107662.	0.9	2
10764	Homo pair formations of thiobarbituric acid: DFT calculations and QTAIM analysis. <i>Main Group Chemistry</i> , 2022, 21, 303-313.	0.4	1
10765	Interaction mechanism of cholesterol/ β -cyclodextrin complexation by combined experimental and computational approaches. <i>Food Hydrocolloids</i> , 2022, 130, 107725.	5.6	9
10766	A new strategy of thin oil film extraction for enhanced recovery and separation of praseodymium and neodymium. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 107692.	3.3	1
10767	Electronic Tuning in Reaction-Based Fluorescent Sensing for Instantaneous and Ultrasensitive Visualization of Ethylenediamine. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	3
10768	A foundational theoretical Al ₁₂ E ₁₂ (E = N, P) adsorption and quinolone docking study: cage quinolone pairs, optics and possible therapeutic and diagnostic applications. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 3630-3646.	2.0	17
10769	Tuning Catalyst-Free Photocontrolled Polymerization by Substitution: A Quantitative and Qualitative Interpretation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3290-3296.	2.1	2
10770	Host-guest liquid gating mechanism with specific recognition interface behavior for universal quantitative chemical detection. <i>Nature Communications</i> , 2022, 13, 1906.	5.8	22
10771	New 3-Acyl Tetramic Acid Derivatives from the Deep-Sea-Derived Fungus <i>Lecanicillium fusisporum</i> . <i>Marine Drugs</i> , 2022, 20, 255.	2.2	3
10772	Synthesis, structure, and bonding of spiro rare-earth metallacyclopent-3-enes via the reduction of metallacyclopentadienes. <i>Cell Reports Physical Science</i> , 2022, 3, 100831.	2.8	9
10773	Influence of particle size on the magneto-refractive effect in PbS quantum dots-doped liquid core fiber. <i>Optical Materials Express</i> , 2022, 12, 1838.	1.6	7
10774	Highly selective, rapid and simple colorimetric detection of Fe ³⁺ in fortified foods by L-Cysteine modified AuNP. <i>Microchemical Journal</i> , 2022, 179, 107480.	2.3	6
10775	Effect of polystyrene microplastics on the degradation of sulfamethazine: The role of persistent free radicals. <i>Science of the Total Environment</i> , 2022, 833, 155024.	3.9	19
10776	The Mechanochemistry of Carboranes. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	14
10777	The Mechanochemistry of Carboranes. <i>Angewandte Chemie</i> , 0, , .	1.6	2
10778	The study of Letrozole adsorption upon CCT nanotube: A DFT/TD-DFT and spectroscopic (excited states) study. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 107780.	0.4	0

#	ARTICLE	IF	CITATIONS
10779	Monitoring Methionine Decarboxylase by a Supramolecular Tandem Assay. Chemistry - an Asian Journal, 2022, 17, .	1.7	4
10780	Au ₁₂ C ₆₈ : a hollow noble metal carbide. Theoretical Chemistry Accounts, 2022, 141, 1.	0.5	0
10781	Effect of weak intermolecular interactions in micro/nanoscale polyphosphazenes and polyethylene terephthalate composites on flame retardancy. Polymers for Advanced Technologies, 2022, 33, 2231-2243.	1.6	5
10782	Accelerating Nickel-Based Molecular Construction via DFT Guidance for Advanced Photocatalytic Hydrogen Production. ACS Applied Materials & Interfaces, 2022, 14, 17486-17499.	4.0	4
10783	Low-Basis Weight Polyacrylonitrile/Polyvinylpyrrolidone Blend Nanofiber Membranes for Efficient Particulate Matter Capture. ACS Applied Polymer Materials, 2022, 4, 3971-3981.	2.0	7
10784	Toward Density-Based and Simultaneous Description of Chemical Bonding and Noncovalent Interactions with Pauli Energy. Journal of Physical Chemistry A, 2022, 126, 2437-2444.	1.1	14
10785	Facilely-prepared sulfide-doped Co ₃ O ₄ nanocomposite as a boosted catalyst for activating Oxone to degrade a sunscreen agent. Journal of the Taiwan Institute of Chemical Engineers, 2022, 133, 104253.	2.7	18
10786	Theoretical insights into the transformation mechanism and eco-toxicity effects of 5-Fluorouracil by O ₃ and \cdot OH in waters. Chemical Engineering Research and Design, 2022, 160, 541-550.	2.7	5
10787	Structure and reactivity of germylene-bridged digold complexes. Nature Communications, 2022, 13, 1785.	5.8	4
10788	Separation of magnesium from lithium in salt-lake brine through struvite precipitation. Minerals Engineering, 2022, 180, 107468.	1.8	14
10789	Hydrogen-Bond-Assisted Solution Discharge in Aprotic Li ⁺ Batteries. Advanced Materials, 2022, 34, e2110416.	11.1	24
10790	Regulating donor-acceptor interactions in triazine-based conjugated polymers for boosted photocatalytic hydrogen production. Applied Catalysis B: Environmental, 2022, 312, 121374.	10.8	28
10791	Enhancing Perfluorinated electron specialty gases separation selectivity in ultra-microporous metal organic framework. Separation and Purification Technology, 2022, 289, 120739.	3.9	16
10792	Enhancing the CO ₂ plasticization resistance of thin polymeric membranes by designing Metal-polymer complexes. Separation and Purification Technology, 2022, 289, 120699.	3.9	10
10793	Thiourea derivatives acting as functional monomers of As(III) molecular imprinted polymers: A theoretical and experimental study on binding mechanisms. Journal of Hazardous Materials, 2022, 430, 128508.	6.5	7
10794	Hydrogen-bonding and π - π interaction promoted solution-processable mixed matrix membranes for aromatic amines detection. Journal of Hazardous Materials, 2022, 430, 128490.	6.5	8
10795	Structural, electronic properties (different solvents), chemical reactivity, ELF, LOL, spectroscopic insights, molecular docking and in vitro anticancer activity studies on methyl (4-nitro-1-imidazolyl)acetate. Journal of the Indian Chemical Society, 2022, 99, 100438.	1.3	12
10796	Impact of regiochemistry on thermal stability of trifuroxan based energetic materials: A theoretical perspective. Computational and Theoretical Chemistry, 2022, 1211, 113686.	1.1	4

#	ARTICLE	IF	CITATIONS
10797	Novel Fe ²⁺ responsive nanofibrous membrane for corrosion detection and adsorption. <i>Polymer</i> , 2022, 248, 124817.	1.8	0
10798	Mechanistic insights into the removal of PFOA by 2D MXene/CNT membrane with the influence of Ca ²⁺ and humic acid. <i>Desalination</i> , 2022, 529, 115643.	4.0	12
10799	Molecular mechanism and extraction performance evaluation of diethylene glycol-based DES for extraction desulfurization process of fuel oil. <i>Journal of Molecular Liquids</i> , 2022, 353, 118785.	2.3	8
10800	Theoretical analysis of the uptake of CO, CO ₂ , and NO ₂ on pristine and BN-doped carbon nanocones. <i>Chemical Physics Letters</i> , 2022, 795, 139531.	1.2	7
10801	Synthesis, spectral analysis, antibacterial activity, quantum chemical studies and supporting molecular docking of Schiff base (E)-4-((4-bromobenzylidene) amino)benzenesulfonamide. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100405.	1.3	43
10802	Engineering of A2-D-A1-D-A2 type BT-dIDT based non-fullerene acceptors for effective organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2022, 1211, 113666.	1.1	12
10803	Insight into the spatial interaction of D- π -A bridge derived cyanines and nitroreductase for fluorescent cancer hypoxia detection. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 273, 121031.	2.0	0
10804	P-Hydroxybenzoic acid (HBA) as a functional electrolyte additive to regulate the electrode/electrolyte interfacial films and improve the electrochemical performance of lithium metal batteries. <i>Electrochimica Acta</i> , 2022, 414, 140212.	2.6	7
10805	Separation and recovery of iridium(IV) from simulated secondary resource leachate by extraction - electrodeposition. <i>Separation and Purification Technology</i> , 2022, 289, 120765.	3.9	5
10806	Quantum chemical studies of the electronic structures of anti-tumor agents: AuIII+ (L ^A = \hat{A} porphine,) Tj ETQq1 1 0.784314 rgBT /Over	1.1	1
10807	Hydrogen bonds between valsartan and solvents (water and methanol): Evidences for solvation dynamics using local energy decomposition and abinitio molecular dynamics analysis. <i>Journal of Molecular Liquids</i> , 2022, 354, 118856.	2.3	14
10808	Spectroscopy and laser cooling of SiBr ⁺ : A computational perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 273, 121042.	2.0	2
10809	Synthesis, XRD, hirshfeld surface analysis, ESP, HOMO-LUMO, quantum chemical modeling and anticancer activity of di(p-methyl benzyl)(dibromo)(1,10-phenanthroline) tin(IV) complex. <i>Inorganic Chemistry Communication</i> , 2022, 139, 109324.	1.8	51
10810	An electrochemical chiral sensor based on glutamic acid functionalized graphene-gold nanocomposites for chiral recognition of tryptophan enantiomers. <i>Journal of Electroanalytical Chemistry</i> , 2022, 913, 116283.	1.9	14
10811	New trans-[Ru(NO)(NO ₂)(dppb)(o-bdqi)] ⁺ complex as NO donor encapsulated Pluronic F-127 micelles. <i>Polyhedron</i> , 2022, 218, 115770.	1.0	4
10812	A fundamental study on selective extraction of Li ⁺ with dibenzo-14-crown-4 ether: Toward new technology development for lithium recovery from brines. <i>Journal of Environmental Management</i> , 2022, 310, 114705.	3.8	14
10813	Triple proton transfer after water rearrangement in (2,6-aza)Ind \hat{A} ·(H ₂ O) ₂ . <i>Journal of Molecular Liquids</i> , 2022, 353, 118847.	2.3	2
10814	Restriction of intramolecular torsion induces abnormal blue-shifted fluorescence in the aggregate state. <i>Dyes and Pigments</i> , 2022, 201, 110192.	2.0	16

#	ARTICLE	IF	CITATIONS
10815	Depicting the role of end-capped acceptors to amplify the photovoltaic properties of benzothiadiazole core-based molecules for high-performance organic solar cell applications. <i>Computational and Theoretical Chemistry</i> , 2022, 1211, 113669.	1.1	14
10816	Machine learning aided high-throughput prediction of ionic liquid@MOF composites for membrane-based CO ₂ capture. <i>Journal of Membrane Science</i> , 2022, 650, 120399.	4.1	24
10817	The sensing mechanism of HCHO gas sensor based on transition metal doped graphene: Insights from DFT study. <i>Sensors and Actuators A: Physical</i> , 2022, 338, 113460.	2.0	12
10818	Solubility study of m-aminobenzoic acid form III in different mono-solvents by thermodynamic analysis and molecular simulation. <i>Journal of Molecular Liquids</i> , 2022, 354, 118871.	2.3	1
10819	Quantum chemical approach to study TIPSTAP derivatives with anticipated minimized crystal roughness for photovoltaic application with estimated PCE of over 20%. <i>Solar Energy</i> , 2022, 237, 96-107.	2.9	13
10820	Solvent effect on mechanistic pathways in Rh-catalyzed hydroformylation of formaldehyde. <i>Molecular Catalysis</i> , 2022, 524, 112248.	1.0	2
10821	Adsorption of polychlorinated biphenyls on gold colloid by surface-enhanced Raman spectroscopy and density functional theory. <i>Vibrational Spectroscopy</i> , 2022, 120, 103369.	1.2	3
10822	Computational studies and experimental fabrication of DSSC device assembly on 2D-layered TiO ₂ and MoS ₂ @TiO ₂ nanomaterials. <i>Physica B: Condensed Matter</i> , 2022, 633, 413770.	1.3	9
10823	Construction of a novel metal-organic framework adenine-Uio-66 piezocatalyst for efficient diclofenac removal. <i>Separation and Purification Technology</i> , 2022, 289, 120743.	3.9	22
10824	Three-coordinated mononuclear Cu(I) complexes with crystallization-enhanced thermally activated delayed fluorescence characteristics. <i>Polyhedron</i> , 2022, 218, 115761.	1.0	5
10825	Degradation of bisphenol A by UV/persulfate process in the presence of bromide: Role of reactive bromine. <i>Water Research</i> , 2022, 215, 118288.	5.3	60
10826	Incorporating amino acids functionalized graphene oxide nanosheets into Pebax membranes for CO ₂ separation. <i>Separation and Purification Technology</i> , 2022, 288, 120682.	3.9	23
10827	Designing on solvent composition of dual-salt low concentration electrolyte for inhibiting lithium dendrite growth at ~20Å ² ,f. <i>Electrochimica Acta</i> , 2022, 414, 140238.	2.6	8
10828	NASICON-based solid state Li-Fe-F conversion batteries enabled by multi-interface-compatible sericin protein buffer layer. <i>Energy Storage Materials</i> , 2022, 47, 551-560.	9.5	31
10829	Analysis of the behavior of Sn ²⁺ and In ³⁺ ions in DES and in water: A theoretical approach. <i>Journal of Molecular Liquids</i> , 2022, 353, 118774.	2.3	2
10830	Degradation of microcystin-LR with expanded graphite based photocatalysts: Performance and mechanism based on active sites-radicals interaction. <i>Separation and Purification Technology</i> , 2022, 288, 120674.	3.9	6
10831	DNA damage, cell cycle perturbation and cell death by naphthalene diimide derivative in gastric cancer cells. <i>Chemico-Biological Interactions</i> , 2022, 358, 109881.	1.7	4
10832	Microscopic mechanism for electrocoalescence of water droplets in water-in-oil emulsions containing surfactant: A molecular dynamics study. <i>Separation and Purification Technology</i> , 2022, 289, 120756.	3.9	28

#	ARTICLE	IF	CITATIONS
10833	High performance nonlinear optical materials with simple aromatic hydrocarbons. <i>FlatChem</i> , 2022, 33, 100362.	2.8	10
10834	Alkali hydrolysis and Lewis acids assisted enhancement based highly sensitive and quantitative detection of malathion in tea using SERS and multivariate analysis. <i>Sensors and Actuators B: Chemical</i> , 2022, 359, 131584.	4.0	4
10835	Rich fluorine-bridged type rigid donor-acceptor (D-A) tricarbazoles-triazine structures: An effective strong acid affinity fluorescent dye. <i>Dyes and Pigments</i> , 2022, 201, 110254.	2.0	2
10836	Atypical adsorption of polycarboxylate superplasticizers on calcium silicate hydrate surface: Converting interaction by solvent effects. <i>Construction and Building Materials</i> , 2022, 330, 127160.	3.2	14
10837	Tuning the surface electronic state by the introduction of Mn on Fe ₂ O ₃ to boost the activity of peroxymonosulfate. <i>Separation and Purification Technology</i> , 2022, 289, 120625.	3.9	12
10838	Luminescent copper(I) complexes bearing benzothiazole-imidazolylidene ligand with various substituents: Synthesis, photophysical properties and computational studies. <i>Polyhedron</i> , 2022, 218, 115785.	1.0	3
10839	Natural quinone molecules as effective cathode materials for nonaqueous lithium-ion batteries. <i>Journal of Power Sources</i> , 2022, 531, 231291.	4.0	15
10840	Passivating defects via 4-cyanobenzenaminium iodide enables 22.44% efficiency perovskite solar cells. <i>Electrochimica Acta</i> , 2022, 413, 140172.	2.6	12
10841	Adsorption of volatile organic compounds on pristine and defected nanographene. <i>Computational and Theoretical Chemistry</i> , 2022, 1211, 113664.	1.1	9
10842	Exploration of perfluorooctane sulfonate degradation properties and mechanism via electron-transfer dominated radical process. <i>Water Research</i> , 2022, 215, 118259.	5.3	26
10843	Rational design of electrolytes operating at low temperatures: Does the co-solvent with a lower melting point correspond to better performance?. <i>Electrochimica Acta</i> , 2022, 415, 140268.	2.6	5
10844	Understanding the effect of vitamin B3, B6 and C as a corrosion inhibitor on the ordinary Portland cement hydration: Experiments and DFT study. <i>Construction and Building Materials</i> , 2022, 331, 127294.	3.2	8
10845	Preparation of activated coke by carbonization, activation, ammonization and thermal treatment of sewage sludge and waste biomass for SO ₂ absorption applications. <i>Fuel Processing Technology</i> , 2022, 231, 107233.	3.7	24
10846	Sensing behaviour of monocyclic C18 and B9N9 analogues toward chemical warfare agents (CWAs); quantum chemical approach. <i>Surfaces and Interfaces</i> , 2022, 30, 101912.	1.5	13
10847	Novel artificial ionic cofactors for efficient electro-enzymatic conversion of CO ₂ to formic acid. <i>Journal of CO₂ Utilization</i> , 2022, 60, 101978.	3.3	9
10848	Experimental spectra, electronic energies (liquid and gaseous phases) quantum computational strategies and potential biological activity studies of (1E, 4E)-1, 5-bis (4-methoxyphenyl) penta-1,4-dien-3-one: An antiviral agent. <i>Journal of Molecular Liquids</i> , 2022, 356, 119012.	2.3	2
10849	Computational data of molybdenum disulfide/graphene bilayer heterojunction under strain. <i>Data in Brief</i> , 2022, 42, 108054.	0.5	3
10850	A new nitrogen-enriched biochar modified by ZIF-8 grafting and annealing for enhancing CO ₂ adsorption. <i>Fuel Processing Technology</i> , 2022, 231, 107250.	3.7	32

#	ARTICLE	IF	CITATIONS
10851	Olympicene as a high-performance sensor for lung irritants: A dispersion corrected DFT insight. <i>Materials Science in Semiconductor Processing</i> , 2022, 144, 106620.	1.9	17
10852	Near-Infrared Light-Boosted Photodynamic-Immunotherapy based on sulfonated Metal-Organic framework nanospindle. <i>Chemical Engineering Journal</i> , 2022, 437, 135370.	6.6	10
10853	Effect of a lone electron pair and tetrel interactions on the structure of Pb(II) CPs constructed from pyrimidine carboxylates and auxiliary inorganic ions. <i>Polyhedron</i> , 2022, 219, 115818.	1.0	10
10854	Degradation of 3-chlorocarbazole in water by sulfidated zero-valent iron/peroxymonosulfate system: Kinetics, influential factors, degradation products and pathways. <i>Chemosphere</i> , 2022, 296, 134016.	4.2	11
10855	End-capped modification of Y-Shaped dithienothiophen[3,2-b]-pyrrolobenzothiadiazole (TPBT) based non-fullerene acceptors for high performance organic solar cells by using DFT approach. <i>Surfaces and Interfaces</i> , 2022, 30, 101875.	1.5	31
10856	Sofosbuvir adsorption onto activated carbon derived from argan shell residue: Optimization, kinetic, thermodynamic and theoretical approaches. <i>Journal of Molecular Liquids</i> , 2022, 356, 119019.	2.3	28
10857	Mechanisms and product toxicity of activated carbon/peracetic acid for degradation of sulfamethoxazole: implications for groundwater remediation. <i>Water Research</i> , 2022, 216, 118347.	5.3	73
10858	Transformation of amino acids and formation of nitrophenolic byproducts in sulfate radical oxidation processes. <i>Journal of Hazardous Materials</i> , 2022, 431, 128648.	6.5	9
10859	Terthiophene based non-fused electron acceptors for efficient organic solar cells. <i>Organic Electronics</i> , 2022, 105, 106512.	1.4	17
10860	Conferring all-nitrogen aromatics extra stability by acidic trapping. <i>Journal of Molecular Liquids</i> , 2022, 355, 118939.	2.3	1
10861	Theoretical study on the extraction behaviors of MoO ₂ ²⁺ with organophosphorous extractants. <i>Journal of Molecular Liquids</i> , 2022, 355, 118969.	2.3	5
10862	Shedding light on the second order nonlinear optical responses of commercially available acidic azo dyes for laser applications. <i>Dyes and Pigments</i> , 2022, 202, 110284.	2.0	8
10863	Structure analysis and insight into hydrogen bond and van der waals interactions of etoricoxib cocrystals and cocrystal solvate. <i>Journal of Molecular Structure</i> , 2022, 1258, 132665.	1.8	8
10864	Exploring the synergism of sunlight and electrooxidation on persulfate activation for efficient degradation of bisphenol S: Performance, Pathway, and mechanism. <i>Chemical Engineering Journal</i> , 2022, 437, 135318.	6.6	26
10865	Theoretical spectroscopic electronic elucidation with different solvents (IEFPCM model), biological assessment and molecular docking studies on Moroxydine-Antiviral drug agent. <i>Journal of Molecular Liquids</i> , 2022, 355, 118946.	2.3	14
10866	The inhibiting water uptake mechanism of main-chain type N-spirocyclic quaternary ammonium ionene blended with polybenzimidazole as anion exchange membrane. <i>Separation and Purification Technology</i> , 2022, 291, 120950.	3.9	12
10867	Modulating LUMO extension of Spiro-junction TADF emitters for efficient OLEDs with relieved efficiency Roll-Off. <i>Chemical Engineering Journal</i> , 2022, 437, 135222.	6.6	17
10868	DFT insights into the degradation mechanism of carbendazim by hydroxyl radicals in aqueous solution. <i>Journal of Hazardous Materials</i> , 2022, 431, 128577.	6.5	20

#	ARTICLE	IF	CITATIONS
10869	Lignin peroxidase-catalyzed direct oxidation of trace organic pollutants through a long-range electron transfer mechanism: Using propranolol as an example. <i>Journal of Hazardous Materials</i> , 2022, 431, 128544.	6.5	7
10870	Ultrafast nonadiabatic mechanism of plant sunscreens biflavonoids with two excited-state intramolecular proton transfer structures. <i>Journal of Luminescence</i> , 2022, 246, 118816.	1.5	2
10871	In-depth insight into the inhibition mechanism of the modified and combined amino acids corrosion inhibitors: "intramolecular synergism" vs. "intermolecular synergism". <i>Chemical Engineering Journal</i> , 2022, 437, 135439.	6.6	32
10872	Electrochemical activation of peroxymonosulfate with titanium suboxide anode for 4-chlorophenol degradation: Influencing factors, kinetics, and degradation mechanism. <i>Separation and Purification Technology</i> , 2022, 291, 120964.	3.9	10
10873	Synthesis, structures, and photophysical properties of three-coordinate copper(I) complexes bearing bidentate bis[(2-diphenylphosphino)phenyl]ether (POP) ligand and monodentate substituted-quinoline ligand. <i>Journal of Molecular Structure</i> , 2022, 1257, 132642.	1.8	6
10874	Robust fluorescent detection of iodine vapor by a film sensor based on a polymer of intrinsic microporosity. <i>Chemical Engineering Journal</i> , 2022, 438, 135641.	6.6	14
10875	Interaction of Fluorouracil drug with boron nitride nanotube, Al doped boron nitride nanotube and BC2N nanotube. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113699.	1.1	22
10876	Simulation guided prediction of zeolites for the sorption of selected anions from water: Machine learning predictors for enhanced loading. <i>Journal of Molecular Liquids</i> , 2022, 355, 118913.	2.3	6
10877	Boosting the cycling stability of hard carbon with NaODFB-based electrolyte at high temperature. <i>Materials Today Chemistry</i> , 2022, 24, 100866.	1.7	6
10878	Equilibrium solubility of amrinone in aqueous co-solvent solutions reconsidered: Quantitative molecular surface, inter/intra-molecular interactions and solvation thermodynamics analysis. <i>Journal of Molecular Liquids</i> , 2022, 355, 118995.	2.3	11
10879	Exploring the potential energy surface of nCO ₂ (n=1-5) capture by imidazole-and fluorine-based ionic liquids: A DFT study. <i>Journal of Molecular Liquids</i> , 2022, 356, 119022.	2.3	1
10880	Investigation on solubility behavior of 2-chloronicotinamide in ten mono-solvents: Measurement, correlation, molecular simulation and thermodynamic analysis. <i>Journal of Molecular Liquids</i> , 2022, 356, 119054.	2.3	4
10881	Strained carbocycle based hypergolic ionic fuels with the improved energy capacity. <i>Fuel Processing Technology</i> , 2022, 231, 107248.	3.7	2
10882	Efficient separation of methanol/dimethyl carbonate mixtures by UiO-66 MOF incorporated chitosan mixed-matrix membrane. <i>Journal of Membrane Science</i> , 2022, 652, 120473.	4.1	20
10883	Biomass-derived carbon quantum dots modified Bi ₂ MoO ₆ /Bi ₂ S ₃ heterojunction for efficient photocatalytic removal of organic pollutants and Cr (VI). <i>Separation and Purification Technology</i> , 2022, 291, 120901.	3.9	37
10884	Mechanistic insight into the electron-donation effect of modified ZIF-8 on Ru for CO ₂ hydrogenation to formic acid. <i>Journal of CO₂ Utilization</i> , 2022, 60, 101992.	3.3	14
10885	Isolation of chemical compositions as dietary antioxidant supplements and neuroprotectants from Chaga mushroom (<i>Inonotus obliquus</i>). <i>Food Bioscience</i> , 2022, 47, 101623.	2.0	11
10886	End-capped group modification on cyclopentadithiophene based non-fullerene small molecule acceptors for efficient organic solar cells; a DFT approach. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 113, 108162.	1.3	46

#	ARTICLE	IF	CITATIONS
10887	Ab initio metadynamics simulations on the formation of calcium silicate aqua complexes prior to the nucleation of calcium silicate hydrate. <i>Cement and Concrete Research</i> , 2022, 156, 106767.	4.6	9
10888	The role of hydroxylation on $\cdot\text{OH}$ generation for enhanced ozonation of benzoic acids: Reactivity, ozonation efficiency and radical formation mechanism. <i>Journal of Hazardous Materials</i> , 2022, 431, 128620.	6.5	16
10889	Effect of halide/pseudohalide anions on the association and semimicroextraction of substituted chloroaurates with a symmetric carbocyanine dye: A complex study and analytical application. <i>Journal of Molecular Liquids</i> , 2022, 356, 119037.	2.3	0
10890	Selective extraction of lithium from seawater desalination concentrates: Study of thermodynamic and equilibrium properties using Density Functional Theory (DFT). <i>Desalination</i> , 2022, 532, 115704.	4.0	14
10891	Investigating the mechanism of fluorescence probe of quinoline derivatives for detecting phosgene in gas and liquid phases. <i>Chemical Physics Letters</i> , 2022, 797, 139577.	1.2	2
10892	Fast coupling and detoxification of aqueous halobenzoquinones by extracellular nucleophiles: The relationship among structures, pathways and toxicity. <i>Chemical Engineering Journal</i> , 2022, 438, 135525.	6.6	5
10893	Theoretical modeling of hydrochar precursor formation during the hydrothermal carbonization of sewage sludge. <i>Fuel Processing Technology</i> , 2022, 231, 107212.	3.7	10
10894	Pyrolysis mechanism law of β -O-4 lignin dimer model compounds: A density functional theory study. <i>Industrial Crops and Products</i> , 2022, 180, 114746.	2.5	10
10895	Simulated preparation and hydration property of a new-generation zwitterionic modified PVDF membrane. <i>Journal of Membrane Science</i> , 2022, 652, 120498.	4.1	10
10896	Rate constant of hydrogen transfer from H-donor solvents to coal radicals. <i>Fuel</i> , 2022, 318, 123621.	3.4	9
10897	Study of quantum chemistry calculation simulation for the effect of electric field on the kerogen molecular decomposition. <i>Fuel</i> , 2022, 318, 123584.	3.4	8
10898	Research on the degradation behaviors of wood pulp cellulose in ionic liquids. <i>Journal of Molecular Liquids</i> , 2022, 356, 119071.	2.3	13
10899	Sustainable composite material based on glutenin biopolymeric-clay for efficient separation of rare earth elements. <i>Chemical Engineering Journal</i> , 2022, 440, 135959.	6.6	10
10900	Spectroscopic analyses on an azatricycloderivative by DFT with different solvents, reactivity analysis and MD simulations. <i>Journal of Molecular Structure</i> , 2022, 1260, 132845.	1.8	0
10901	Theoretical correction on the existing understanding for hydroper-oxymethyl formate dissociation in DME low temperature oxidation. <i>Combustion and Flame</i> , 2022, 241, 112065.	2.8	2
10902	Mechanistic study on the radical scavenging activity of viniferins. <i>Journal of Molecular Structure</i> , 2022, 1260, 132830.	1.8	4
10903	Self-activated Ni(OH) ₂ cathode for complete electrochemical reduction of trichloroethylene to ethane in low-conductivity groundwater. <i>Applied Catalysis B: Environmental</i> , 2022, 309, 121258.	10.8	15
10904	Effect of pH on caffeine removal from aqueous media by graphene/graphene oxide adsorption. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 644, 128864.	2.3	15

#	ARTICLE	IF	CITATIONS
10905	Unveiling the effects of atomic electronegativity on the ESIPT mechanism and luminescence property of new coumarin benzothiazole Fluorophore: A TD-DFT exploration. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 275, 121118.	2.0	12
10906	Single-atom iron on penta-graphene assisted with non-bonding interaction as superior demercurizer: A DFT exploration. <i>Applied Surface Science</i> , 2022, 590, 153060.	3.1	8
10907	Microscopic mechanism and kinetics of NO heterogeneous reduction on char surface: A density functional theory study. <i>Energy</i> , 2022, 250, 123861.	4.5	7
10908	Polyethersulfone/polyvinylpyrrolidone/boron nitride composite membranes for high proton conductivity and long-term stability high-temperature proton exchange membrane fuel cells. <i>Journal of Membrane Science</i> , 2022, 653, 120512.	4.1	19
10909	DFT of 5-Fluoro-2-Oxo-1H-Pyrazine-3-Carboxamide (OPC) Adsorption, Spectroscopic, Solvent Effect, and SERS Analysis. <i>Journal of Molecular Liquids</i> , 2022, 357, 119076.	2.3	35
10910	Estimations of OHâ€N hydrogen bond length from positions and intensities of IR bands. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 275, 121172.	2.0	4
10911	Experimental and theoretical investigation on the adsorption properties of benzene on graphene surface: Influence of pH and edge effects. <i>Chemical Engineering Journal</i> , 2022, 440, 135794.	6.6	9
10912	Refine the evaluation of photophysical properties of organometallic chromophores under confined molecular crystal conditions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 275, 121168.	2.0	1
10913	From normal crosslinking to coreâ€shell structure: Improved performance of Î²-cyclodextrin based adsorbent toward efficient separation of acetophenone and 1-phenylethanol. <i>Separation and Purification Technology</i> , 2022, 292, 120955.	3.9	3
10914	Feâ€Oâ€Zr in MOF for effective photo-Fenton Bisphenol A degradation: Boosting mechanism of electronic transmission. <i>Chemosphere</i> , 2022, 299, 134481.	4.2	20
10915	A high-sensitive dopamine electrochemical sensor based on multilayer Ti3C2 MXene, graphitized multi-walled carbon nanotubes and ZnO nanospheres. <i>Microchemical Journal</i> , 2022, 178, 107410.	2.3	66
10916	N,N-di(4-methoxyphenyl)hydrazones of carbazole and phenothiazine carbaldehydes containing 4-methoxyphenyl groups as hole transporting materials. <i>Synthetic Metals</i> , 2022, 287, 117057.	2.1	2
10917	Imidazole functionalized graphene and carbon nanotubes for CO2 detection. <i>Journal of Molecular Structure</i> , 2022, 1259, 132719.	1.8	0
10918	Highly efficient hybridized local and Charge-transfer (HLCT) Deep-blue electroluminescence with excellent molecular horizontal orientation. <i>Chemical Engineering Journal</i> , 2022, 440, 135911.	6.6	52
10919	Quantitative surface analysis of paclobutrazol molecule and comprehensive insight into its solubility in aqueous co-solvent solutions. <i>Journal of Chemical Thermodynamics</i> , 2022, 170, 106787.	1.0	12
10920	Fabrication of Novel Potentiometric Sensor for Lead Ion Detection in Blood Samples: Experimental and Theoretical Approaches. <i>Microchemical Journal</i> , 2022, 178, 107383.	2.3	1
10921	Exploration of catalytic species for highly efficient preparation of quinazoline-2,4(1H,3H)-diones by succinimide-based ionic liquids under atmospheric pressure: Combination of experimental and theoretical study. <i>Fuel</i> , 2022, 319, 123628.	3.4	9
10922	Antispasmodic activity of carnosic acid extracted from <i>rosmarinus officinalis</i> : Isolation, spectroscopic characterization, DFT studies, and in silico molecular docking investigations. <i>Journal of Molecular Structure</i> , 2022, 1260, 132795.	1.8	43

#	ARTICLE	IF	CITATIONS
10923	Naked-eye colorimetric anion probing and fluorescent switching features of conjugated Schiff Bases derived from 4-(Trifluoromethyl) benzenesulfonamide. <i>Journal of Luminescence</i> , 2022, 247, 118849.	1.5	5
10924	Effects of linkage between donors on photoinduced charge transfer in one-photon and two-photon absorption of Donor- π -Donor- π -Acceptor conjugates. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 275, 121179.	2.0	2
10925	Functional group substitutions influence the binding of benzophenone-type UV filters with DNA. <i>Chemosphere</i> , 2022, 299, 134490.	4.2	6
10926	New insights into ferric iron-facilitated UV254 photolytic defluorination of perfluorooctanoic acid (PFOA): Combined experimental and theoretical study. <i>Journal of Hazardous Materials</i> , 2022, 434, 128865.	6.5	10
10927	Electronic transitions in noncovalent BODIPY dimers: TD-DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 275, 121151.	2.0	2
10928	Halogen bonding (C-F \cdots X) and its effect on creating ideal insensitive energetic materials. <i>Chemical Engineering Journal</i> , 2022, 440, 135969.	6.6	18
10929	Solvothermal synthesis, crystal structure, thermal, magnetic properties and DFT computations of a Ytterbium(III) complex derived from pyridine-2,6-dicarboxylic acid. <i>Journal of Molecular Structure</i> , 2022, 1260, 132877.	1.8	10
10930	A new naphthalimide-picolinohydrazide derived fluorescent "turn-on" probe for hypersensitive detection of Al ³⁺ ions and applications of real water analysis and bio-imaging. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 275, 121193.	2.0	12
10931	Synthesis, crystal structure, DFT and molecular docking studies of N-acetyl-2,4-[diaryl-3-azabicyclo[3.3.1]nonan-9-yl]-9-spiro-4'-acetyl-2'-acetyl-(acetylamino)-4'-9-dihydro-[1,3,4]thiadiazoles: A potential SARS-nCoV-2 Mpro (COVID-19) inhibitor. <i>Journal of Molecular Structure</i> , 2022, 1259, 132747.	1.8	3
10932	Hydrogen vs. halogen bonding in crystals of 2,5-dibromothiophene-3-carboxylic acid derivatives. <i>Journal of Molecular Structure</i> , 2022, 1260, 132785.	1.8	2
10933	Designing sub-nanometer pores for efficient boron removal. <i>Desalination</i> , 2022, 533, 115755.	4.0	13
10934	Nanocellulose bio-based composites for the removal of methylene blue from water: An experimental and theoretical exploration. <i>Journal of Molecular Liquids</i> , 2022, 357, 119089.	2.3	6
10935	Functional group modified 1D interpenetrated metal-organic frameworks on perfluorooctanoic acid adsorption: Experimental and theoretical calculation study. <i>Environmental Research</i> , 2022, 211, 113083.	3.7	4
10936	Synthesis, crystal structure, characterization, Hirshfeld analysis, molecular docking and DFT calculations of 5-Phenylamino-isophthalic acid: A good NLO material. <i>Journal of Molecular Structure</i> , 2022, 1261, 132791.	1.8	23
10937	Dualism of 1,2,4-oxadiazole ring in noncovalent interactions with carboxylic group. <i>Journal of Molecular Structure</i> , 2022, 1262, 132974.	1.8	4
10938	Optimizing porous structure of carbon electrodes for temperature-independent capacitance at sub-zero temperatures. <i>Chemical Engineering Journal</i> , 2022, 441, 136053.	6.6	8
10939	Consequence of Proton Transfer and Hydrogen Bonding Interactions on the Molecular, Vibrational and Biological properties of the Novelty Synthesized Antibacterial Compound bis-(4-Dimethylaminopyridinium) bis-(3, 5-Dinitrobenzoate) monohydrate using DFT Study. <i>Journal of Molecular Structure</i> , 2022, 1261, 132914.	1.8	5
10940	Two nickel (II) complexes with side chain isomeric ligands: L-leucine and L-isoleucine to study non-covalent interactions and metal-ligand bonding. <i>Journal of Molecular Structure</i> , 2022, 1261, 132898.	1.8	2

#	ARTICLE	IF	CITATIONS
10941	Grape seed oligomeric proanthocyanidins-assembled membranes with a highly negatively charged surface for high-performance nanofiltration. <i>Chemical Engineering Journal</i> , 2022, 441, 136113.	6.6	2
10942	Synergetic promoting/inhibiting mechanisms of copper/calcium compounds in the formation of persistent organic pollutants and environmentally persistent free radicals from anthracene. <i>Chemical Engineering Journal</i> , 2022, 441, 136102.	6.6	6
10943	Multi-armed imide-based molecules promote interfacial charge transfer for efficient organic solar cells. <i>Chemical Engineering Journal</i> , 2022, 441, 135894.	6.6	9
10944	New silver(I) complex as antibiotic candidate: Synthesis, spectral characterization, DFT, QTAIM and antibacterial investigations and docking properties. <i>Journal of Molecular Structure</i> , 2022, 1261, 132902.	1.8	13
10945	Experimental investigations and quantum chemical calculations of methylene diphenyl diisocyanate (MDI)-based chemically modified bitumen and its crosslinking behaviours. <i>Fuel</i> , 2022, 321, 124084.	3.4	16
10946	Synthesis, photophysical, electrochemical and computational studies of novel 2-aminoimidazolones with D-π-A framework. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 429, 113918.	2.0	5
10947	The role of regioisomerism on thermal stability of furoxan based energetic materials. <i>Journal of Molecular Structure</i> , 2022, 1262, 132955.	1.8	5
10948	Synthesis and characterization of hypergolic salts based on bis(1H-1,2,3-triazole-1-yl) dihydroborate anion. <i>Journal of Molecular Structure</i> , 2022, 1261, 132850.	1.8	2
10949	Insights into the synergistic effect of catalyst acidity and solvent basicity for effective production of pentose from glucose. <i>Chemical Engineering Journal</i> , 2022, 442, 136224.	6.6	9
10950	A novel π-d conjugated cobalt tetraaza[14]annulene based atomically dispersed electrocatalyst for efficient CO ₂ reduction. <i>Chemical Engineering Journal</i> , 2022, 442, 136129.	6.6	16
10951	Hydroxyl group-enriched microporous organic network for high-performance solid-phase extraction of triazine herbicides: Experiment and DFT calculation on adsorption behavior. <i>Chemical Engineering Journal</i> , 2022, 442, 136171.	6.6	15
10952	Structural Elucidation, Growth and Characterization of (E)-2-(4-dimethylamino) benzylidene-3,4-dihydranaphthalen-1(2H)-one Single Crystal for Nonlinear Optical Applications. <i>Journal of Molecular Structure</i> , 2022, 1261, 132942.	1.8	2
10953	Rationalizing the role of electron/charge transfer in the intramolecular chemiexcitation of dioxetanone-based chemi-/bioluminescent systems. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 429, 113904.	2.0	5
10954	Theoretical and experimental investigation of 1,4-dihydropyridine-based hexahydroquinoline-3-carboxylates: Photophysics and bovine serum albumin binding studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 429, 113915.	2.0	3
10955	Molecular Docking, Structural Examination, Reactive Sites Identification (HOMO-LUMO, MEP) of 6-Phenylpteridine 2, 4, 7-triamine: Potential Bacterial Inhibitor. <i>Analytical Chemistry Letters</i> , 2021, 11, 886-898.	0.4	2
10956	Spectroscopic (FT-IR, FT Raman and UV-Vis), Quantum Computational and Molecular Docking studies on Propylthiouracil. <i>Analytical Chemistry Letters</i> , 2021, 11, 771-791.	0.4	2
10957	Construction of High-Performance Carbene-Metal-Amide-Like TADF Materials: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 26770-26777.	1.5	7
10958	Application of Group Theory for Evaluating the Jahn-Teller Effect and Analyzing the Stability Structure of Boron B_n Clusters. <i>Russian Journal of Inorganic Chemistry</i> , 2021, 66, 2091-2104.	0.3	1

#	ARTICLE	IF	CITATIONS
10959	Simulation of Gas Production Mechanisms in Shear Deformation of Medium-Rank Coal. ACS Omega, 2022, 7, 342-350.	1.6	3
10960	The Halogenation Effects of Electron Acceptor ITIC for Organic Photovoltaic Nano-Heterojunctions. Nanomaterials, 2021, 11, 3417.	1.9	8
10961	N-Heterocyclic Carbene-Photocatalyzed Tricomponent Regioselective 1,2-Diacylation of Alkenes Illuminates the Mechanistic Details of the Electron Donor-Acceptor Complex-Mediated Radical Relay Processes. ACS Catalysis, 2022, 12, 285-294.	5.5	41
10962	On Electron Pair Rearrangements in Photochemical Reactions: 1,3-Cyclohexadiene Ring Opening. Journal of Physical Chemistry A, 2022, 126, 395-405.	1.1	12
10963	The role of cysteine residues in the allosteric modulation of the chromophore phototransformations of biphotochromic fluorescent protein SAASoti. Scientific Reports, 2021, 11, 24314.	1.6	5
10964	Influence of co-ligand on the biological properties of Schiff base metal complexes: Synthesis, characterization, cytotoxicity, and antimicrobial studies. Applied Organometallic Chemistry, 2022, 36, .	1.7	9
10965	Linear and second-order nonlinear optical properties of non-fullerene acceptor derivatives with A structure. International Journal of Quantum Chemistry, 2022, 122, .	1.0	0
10966	High-Fidelity Dimerization of Xanthenyl Radicals and Dynamic Qualities of a Congested Ethane: Diethyl Dixanthenyl-9,9-dicarboxylate. European Journal of Organic Chemistry, 2022, 2022, .	1.2	1
10967	Incorporation of Different Metal Ion for Tuning Color and Enhancing Antioxidant Activity of Curcumin/Palygorskite Hybrid Materials. Frontiers in Chemistry, 2021, 9, 760941.	1.8	6
10968	A General Method to Develop Highly Environmentally Sensitive Fluorescent Probes and AIEgens. Advanced Science, 2022, 9, e2104609.	5.6	35
10969	Understanding the Photocatalytic Reduction of CO ₂ with Heterometallic Molybdenum(V) Phosphate Polyoxometalates in Aqueous Media. ACS Catalysis, 2022, 12, 453-464.	5.5	27
10970	Methane and Acetylene Detection in Transformer Oil Based on Raman Spectroscopy. , 2021, , .		0
10971	A Carbene Strategy for Progressive (Deutero)Hydrodefluorination of Fluoroalkyl Ketones. Angewandte Chemie, 2022, 134, .	1.6	9
10972	Theoretical probe of absorption and fluorescence emission characteristics of highly luminescent ReL(CO) ₃ X (L=1H-indazolo[5,6-f][1,10]phenanthroline and X=F, Cl, Br, I): a DFT/TD-DFT study. Molecular Physics, 2022, 120, .		
10973	Mechanistic study of cobalt(I)-catalyzed asymmetric coupling of ethylene and enynes to functionalized cyclobutanes. Journal of Computational Chemistry, 2022, 43, 440-447.	1.5	0
10974	Combination multi-nitrogen with high heat of formation: theoretical studies on the performance of bridged 1,2,4,5-tetrazine derivatives. Journal of Molecular Modeling, 2022, 28, 3.	0.8	1
10975	Ability of B ₁₂ N ₁₂ fullerene like nano-cage for sensing and improving the antioxidant activity of juglone and its derivative: Density functional theory investigation. International Journal of Quantum Chemistry, 2022, 122, .	1.0	7
10976	Salt Formation, to Realize a Good Combination of High Energy and Low Sensitivity of Nitroform-Based Energetic Compounds. Crystal Growth and Design, 2022, 22, 167-173.	1.4	4

#	ARTICLE	IF	CITATIONS
10977	Latent Nucleophilic Carbenes. <i>Journal of Organic Chemistry</i> , 2022, 87, 373-385.	1.7	5
10978	Regulation of Silver Precursor Reactivity via Tertiary Phosphine to Synthesize Near-Infrared Ag ₂ Te with Photoluminescence Quantum Yield of up to 14.7%. <i>Chemistry of Materials</i> , 2021, 33, 9524-9533.	3.2	10
10979	Exploitation of a Half-Conjugate Polydentate Salamo-Salen Hybrid Ligand and Its Two Phenoxide-Bridged Heterohexanuclear 3d's Double-Helical Cluster Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 1018-1030.	1.9	80
10980	Chemical Cutting of Network Nodes in Polymeric Carbon Nitride for Enhanced Visible-Light Photocatalytic Hydrogen Generation. <i>ACS Applied Nano Materials</i> , 2022, 5, 691-701.	2.4	8
10981	Sulfide with Oxygen-Rich Carbon Network for Good Lithium-Storage Kinetics. <i>ACS Nano</i> , 2022, 16, 2651-2660.	7.3	22
10982	Local Spatial Polarization Induced Efficient Charge Separation of Squaraine-Linked COF for Enhanced Photocatalytic Performance. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	56
10983	Li ₄ EPc: A metallo-organic electride comprising metal-nitrogen bonds. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	2
10984	Adsorption of Lewisite Warfare Agent on B12N12 Nano-Cluster: A Computational Investigation. <i>Russian Journal of Physical Chemistry A</i> , 2021, 95, 2637-2642.	0.1	2
10985	Stabilizing the Exotic Carbonic Acid by Bisulfate Ion. <i>Molecules</i> , 2022, 27, 8.	1.7	4
10986	The Effects of Benzene on the Structure and Properties of Triethylamine Hydrochloride/Chloroaluminate. <i>Crystals</i> , 2021, 11, 1532.	1.0	0
10987	A Discrete Platinum(II) Metallacycle Harvesting Triplet Excitons for Solution-Processed Deep-Red Organic Light-Emitting Diodes. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	5
10988	CO ₂ Adsorption on PtCu Sub-Nanoclusters Deposited on Pyridinic N-Doped Graphene: A DFT Investigation. <i>Materials</i> , 2021, 14, 7619.	1.3	6
10989	The mechanism of sugar produced from simple glycolaldehyde derivative at ambient conditions. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	0
10990	Enhanced Solubility, Dissolution, and Permeability of Abacavir by Salt and Cocrystal Formation. <i>Crystal Growth and Design</i> , 2022, 22, 428-440.	1.4	21
10991	Long-Life and High-Rate-Charging Lithium Metal Batteries Enabled by a Flexible Active Solid Electrolyte Interphase Layer. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 60678-60688.	4.0	9
10992	Energetic Co-Crystal of a Primary Metal-Free Explosive with BTF. Ideal Pair for Co-Crystallization. <i>Molecules</i> , 2021, 26, 7452.	1.7	10
10993	A Mechanochromic and Vapochromic Luminescent Cuprous Complex Based on a Switchable Intramolecular H \cdots A \cdots A Interaction. <i>Inorganic Chemistry</i> , 2022, 61, 254-264.	1.9	17
10994	Reaction Path Determination of Rhodium(I)-Catalyzed C-H Alkylation of <i>N</i> -8-Aminoquinoliny Aromatic Amides with Maleimides. <i>Journal of Organic Chemistry</i> , 2022, 87, 737-743.	1.7	5

#	ARTICLE	IF	CITATIONS
10995	Theoretical Study on the Structures, Spectral Properties, and Drugability of Xenicane-type Diterpenoids from <i>Dictyota dichotoma</i> . <i>Chemical Research in Chinese Universities</i> , 2022, 38, 622-631.	1.3	1
10996	Chiral 1D Metal-Organic Materials Based on Cu(II) and Amino Acid Schiff Bases. <i>Crystal Growth and Design</i> , 2022, 22, 237-250.	1.4	6
10997	M ^{II} -Cl Interaction Supported Heterometallic {Ni ^{II} Sn ^{II} } ₂ {Sn ^{IV} } and {Ni ^{II} Sn ^{II} } ₂ {Sn ^{II} } Complex Salts: Possibility of Ion-Pair-Assisted Tetrel Bonds. <i>Crystal Growth and Design</i> , 2022, 22, 341-355.	1.4	3
10998	CO ₂ Cleavage Reaction Driven by Alkylidyne Complexes of Group 6 Metals and Uranium: A Density Functional Theory Study on Energetics, Reaction Mechanism, and Structural/Bonding Properties. <i>Inorganic Chemistry</i> , 2021, 60, 18859-18869.	1.9	0
10999	Structural Isomerization Effect on the Triplet Energy Consumption Process of Organic Room-Temperature Phosphorescence Molecules: A QM/MM Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27810-27819.	1.5	10
11000	Boosting Palladium-Catalyzed Aryl Nitro Bond Activation Reaction by Understanding the Electronic, Electrostatic, and Polarization Effect: A Computational Study from a Basic Understanding to Ligand Design. <i>Journal of Organic Chemistry</i> , 2022, 87, 531-539.	1.7	2
11001	Manipulating Interfacial Stability Via Absorption-Competition Mechanism for Long-Lifespan Zn Anode. <i>Nano-Micro Letters</i> , 2022, 14, 31.	14.4	30
11002	Using Solid Catalysts in Disulfide-Based Dynamic Combinatorial Solution and Mechanochemistry. <i>ChemSusChem</i> , 2022, 15, .	3.6	5
11003	Novel quad-rotor-shaped photovoltaic materials: first example of fused-ring non-fullerene acceptors with proficient photovoltaic properties for high-performance solar cells. <i>Journal of Molecular Modeling</i> , 2022, 28, 18.	0.8	2
11004	Theoretical Study of CO Adsorption Interactions with Cr-Doped Tungsten Oxide/Graphene Composites for Gas Sensor Application. <i>ACS Omega</i> , 2022, 7, 528-539.	1.6	8
11005	Hapten Synthesis and Monoclonal Antibody Preparation for Simultaneous Detection of Albendazole and Its Metabolites in Animal-Origin Food. <i>Foods</i> , 2021, 10, 3106.	1.9	8
11006	Synthesis and structural characterization of two rotationally flexible bis(benzoxaphosphole)s. Phosphorus, Sulfur and Silicon and the Related Elements, 2022, 197, 426-433.	0.8	1
11007	Spectroscopic profiling, DFT computations, molecular docking and molecular dynamic simulation of biologically active 5-isoquinolinesulfonic acid. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 722-735.	2.0	10
11008	Bonding Character, Electron Delocalization, and Aromaticity of Cyclo[18]Carbon (C ₁₈) Precursors, C ₁₈ -n(CO) _n (n=6, 4, and 2): Focusing on the Effect of Carbonyl (CO) Groups**. <i>Chemistry - A European Journal</i> , 2022, 28, e202103815.	1.7	30
11009	A theoretical approach on the ability of functionalized gold nanoparticles for detection of Cd ²⁺ . <i>Scientific Reports</i> , 2021, 11, 23422.	1.6	6
11010	Enhancement of superexchange due to synergetic breathing and hopping in corner-sharing cuprates. <i>Nature Physics</i> , 2022, 18, 190-195.	6.5	10
11011	Extraction of phenols from bio-oil aqueous fraction by hydrophobic ionic liquids. <i>Journal of Fuel Chemistry and Technology</i> , 2021, 49, 1832-1839.	0.9	9
11012	Exploring Nonemissive Excited-State Intramolecular Proton Transfer by Plasmon-Enhanced Hyper-Raman Scattering and Two-Photon Excitation Fluorescence. <i>Journal of Physical Chemistry C</i> , 2022, 126, 487-492.	1.5	22

#	ARTICLE	IF	CITATIONS
11013	Generation of Phenol and Molecular Hydrogen through Catalyst-Free C-H Activation of Benzene by Water Radical Cations. <i>Journal of the American Society for Mass Spectrometry</i> , 2022, 33, 68-73.	1.2	7
11014	Interaction Types in C ₆ H ₅ (CH ₂) _n OH-CO ₂ (n = 1-10) Tj. <i>ETOP</i> 1 0.784314 rgsB 2.1 10	2.1	10
11015	A Carbene Strategy for Progressive (Deutero)Hydrodefluorination of Fluoroalkyl Ketones. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	27
11016	Azepine- or Oxepine-embedded Double Saddle-Helix Nanographenes. <i>Chemistry - an Asian Journal</i> , 2022, 17, e202101365.	1.7	6
11017	Carbazochrome carbon nanotube as drug delivery nanocarrier for anti-bleeding drug: quantum chemical study. <i>Journal of Molecular Modeling</i> , 2022, 28, 11.	0.8	17
11018	A Dispersion Corrected DFT Investigation of the Inclusion Complexation of Dexamethasone with β -Cyclodextrin and Molecular Docking Study of Its Potential Activity against COVID-19. <i>Molecules</i> , 2021, 26, 7622.	1.7	9
11019	PAHs Containing both Heptagon and Pentagon: Corannulene Extension by [5+2] Annulation. <i>European Journal of Organic Chemistry</i> , 2022, 2022, .	1.2	8
11020	pH-Responsive N-Cyclometalated Iridium(III) Complexes: Synthesis, Photophysical Properties, Computational Results, and Bioimaging Application. <i>Molecules</i> , 2022, 27, 232.	1.7	7
11021	Bithieno Thiophene-Based Small Molecules for Application as Donor Materials for Organic Solar Cells and Hole Transport Materials for Perovskite Solar Cells. <i>ACS Omega</i> , 2022, 7, 844-862.	1.6	43
11022	Synthesis, Properties, and Packing Structures of Wing-Shaped N-Doped Nanographene in Various Oxidation States. <i>Organic Letters</i> , 2022, 24, 80-84.	2.4	6
11023	Supramolecule-Originated Emission: A Room-Temperature Phosphorescence 2D Ionic H-Bond Network from Nonemissive Aliphatic Derivatives. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 61528-61535.	4.0	2
11024	Surprising Complexity of the [Gd(AAZTA)(H ₂ O) ₂] ⁺ Chelate Revealed by NMR in the Frequency and Time Domains. <i>Inorganic Chemistry</i> , 2022, 61, 496-506.	1.9	4
11025	The Covalent Au ^I -Au ^I Bond in (AuF) ₂ (n = 2 ^{1/4}): A Perspective to Understand the Closed-Shell Au ^I -Au ^I Interaction. <i>Inorganic Chemistry</i> , 2022, 61, 1051-1058.	1.9	7
11026	Conformation and Metal Cation Binding of Zwitterionic Alanine Tripeptide in Saline Solutions by Infrared Vibrational Spectroscopy and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2022, 126, 161-173.	1.2	2
11027	1,2,3,4-Tetrakis(2-cyanoethoxy)butane (TCEB)-Assisted Construction of Self-Repair Electrode Interface Films to Improve the Performance of 4.5 V Pouch LiCoO ₂ /Artificial Graphite Full Cells Operating at 45 °C. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 59925-59936.	4.0	7
11028	DFT-D4 Insight into the Inclusion of Amphetamine and Methamphetamine in Cucurbit[7]uril: Energetic, Structural and Biosensing Properties. <i>Molecules</i> , 2021, 26, 7479.	1.7	11
11029	PDMS with Tunable Side Group Mobility and Its Highly Permeable Membrane for Removal of Aromatic Compounds. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	22
11030	A comparative conformational study of (C ₆ H ₅ O) ₂ P(O)(NHCS)NHCH ₂ C ₆ H ₅ and analogous X-ray structures: energy calculations (solid-state/gas phase). <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 0, 1-11.	0.8	0

#	ARTICLE	IF	CITATIONS
11031	Interaction between Phosgene and B12N12 Nano-Cluster: A Computational Investigation. Russian Journal of Physical Chemistry A, 2021, 95, S323-S330.	0.1	3
11032	Anion Complexation Strongly Influences the Reactivity of Octafluorocyclooctatetraene. ChemistrySelect, 2021, 6, 13897-13905.	0.7	0
11033	A promising strategy for increasing phosphorescent quantum yield: The ligand 10- β -cyclic chelate of the tetradentate Pt(II) complex. Applied Organometallic Chemistry, 2022, 36, .	1.7	1
11034	Effect of the Defect Modulator and Ligand Length of Metal-Organic Frameworks on Carbon Dioxide Photoreduction. ACS Applied Materials & Interfaces, 2021, 13, 61578-61586.	4.0	21
11035	Three-Dimensional Graphene-Based Foams with π -Greater Electron Transferring Areas- π -Deriving High Gas Sensitivity. ACS Applied Nano Materials, 2021, 4, 13234-13245.	2.4	6
11036	Self-Healable, Malleable, and Flexible Ionic Polyimine as an Environmental Sensor for Portable Exogenous Pollutant Detection. , 2022, 4, 136-144.		30
11037	Through-Space Charge-Transfer Emitters Developed by Fixing the Acceptor for High-Efficiency Thermally Activated Delayed Fluorescence. ACS Applied Materials & Interfaces, 2021, 13, 60269-60278.	4.0	31
11038	Donor-Acceptor Boron-Ketoiminate Complexes with Pendent <i>N</i> -Heterocyclic Arms: Switched-on Luminescence through <i>N</i> -Heterocycle Methylation. Journal of Organic Chemistry, 2022, 87, 184-196.	1.7	5
11039	Reversible Photochromic Coordination Polymer by Phototriggered Subtle Molecular Conformation Variations. Inorganic Chemistry, 2021, 60, 18870-18878.	1.9	7
11040	Structural and Electronic Properties of LaSi _n O ₃ (<i>n</i> = 2-6) Clusters: Anion Photoelectron Spectroscopy and Density Functional Calculations. Journal of Physical Chemistry A, 2021, 125, 10557-10567.	1.1	8
11041	Theoretical Calculation of Cocrystal Components for Explosives: A Similarity Function of Energetic Supramolecules. Crystal Growth and Design, 2022, 22, 293-303.	1.4	2
11042	Molecular Insights into Asphaltene Aggregation in Gas Flooding. Energy & Fuels, 2022, 36, 762-770.	2.5	7
11043	Experimental Methods of Corrosion Inhibition Assessment. ACS Symposium Series, 0, , 49-60.	0.5	1
11044	Modulation of π character upon complexation captured by molecular rotation spectra. Physical Chemistry Chemical Physics, 2022, , .	1.3	0
11045	Synthesis and characterization of rhenia[10]annulynes. Inorganic Chemistry Frontiers, 2022, 9, 2895-2902.	3.0	3
11046	Cytotoxic properties of rhenium(<i>n</i>) tricarbonyl complexes of <i>N</i> -heterocyclic carbene ligands. Dalton Transactions, 2022, 51, 7630-7643.	1.6	3
11047	Inorganic-organic {d _z ² -M _{II} S ₄ } π -hole stacking in reverse sandwich structures: the case of cocrystals of group 10 metal dithiocarbamates with electron-deficient arenes. Inorganic Chemistry Frontiers, 2022, 9, 2869-2879.	3.0	9
11048	Structure, Bonding and Adaptive Aromaticity in Rhenium-oxo Complexes: A DFT Study. New Journal of Chemistry, 0, , .	1.4	5

#	ARTICLE	IF	CITATIONS
11049	Modulation of Epoxy Polymer Trapping Energy Levels by Fluorinated Diluents to Improve Insulation Properties. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2022, 29, 1062-1069.	1.8	5
11050	Al-Embedded C ₂ N: a DFT study on a promising catalyst for CO oxidation. <i>New Journal of Chemistry</i> , 2022, 46, 9250-9257.	1.4	3
11051	Theoretical unraveling of the separation of trivalent Am and Eu ions by phosphine oxide ligands with different central heterocyclic moieties. <i>Dalton Transactions</i> , 2022, 51, 7118-7126.	1.6	10
11052	A DFT study of NHC-catalyzed reactions between 2-bromo-2-enals and acylhydrazones: mechanisms, and chemo- and stereoselectivities. <i>New Journal of Chemistry</i> , 2022, 46, 9146-9154.	1.4	3
11053	Experimental and theoretical insights into trans influence of organo-sulfur and -selenium ligands in 5,6-membered palladium(II) cationic pincer complexes based on iminophosphoranes. <i>New Journal of Chemistry</i> , 0, , .	1.4	1
11054	Nitro rotation tuned dissociative electron attachment upon targeted radiosensitizer 4-substituted Z bases. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 10356-10364.	1.3	6
11055	Nonlinear plexcitons: excitons coupled with plasmons in two-photon absorption. <i>Nanoscale</i> , 2022, 14, 7269-7279.	2.8	27
11056	Strong visible light-absorbing BODIPY-based Cu(<i>scp</i>) cyclic trinuclear sensitizer for photocatalysis. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 2928-2937.	3.0	7
11057	Density Functional Theory Study on the Mechanism of Organophosphine-Catalyzed [4+2] Cycloaddition Reaction. <i>Chinese Journal of Organic Chemistry</i> , 2022, 42, 830.	0.6	3
11058	A theoretical approach for homogeneous CO ₂ reduction by Ni(cyclam): substituents with intra-molecular hydrogen transfer. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 2691-2696.	3.0	3
11059	Synthesis of an advanced metal-guided photochromic system for molecular keypad lock: detailed experimental findings and theoretical understanding. <i>New Journal of Chemistry</i> , 2022, 46, 8284-8302.	1.4	5
11060	UV-selective organic absorbers for the cosensitization of greenhouse-integrated dye-sensitized solar cells: synthesis and computational study. <i>RSC Advances</i> , 2022, 12, 11420-11435.	1.7	8
11061	Realizing high-rate aqueous zinc-ion batteries using organic cathode materials containing electron-withdrawing groups. <i>Sustainable Energy and Fuels</i> , 2022, 6, 2523-2531.	2.5	21
11062	The role of the donor group and electron-accepting substitutions inserted in ĩ-linkers in tuning the optoelectronic properties of DĩA dye-sensitized solar cells: a DFT/TDDFT study. <i>RSC Advances</i> , 2022, 12, 11557-11573.	1.7	19
11063	Highly-fluorescent BODIPY-functionalised metallacages as drug delivery systems: synthesis, characterisation and cellular accumulation studies. <i>Dalton Transactions</i> , 2022, 51, 7476-7490.	1.6	8
11064	Research on the evaluation method of eco-friendly gas in the application of high voltage circuit breaker. , 2022, , .		0
11065	Intercalation of metalĩaluminum layered double hydroxides with anionic surfactants: Experimental and density functional theory studies. <i>AIP Advances</i> , 2022, 12, 045217.	0.6	1
11066	Radical Reactivity of the Biradical [ĩ...P(ĩĩTer) ₂ Pĩ...] and Isolation of a Persistent PhosphorusĩCantered Monoradical [ĩ...P(ĩĩTer) ₂ PĩEt]. <i>Chemistry - A European Journal</i> , 2022, 28, .		9

#	ARTICLE	IF	CITATIONS
11067	Mapping the energy level alignment at donor/acceptor interfaces in non-fullerene organic solar cells. <i>Nature Communications</i> , 2022, 13, 2046.	5.8	41
11068	Modified <sc>COSMOÜNIFAC</sc> model for ionic liquidâ<sc>CO₂</sc> systems and molecular dynamic simulation. <i>AIChE Journal</i> , 2022, 68, .	1.8	5
11069	Substitution-induced Nonplanarity of 3-Fluorothioanisole in the First Electronically Excited State. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2541-2550.	1.1	0
11070	An unusual reaction of 1,1-diamino-2-nitro-2-(1H-triazol-5-yl)ethene and hydrazine: The synthesis of a dihydrotetrazine bridged energetic compound. <i>Energetic Materials Frontiers</i> , 2022, 3, 172-176.	1.3	1
11071	Revisiting the trapping of noble gases (HeâKr) by the triatomic H3+ and Li3+ species: a density functional reactivity theory study. <i>Journal of Molecular Modeling</i> , 2022, 28, 122.	0.8	2
11072	Tuning the structures of polypyridinium salts as bifunctional cathode interfacial layers for all-solution-processed red quantum-dot light-emitting diodes. <i>Chinese Chemical Letters</i> , 2023, 34, 107411.	4.8	0
11073	Experimental spectroscopic, molecular structure, electronic solvation, biological prediction and topological analysis of 2, 4, 6-tri (propan-2-yl) benzenesulfonyl chloride: An antidepressant agent. <i>Journal of Molecular Liquids</i> , 2022, 358, 119166.	2.3	9
11075	Competitive Delocalized Charge Transfer Boosted by Solvent Induction Strategy for Survivable Colorimetric Detection of ng-Level Urea. <i>Analytical Chemistry</i> , 2022, 94, 6318-6328.	3.2	7
11076	Efficient lamellar twoâdimensional proton channels derived from dipole interactions in a polyelectrolyte membrane. <i>AIChE Journal</i> , 2022, 68, .	1.8	8
11077	Superalkali Coated Rydberg Molecules. <i>Frontiers in Chemistry</i> , 2022, 10, 880804.	1.8	0
11078	A simple spectrophotometric method for the determination of zirconium in UâZr alloy samples in presence of fluoride ions. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2022, 331, 2383-2391.	0.7	1
11079	Meta-Hybrid Density Functional Theory Prediction of the Reactivity, Stability, and IGM of Azepane, Oxepane, Thiepane, and Halogenated Cycloheptane. <i>ACS Omega</i> , 2022, 7, 13704-13720.	1.6	60
11080	The effects of ï€-conjugation-substitution on ESIPT process for Oxazoline-substituted hydroxyfluorenes. <i>Chinese Physics B</i> , 0, , .	0.7	0
11082	Assessing Alkene Reactivity toward Cytochrome P450-Mediated Epoxidation through Localized Descriptors and Regression Modeling. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1979-1987.	2.5	4
11083	Probing the Difference in the Complexation of Trivalent Actinides and Lanthanides with a Tridentate N,O-Hybrid Ligand: Spectroscopy, Thermodynamics, and Coordination Modes. <i>Inorganic Chemistry</i> , 2022, 61, 6063-6072.	1.9	4
11084	Through-Space Interaction of Tetraphenylethylene: What, Where, and How. <i>Journal of the American Chemical Society</i> , 2022, 144, 7901-7910.	6.6	72
11085	Enchant O Hâ...âO interactions in hydrated 6-amino-2-methoxypyrimidin-4(3H)one resembles as water flow in the channel: Crystallographic and theoretical investigations. <i>Journal of Molecular Structure</i> , 2022, 1263, 133098.	1.8	2
11086	Odd-Number Cyclo[<i>n</i>]Carbons Sustaining Alternating Aromaticity. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2445-2452.	1.1	7

#	ARTICLE	IF	CITATIONS
11087	Engineering a passivating electric double layer for high performance lithium metal batteries. <i>Nature Communications</i> , 2022, 13, 2029.	5.8	113
11088	Synthesis and Application of Poly Methyl Indole-4-Carboxylate with Blue Light Blocking Properties. <i>European Polymer Journal</i> , 2022, , 111198.	2.6	0
11089	Tetraanionic arachno- β -Carboranyl Ligand Imparts Strong Axiality to Terbium(III) Single-Molecule Magnets. <i>Angewandte Chemie</i> , 0, , .	1.6	0
11090	Constructing Planar C-N Bond-Linked Bi-Triazole High-Energy Explosives via the Formation of Salts. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 898-908.	2.0	3
11091	B ₆ C ₈ and its anion: a planar dodecagon reinforced by the central strong B-B single bond and aromaticity. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1.	0.5	1
11092	Chloride substitution on 2-hydroxy-3,4,6-trimethoxyphenylchalcones improves in vitro selectivity on <i>Trypanosoma cruzi</i> strain Y. <i>Chemico-Biological Interactions</i> , 2022, 361, 109920.	1.7	7
11093	Density functional theory, Monte Carlo simulation and non-covalent interaction study for exploring the adsorption and corrosion inhibiting property of double azomethine functionalised organic molecules. <i>Journal of Adhesion Science and Technology</i> , 2022, 36, 2732-2760.	1.4	15
11094	Partial Metalation of Porphyrin Moieties in Hydrogen-Bonded Organic Frameworks Provides Enhanced CO ₂ Photoreduction Activity. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	4
11095	Inactivation Mechanism of Algal Chlorophyll by Allelochemical Quercetin. <i>Bulletin of Environmental Contamination and Toxicology</i> , 2022, , 1.	1.3	0
11096	Pd-Catalyzed ¹³ C-Acetoxylation of Alkylamides: Structural Influence of Directing Groups. <i>Journal of Organic Chemistry</i> , 2022, 87, 6378-6386.	1.7	5
11097	Theoretically exploring the bonding properties of trivalent transuranic elements with 2-amino-2-oxyethoxy) acetic acid. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	4
11098	Physicochemical Insights on Terahertz Wave Diminished Side Effects of Drugs from Slow Dissociation. <i>ACS Nano</i> , 2022, 16, 8419-8426.	7.3	14
11099	Theoretical Insights into the Selective Separation of Am(III)/Eu(III) Using Hydrophilic Triazolyl-Based Ligands. <i>Inorganic Chemistry</i> , 2022, 61, 6110-6119.	1.9	18
11100	Theoretical insight of ciprofloxacin removal from water using boron nitride (B ₁₂ N ₁₂) nanocage. <i>Surfaces and Interfaces</i> , 2022, 31, 101982.	1.5	5
11101	Insights into solvation, chemical reactivity, structural, vibrational and anti-hypertensive properties of a thiazolopyrimidine derivative by DFT and MD simulations. <i>Structural Chemistry</i> , 0, , 1.	1.0	2
11102	Using Physical Organic Chemistry Knowledge to Predict Unusual Metabolites of Synthetic Phenolic Antioxidants by Cytochrome P450. <i>Chemical Research in Toxicology</i> , 2022, 35, 840-848.	1.7	3
11103	Theoretical Approach for the Luminescent Properties of Ir(III) Complexes to Produce Red-Green-Blue LEC Devices. <i>Molecules</i> , 2022, 27, 2623.	1.7	1
11104	Designing of small organic non-fullerene (NFAs) acceptor molecules with an A-D-A framework for high-performance organic solar cells: A DFT and TD-DFT method. <i>Oxford Open Materials Science</i> , 2022, 2, .	0.5	1

#	ARTICLE	IF	CITATIONS
11105	Efficient demethylation of lignin for polyphenol production enabled by low-cost bifunctional protic ionic liquid under mild and halogen-free conditions. <i>Chemical Engineering Journal</i> , 2022, 443, 136486.	6.6	25
11106	Computational investigation, effects of polar and non-polar solvents on optimized structure with topological parameters (ELF, LOL, AIM, and RDG) of three glycine derivative compounds. <i>Structural Chemistry</i> , 2022, 33, 1295-1319.	1.0	4
11107	Current Trends in Computational Quantum Chemistry Studies on Antioxidant Radical Scavenging Activity. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2639-2658.	2.5	33
11108	Microscopic Insights Into the Formation of Methanesulfonic Acid "Methylamine" Ammonia Particles Under Acid-Rich Conditions. <i>Frontiers in Ecology and Evolution</i> , 2022, 10, .	1.1	1
11109	Confinement-Enhanced Selective Oxidation of Lignin Derivatives to Formic Acid Over Fe-Cu/ZSM-5 Catalysts Under Mild Conditions. <i>ChemSusChem</i> , 2022, 15, .	3.6	1
11110	Superalkali X ₃ O (X = Li, Na, K) doped B ₁₂ N ₁₂ nano-cages as a new drug delivery platform for chlormethine: A DFT approach. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113722.	1.1	18
11111	Mechanism and Origins of Enantioselectivity of Cobalt-Catalyzed Intermolecular Hydroarylation/Cyclization of 1,6-Enynes with <i>N</i> -Pyridylindoles. <i>Journal of Organic Chemistry</i> , 2022, 87, 6438-6443.	1.7	15
11112	First example of N-shaped dipyrrolo[2,3-b:2',3'-e]pyrazine-2,6(1H,5H)-dione based small acceptor materials: Role of cyano (C≡N) free guest acceptors for developing environmental friendly organic solar cells. <i>European Physical Journal Plus</i> , 2022, 137, .	1.2	4
11113	Metal-Free Boron/Phosphorus Co-Doped Nanoporous Carbon for Highly Efficient Benzyl Alcohol Oxidation. <i>Advanced Science</i> , 2022, 9, e2200518.	5.6	16
11114	Reactivity, stability, and thermodynamics of para-methylpyridinium-based ionic liquids: Insight from DFT, NCI, and QTAIM. <i>Journal of Ionic Liquids</i> , 2022, 2, 100030.	1.0	65
11115	Keto-enol tautomerism from the electron delocalization perspective. <i>Journal of Computational Chemistry</i> , 2022, , .	1.5	6
11116	Possible catalytic activity of N,N-coordinated mono-cationic copper bound Pyrazol-1-yl(1H-pyrrol-2-yl)methanone complex: a computational study. <i>Proceedings of the Indian National Science Academy</i> , 0, , 1.	0.5	0
11117	New Insight into a Fenton-like Reaction Mechanism over Sulfidated ^{II} -FeOOH: Key Role of Sulfidation in Efficient Iron(III) Reduction and Sulfate Radical Generation. <i>Environmental Science & Technology</i> , 2022, 56, 5542-5551.	4.6	35
11118	Scaffold-Hopping Approach To Identify New Chemotypes of Dimpropyridaz. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 11109-11122.	2.4	5
11119	Tetraanionic arachno-Carboranyl Ligand Imparts Strong Axiality to Terbium(III) Single-Molecule Magnets. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	11
11120	Photodeprotection Reaction Mechanisms of Caged Species Utilizing a Photochromism Function. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3417-3423.	2.1	1
11121	Phosphoric acid assisted synthesis of fluorescent carbon dots from waste biomass for detection of Cr(VI) in aqueous media. <i>Materials Chemistry and Physics</i> , 2022, 286, 126133.	2.0	25
11122	Insights into the Mechanism of Enantioselective Copper-Catalyzed Ring-Opening Allylic Alkylation of Cyclopropanols. <i>Advanced Synthesis and Catalysis</i> , 2022, 364, 1855-1862.	2.1	5

#	ARTICLE	IF	CITATIONS
11123	Engineering and Structural Insights of a Novel BBI-like Protease Inhibitor Livisin from the Frog Skin Secretion. <i>Toxins</i> , 2022, 14, 273.	1.5	5
11124	Origin of iodine preferential attack at sulfur in phosphorothioate and subsequent P-O or P-S bond dissociation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2119032119.	3.3	8
11125	Accurate Ring Strain Energies of Unsaturated Three-Membered Heterocycles with One Group 13 ⁺ 16 Element. <i>Inorganic Chemistry</i> , 2022, 61, 6459-6468.	1.9	13
11126	Experimental Spectroscopic, Quantum Computational, Hirshfeld Surface, Molecular Docking, and Electronic Excitation Studies on an Antibiotic Agent: SDZ. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 3122-3146.	1.4	1
11127	Electron transfer and energy barrier co-modulation: Unravelling the role of sequential fluorination in high-rate CO ₂ photoreduction on conjugated organic polymers. <i>Applied Catalysis A: General</i> , 2022, 638, 118618.	2.2	3
11128	Impact of donor acidity on $\hat{1}/2$ \langle sub \rangle C \hat{a} $\%_{i}$ N \langle sub \rangle and $\hat{1}/2$ \langle sub \rangle O \hat{a} $\%_{i}$ H \langle sub \rangle spectral shifts in O-H \hat{A} \cdot \hat{A} \cdot N \hat{a} $\%_{i}$ C H-bonded complexes between nitriles and alcohols: a combined IR spectroscopic and quantum chemical investigation. <i>Molecular Physics</i> , 0, , .	0.8	0
11129	Early Transition Metals Strengthen the B ₂ Bond in MB ₂ Complexes. <i>Journal of the American Chemical Society</i> , 2022, 144, 7557-7561.	6.6	4
11130	Non-Stabilized Vinyl Anion Equivalents from Styrenes by N-Heterocyclic Carbene Catalysis and Its Use in Catalytic Nucleophilic Aromatic Substitution. <i>Journal of the American Chemical Society</i> , 2022, 144, 6714-6718.	6.6	17
11131	A combined experimental and theoretical studies of two new decavanadate: (C ₆ N ₂ H ₉) ₄ [H ₂ V ₁₀ O ₂₈] \hat{A} \cdot 4H ₂ O and (C ₇ H ₉ NF) ₄ [H ₂ V ₁₀ O ₂₈] \hat{A} \cdot 2H ₂ O. <i>Journal of Molecular Structure</i> , 2022, 1262, 133085.	1.8	3
11132	Synthesis, structures, and photophysical properties of orange-red emissive Cu(I) complexes of 9,9-dimethyl-4,5-bis(diphenylphosphino)-9H-xanthene (Xantphos) with the substituted N-heterocycle carbene (NHC) ligand. <i>Journal of Organometallic Chemistry</i> , 2022, , 122356.	0.8	0
11133	Selenization governs the intrinsic activity of copper-cobalt complexes for enhanced non-radical Fenton-like oxidation toward organic contaminants. <i>Journal of Hazardous Materials</i> , 2022, 435, 128958.	6.5	17
11134	Partial Metalation of Porphyrin Moieties in Hydrogen \hat{B} Bonded Organic Frameworks Provides Enhanced CO ₂ Photoreduction Activity. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	42
11135	Impact of Covalent Modifications on the Hydrogen Bond Strengths in Diaminotriazine Supramolecules. <i>ChemPhysChem</i> , 2022, 23, .	1.0	2
11136	A potent anesthetic drug salt: experimental and computational studies. <i>Journal of Molecular Structure</i> , 2022, 1263, 133049.	1.8	3
11137	A DFT/TD-DFT Study on the ESIPT-Type Flavonoid Derivatives with High Emission Intensity. <i>Materials</i> , 2022, 15, 2896.	1.3	8
11138	Zinc(II) complex: Spectroscopic, physicochemical calculations, anti-inflammatory and in silico molecular docking studies. <i>Journal of Molecular Structure</i> , 2022, 1263, 133070.	1.8	6
11139	Interaction behavior between bisphenol AP and pepsin: Insights from density functional theory, and spectroscopic and molecular dynamic simulation. <i>Quality Assurance and Safety of Crops and Foods</i> , 2022, 14, 1-12.	1.8	3
11140	Genuine Pores in a Stable Zinc Phosphite for High H ₂ Adsorption and CO ₂ Capture. <i>Chemistry - A European Journal</i> , 2022, , .	1.7	2

#	ARTICLE	IF	CITATIONS
11141	Assessment of alkali and alkaline earth metals doped cubanes as high-performance nonlinear optical materials by first-principles study. <i>Journal of Science: Advanced Materials and Devices</i> , 2022, 7, 100457.	1.5	8
11142	Thermosensitive Microgels Containing AIEgens: Enhanced Luminescence and Distinctive Photochromism for Dynamic Anticounterfeiting. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 17794-17805.	4.0	17
11143	Protonation of Borylated Carboxonium Derivative [2,6-B10H8O2CCH3] ⁺ : Theoretical and Experimental Investigation. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4190.	1.8	8
11144	Ligand Shell Isomerization Induces Different Fluorescence Origins of Two Au ₂₈ Nanoclusters. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3718-3725.	2.1	5
11145	Theoretical study of heptadentate bispidine ligands for radiopharmaceutic applications. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113716.	1.1	1
11146	Mass spectral and theoretical investigations of C [±] bond cleavages in the disulfide-containing peptide TTCPYCKK and its analogues. <i>Rapid Communications in Mass Spectrometry</i> , 2022, 36, e9315.	0.7	0
11147	A Copper(II)-Nitrite Complex Hydrogen-Bonded to a Protonated Amine in the Second-Coordination Sphere. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	3
11148	Origin of enantioselectivity and product-distribution control in isocyanide-based multicomponent reaction catalysed by chiral N, N'-dioxide-Mg(II) complex. <i>Molecular Catalysis</i> , 2022, 524, 112277.	1.0	2
11149	Theoretical study on the synthesis of vinyl acetate from acetylene and acetic acid over nonmetallic catalysts with different carbon-nitrogen ratios. <i>Molecular Catalysis</i> , 2022, 524, 112299.	1.0	0
11150	Insights into the sulfite activation by cobalt(II) sulfide for acetaminophen removal: A synergistic catalysis and DFT calculations. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 107709.	3.3	5
11151	Toxic potential of Poly-hexamethylene biguanide hydrochloride (PHMB): A DFT, AIM and NCI analysis study with solvent effects. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113709.	1.1	13
11152	Reaction mechanism of the gas-phase pyrolysis of N-Acetylthiourea and N,N'-diacetylthiourea: A theoretical study based in density functional theory. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113702.	1.1	0
11153	Structural insights and supramolecular description of Gliclazide and its Impurity F. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113707.	1.1	2
11154	A first-principles study on the adsorption properties of phosphorene oxide for pollutant removal from water. <i>Journal of Molecular Liquids</i> , 2022, 357, 119103.	2.3	2
11155	Optimization, characterization, and evaluation of carrageenan/alginate/poloxamer/curcumin hydrogel film as a functional wound dressing material. <i>Materials Today Communications</i> , 2022, 31, 103528.	0.9	13
11156	Zwitterionic ionic liquids modulating two-dimensional hierarchically porous zeolitic imidazolate framework composites. <i>Journal of Colloid and Interface Science</i> , 2022, 620, 365-375.	5.0	4
11157	Effects of soluble products decomposed from chelato-borate additives on formation of solid electrolyte interface layers. <i>Journal of Power Sources</i> , 2022, 535, 231451.	4.0	17
11158	Aggregation induced emission enhancement and chromism properties of a vinyl bridged naphthalene diimide dimer. <i>Dyes and Pigments</i> , 2022, 203, 110330.	2.0	3

#	ARTICLE	IF	CITATIONS
11159	Energetic material derivatives of insoluble 3,4,5-triamino-1-tetrazolyl-1,2,4-triazole (TATT). Journal of Molecular Structure, 2022, 1262, 133099.	1.8	2
11160	Portable visual assay of Bacillus anthracis biomarker based on ligand-functionalized dual-emission lanthanide metal-organic frameworks and smartphone-integrated mini-device. Journal of Hazardous Materials, 2022, 434, 128914.	6.5	24
11161	Theoretical study for the TADF nature of through-space conjugated [2.2]paracyclophane derivatives and the design for red-light emission. Dyes and Pigments, 2022, 202, 110268.	2.0	5
11162	Preparation, structure and optical properties of mixed stacked cocrystals of 2,2':6''-Terpyridine and 1,2,4,5-tetracyanobenzene. Journal of Luminescence, 2022, 247, 118903.	1.5	1
11163	Improved stability of picric acid: 1-aminopyrene™ charge-transfer complex: Synthesis, characterization, energetic performance and molecular docking study with B-DNA. Journal of Molecular Structure, 2022, 1262, 133058.	1.8	4
11164	Quantitative molecular surface analysis of doxofylline and its thermodynamic solubility behavior in aqueous solutions. Journal of Chemical Thermodynamics, 2022, 171, 106792.	1.0	3
11165	In situ interfacial polymerization of lithiophilic COF@PP and POP@PP separators with lower shuttle effect and higher ion transport for high-performance Li-S batteries. Chemical Engineering Journal, 2022, 442, 136352.	6.6	27
11166	Spin-states-assistance peroxymonosulfate absorption via Mn doped catalyst with/without light for BPA oxidation: The negative contribution of electrons transfer by light. Chemical Engineering Journal, 2022, 443, 136399.	6.6	18
11167	Efficient degradation of organic pollutants by enhanced interfacial internal electric field induced via various crystallinity carbon nitride homojunction. Applied Catalysis B: Environmental, 2022, 312, 121388.	10.8	45
11168	Preparation, characterization and computational study of mosapride solvates. Journal of Molecular Structure, 2022, 1262, 133082.	1.8	1
11169	One-step supramolecular fabrication of ionic liquid/ZIF-8 nanocomposites for low-energy CO ₂ capture from flue gas and conversion. Fuel, 2022, 322, 124175.	3.4	9
11170	The role of intermolecular interactions of aromatic sandwich dimer ligands for the half-titanocene catalysts: Theoretical study. Chemical Physics, 2022, 559, 111556.	0.9	0
11171	Understanding the geometric structure, electronic and stability properties of anionic germanium-doped magnesium clusters: Gas-phase GeMgn ⁻ (n=12) DFT study. Computational Materials Science, 2022, 210, 111444.	1.4	2
11172	2D Benzodithiophene based conjugated polymer/g-C ₃ N ₄ heterostructures with enhanced photocatalytic activity: Synergistic effect of antibacterial carbazole side chain and main chain copolymerization. Applied Catalysis B: Environmental, 2022, 312, 121401.	10.8	22
11173	Unraveling H ₂ O activation by intermolecular frustrated Lewis pair. Chemical Physics Letters, 2022, 799, 139634.	1.2	5
11188	Regiochemistry of Donor Dendrons Controls the Performance of Thermally Activated Delayed Fluorescence Dendrimer Emitters for High Efficiency Solution-Processed Organic Light-Emitting Diodes. Advanced Science, 2022, 9, e2201470.	5.6	19
11189	Highly Robust Rhenium(I) Bipyridyl Complexes Containing Dipyromethene-BF ₂ Chromophores for Visible Light-Driven CO ₂ Reduction. ChemSusChem, 2022, , .	3.6	5
11190	Two-layer molecular rotors: A zinc dimer rotating over planar hypercoordinate motifs. Journal of Computational Chemistry, 2022, , .	1.5	1

#	ARTICLE	IF	CITATIONS
11191	Synthesis and Magnetic Properties of Antimony-Ligated Co(II) Complexes: Stibines versus Phosphines. <i>Inorganic Chemistry</i> , 2022, 61, 6733-6741.	1.9	5
11192	Investigation of Spatial Orientation and Kinetic Energy of Reactive Site Collision between Benzyl Chloride and Piperidine: Novel Insight into the Microwave Nonthermal Effect. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2690-2705.	1.1	5
11193	Study on Excited State Kinetics and Optical Limiting Performance of Triphenylamine-Based Chalcone Derivatives: Effect of the Molecular π -Conjugated Structure. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3327-3337.	1.2	3
11194	Binding methane to a metal centre. <i>Nature Chemistry</i> , 2022, 14, 801-804.	6.6	13
11195	Structures and chemical bonding of boron-based $B_{12}O$ and $B_{11}Au$ clusters. A counterexample in boronyl chemistry. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 10952-10961.	1.3	3
11196	Synthesis and reactivity of an iridium complex based on a tridentate aminophosphano ligand. <i>Dalton Transactions</i> , 2022, 51, 7142-7153.	1.6	2
11197	Application of amino acid ionic liquids for increasing the stability of DNA in long term storage. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 4383-4397.	2.0	0
11198	DFT and MD investigations of the biomolecules of phenothiazine derivatives: interactions with gold and water molecules and investigations in search of effective drug for SARS-CoV-2. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 4522-4533.	2.0	5
11199	Organometallic-functionalized interfaces for highly efficient inverted perovskite solar cells. <i>Science</i> , 2022, 376, 416-420.	6.0	527
11200	Linker engineering in metal-organic frameworks for dark photocatalysis. <i>Chemical Science</i> , 2022, 13, 6696-6703.	3.7	30
11201	Photoelectron velocity-map imaging spectroscopy of nickel carbide: Examination of the low-lying electronic states. <i>New Journal of Chemistry</i> , 0, , .	1.4	1
11202	On the energetic stability of halogen bonds involving metals: implications in crystal engineering. <i>CrystEngComm</i> , 2022, 24, 4440-4446.	1.3	15
11203	Various bond interactions between NO and anionic gold clusters: a theoretical calculation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 13641-13650.	1.3	1
11204	Combustion Kinetics of N-Propylamine: Theoretical Calculations and Ignition Delay Time Measurements. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11205	Synergistic end-capped engineering on non-fused thiophene ring-based acceptors to enhance the photovoltaic properties of organic solar cells. <i>RSC Advances</i> , 2022, 12, 12321-12334.	1.7	19
11206	A straightforward method to quantify the electron-delocalizing ability of π -conjugated molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11486-11490.	1.3	3
11207	Successive protonation of Lindqvist hexaniobate, $[Nb_6O_{19}]^{8-}$: electronic properties and structural distortions. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 13083-13093.	1.3	2
11208	Drug-nutrient cocrystallization-driven strategy towards self-assembly of milrinone and ferulic acid provides an exemplification in perfecting in vitro/vivo characteristics of anti-heart failure drugs. <i>New Journal of Chemistry</i> , 0, , .	1.4	3

#	ARTICLE	IF	CITATIONS
11209	Achieving halogen bonding enhanced ultra-highly efficient AIE and reversible mechanochromism properties of TPE-based luminogens: position of bromine substituents. <i>Journal of Materials Chemistry C</i> , 2022, 10, 8390-8399.	2.7	14
11210	Nonignorable Involvement of Cl ⁻ , NO ₃ ⁻ , Co ³⁺ , and HCO ₃ ⁻ in the Water: Reevaluation on Degradation Pathways and Toxicity Evolution of Uv-Based Aops for Pcmx Decontamination. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11211	Trinuclear anionic gold clusters bridged by dialkylsilylene and dialkylgermylene. <i>Chemical Communications</i> , 2022, 58, 6705-6708.	2.2	4
11212	Symmetry-breaking charge separation in a nitrogen-bridged naphthalene monoimide dimer. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14007-14015.	1.3	8
11213	S-Scheme Cs ₂ AgBr ₆ /Ag ₃ PO ₄ Heterojunction with Efficient Photocatalysis Performance for H ₂ Production and Organic Pollutant Degradation Under Visible Light. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11214	A C,S bonded quasi-two-coordinate chromium(ⁱⁱ /sc ⁱⁱ) complex showing field-induced slow magnetic relaxation behaviour. <i>Dalton Transactions</i> , 2022, 51, 9218-9222.	1.6	5
11215	Phase transition induced by an external electric field as a buffer to facilitate the initial decomposition of a series of catenated nitrogen energetic systems: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12488-12500.	1.3	3
11216	Bimetallic sites and coordination effects: electronic structure engineering of NiCo-based sulfide for 5-hydroxymethylfurfural electrooxidation. <i>Catalysis Science and Technology</i> , 2022, 12, 3817-3825.	2.1	15
11217	Oxygen Vacancies-Mediated Cu@N-Doped Carbon Nanocomposites for Non-Radical-Dominated Photothermal Catalytic Degradation of Contaminants. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11218	Study of polyphenols from <i>Caesalpinia paraguariensis</i> as \pm -glucosidase inhibitors: kinetics and structure-activity relationship. <i>New Journal of Chemistry</i> , 0, , .	1.4	3
11219	Manipulating room-temperature phosphorescence via lone-pair electrons and empty-orbital arrangements and hydrogen bond adjustment. <i>Journal of Materials Chemistry C</i> , 2022, 10, 8854-8859.	2.7	5
11220	Application of Terahertz Spectroscopy in the Detection of Carbohydrate Isomers. <i>Springer Proceedings in Physics</i> , 2022, , 345-352.	0.1	1
11221	Benzothiadiazole based "hot exciton" materials for red electroluminescence with the maximum external quantum efficiency approaching 10%. <i>Journal of Materials Chemistry C</i> , 2022, 10, 8684-8693.	2.7	9
11222	Anion-anion interaction within Ch(CH ₃) ₃ X ₄ ⁺ (Ch = S, Se, Te; X = Cl, Br, I). <i>Tj ETQg</i> 1 1.0784314 rg	1.3	5
11223	Computational insight into the mechanism and stereoselectivity of cycloaddition between donor-acceptor spirocyclopropane and aldehyde catalyzed by Brønsted acid TsOH. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 4006-4015.	1.5	3
11224	A porphyrin-triazatruxene dyad for ratiometric two-photon fluorescent sensing of intracellular viscosity. <i>Journal of Materials Chemistry B</i> , 0, , .	2.9	3
11225	Preference of Adsorption Sites and Electron Transfer Characteristics of Methyl Orange on Hollow Structured Cobalt-Aluminum Layered Double Hydroxides: Experimental and Dft Investigation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11226	Copper(ii) and Zinc(ii) Complexes of Nicotinic Acid Hydrazide Derivative: Synthesis, Characterization, Density Functional Theory, Anti-Tubercular and Molecular Docking Studies. <i>SSRN Electronic Journal</i> , 0, , .	0.4	1

#	ARTICLE	IF	CITATIONS
11227	Conformational Analysis of Psilocybin: A Computational Approach. SSRN Electronic Journal, 0, , .	0.4	0
11228	Platinum(II)-gold(I) heterotrinnuclear complexes with β -diarylamine-functionalized acetylide ligands for red electroluminescence. Inorganic Chemistry Frontiers, 2022, 9, 3156-3164.	3.0	4
11229	Ultrasensitive and Rapid Colorimetric Detection of Urotropin Boosted by Effective Electrostatic Probing and Non-Covalent Sampling. SSRN Electronic Journal, 0, , .	0.4	0
11230	Insight into non-covalent interactions in a [Cu(N ₃) ₄] ²⁺ bridged hetero-pentanuclear copper(II)/sodium complex with special emphasis on the strong CH \cdots [Cu(N ₃) ₃] ₄ interactions. New Journal of Chemistry, 2022, 46, 11286-11295.	1.4	7
11231	Molecular engineering of covalent triazine frameworks for highly enhanced photocatalytic aerobic oxidation of sulfides. Journal of Materials Chemistry A, 2022, 10, 12489-12496.	5.2	35
11232	Regulating Excited State of Sulfone-Locked Triphenylamine Heteroaromatics for High-Efficiency Ultralong Room-Temperature Phosphorescence. SSRN Electronic Journal, 0, , .	0.4	0
11233	Investigation of Charge Accumulation and Decay Processes in Epoxy-Based Composites Using Quantum Chemical Calculations Under the Effect of Electric Field. IEEE Transactions on Dielectrics and Electrical Insulation, 2022, 29, 883-890.	1.8	4
11234	A mitochondria-targeted rhodol fluorescent probe for imaging of hydrogen peroxide in living cells. Analytical Methods, 2022, 14, 2117-2122.	1.3	1
11235	Rational Design of Freestanding and High-Performance Thick Electrode from Carbon Foam Modified with Polypyrrole/Polydopamine for Supercapacitors. SSRN Electronic Journal, 0, , .	0.4	0
11236	Bottom-Up Synthesis of Cationic Porphyrin-Based Porous Organic Polymers for Highly Efficient and Selective Recovery of Gold. SSRN Electronic Journal, 0, , .	0.4	0
11237	Fluoride-Selective Chemosensor Based on an Anion Imprinted Fluorescent Polymer. SSRN Electronic Journal, 0, , .	0.4	0
11238	Structural modification on tetraphenylpyrazine: from polarity enhanced emission to polarity quenching emission and its intramolecular charge transfer mechanism. Journal of Materials Chemistry C, 2022, 10, 8174-8180.	2.7	13
11239	Ultralong blue room-temperature phosphorescence by cycloalkyl engineering. Materials Chemistry Frontiers, 2022, 6, 1606-1614.	3.2	15
11240	Protonation-induced charge transfer and polaron formation in organic semiconductors doped by Lewis acids. RSC Advances, 2022, 12, 13999-14006.	1.7	3
11241	Adsorption properties of pyramidal superatomic molecules based on the structure framework of Au ₂₀ cluster. Physical Chemistry Chemical Physics, 2022, , .	1.3	3
11242	A theoretical study of asymmetric ketone hydrogenation catalyzed by Mn complexes: from the catalytic mechanism to the catalyst design. Physical Chemistry Chemical Physics, 2022, 24, 13365-13375.	1.3	8
11243	Sniffing out camphor: the fine balance between hydrogen bonding and London dispersion in the chirality recognition with \pm -fenchol. Physical Chemistry Chemical Physics, 2022, , .	1.3	1
11244	Vibrationally excited intermolecular potential energy surfaces and the predicted near infrared overtone (ν _{OH} = 2 $\hat{+}$ 0) spectra of a H ₂ O \cdots Ne complex. Physical Chemistry Chemical Physics, 2022, 24, 12937-12949.	1.3	2

#	ARTICLE	IF	CITATIONS
11245	Molecular screening of ionic liquids for CO ₂ absorption and molecular dynamic simulation. <i>Open Chemistry</i> , 2022, 20, 379-387.	1.0	2
11246	Achieving Full-Spectrum-Driven Simultaneous Hydrogen Evolution and Organic Pollutants Degradation Through the Sensitization of Ag ₃ PO ₄ by Double Perovskite Quantum Dots. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11247	Strong second order nonlinear optical properties of azulene-based porphyrin derivatives. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 13275-13285.	1.3	3
11248	Mixed superalkalis are a better choice than pure superalkalis for B ₁₂ N ₁₂ nanocages to design high-performance nonlinear optical materials. <i>Dalton Transactions</i> , 2022, 51, 8437-8453.	1.6	10
11249	Iodous acid is a more efficient nucleation precursor than iodic acid. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 13651-13660.	1.3	11
11250	A Comprehensive DFT Investigation of the Adsorption of Polycyclic Aromatic Hydrocarbons onto Graphene. <i>Computation</i> , 2022, 10, 68.	1.0	6
11251	An optoelectronic study to design better benzodithiophene (BDT) donor unit based non-fullerene organic solar cells (OSCs): the DFT approaches. <i>Chemical Papers</i> , 2022, 76, 4977-4987.	1.0	14
11252	Synthesis, Electrochemical Studies, Molecular Docking, and Biological Evaluation as an Antimicrobial Agent of 5-Amino-6-cyano-3-hydroxybenzo[<i>c</i>]coumarin Using Ni-Cu-Al-CO ₃ Hydroxalcite as a Catalyst. <i>ACS Omega</i> , 2022, 7, 15718-15727.	1.6	1
11253	DFT exploration to tune the silyl group as anchoring unit on the performance of dye-sensitized solar cells: an approach to suppress dye leaching from semiconductor surface. <i>Journal of Molecular Modeling</i> , 2022, 28, 131.	0.8	6
11254	Anticancer effects of dendrocandine (DDCD) against AKT in HepG2 cells using molecular modeling, DFT, and in vitro study. <i>Structural Chemistry</i> , 0, , 1.	1.0	0
11255	Spectroscopic, conformational analysis, structural benchmarking, excited state dynamics, and the photovoltaic properties of Enalapril and Lisinopril. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100500.	1.3	56
11256	Sodium Tanshinone IIA Sulfonate as a Potent IDO1/TDO2 Dual Inhibitor Enhances Anti-PD1 Therapy for Colorectal Cancer in Mice. <i>Frontiers in Pharmacology</i> , 2022, 13, 870848.	1.6	9
11257	Black Titanium-Oxo Clusters with Ultralow Band Gaps and Enhanced Nonlinear Optical Performance. <i>Journal of the American Chemical Society</i> , 2022, 144, 8153-8161.	6.6	39
11258	Feasibility of p-Doped Molecular Crystals as Transparent Conductive Electrodes via Virtual Screening. <i>Chemistry of Materials</i> , 2022, 34, 4050-4061.	3.2	0
11259	A comprehensive theoretical analysis on the intermolecular hydrogen bond interactions with the Lewis bases having multiple hydrogen bonding ability. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	0
11260	Theoretical Study on the Atom-Substituted Quinazoline Derivatives with Faint Emission as Potential Sunscreens. <i>ACS Omega</i> , 2022, 7, 14848-14855.	1.6	5
11261	Type II porous ionic liquid based on metal-organic cages that enables l-tryptophan identification. <i>Nature Communications</i> , 2022, 13, 2353.	5.8	20
11262	Unveiling the nature of interactions in the supramolecular complex of Cucurbit [7-8] uril with ascorbic acid, dopamine and uric acid for biosensing applications: a computational study. <i>Structural Chemistry</i> , 2022, 33, 1321-1330.	1.0	2

#	ARTICLE	IF	CITATIONS
11263	Insight into Spodiumâ€“ Bonding Characteristics of the MX ₂ (M = Zn, Cd and Hg; X = Cl, Br and I) Complexesâ€“ A Theoretical Study. <i>Molecules</i> , 2022, 27, 2885.	1.7	4
11264	Probing fluorination promoted sodiophilic sites with model systems of F16CuPc and CuPc. <i>Frontiers of Optoelectronics</i> , 2022, 15, 1.	1.9	2
11265	Synthesis, X-ray, Hirshfeld, and AIM Studies on Zn(II) and Cd(II) Complexes with Pyridine Ligands. <i>Crystals</i> , 2022, 12, 590.	1.0	1
11266	A fluorescent film sensor for high-performance detection of <i>Listeria monocytogenes</i> via vapor sampling. <i>Aggregate</i> , 2023, 4, .	5.2	8
11267	Are Vanadium Intermediates Suitable Mimics in Non-Heme Iron Enzymes? An Electronic Structure Analysis. <i>ACS Catalysis</i> , 2022, 12, 5489-5501.	5.5	5
11268	Binding and Degradation Reaction of Hydroxide Ions with Several Quaternary Ammonium Head Groups of Anion Exchange Membranes Investigated by the DFT Method. <i>Molecules</i> , 2022, 27, 2686.	1.7	12
11269	Theoretical insights into the reduction mechanism of neptunyl nitrate by hydrazine derivatives. <i>Radiochimica Acta</i> , 2022, 110, 471-480.	0.5	1
11270	Dihydroisatropolone C from <i>Streptomyces</i> and Its Implication in Tropolone-Ring Construction for Isatropolone Biosynthesis. <i>Molecules</i> , 2022, 27, 2882.	1.7	0
11271	Experimental and Molecular Modeling Studies on the Complexation of Chromium(III) with the Angiotensin-Converting Enzyme Inhibitor Captopril. <i>ACS Omega</i> , 2022, 7, 15909-15918.	1.6	0
11272	Boosting the Optical Absorption of Melanin-like Polymers. <i>Macromolecules</i> , 2022, 55, 3493-3501.	2.2	33
11273	Theoretical Study on Nonlinear Optical Properties of M3-Phenalenyl and M3O-Phenalenyl (M = Li, Na, K) Molecules. <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, S95-S100.	0.1	1
11274	Theoretical study on Xeâ€“N non-covalent interactions: Three hybridization N with XeO ₃ and XeOF ₂ . <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 322-330.	0.6	9
11275	Regulation of excited-state intramolecular proton transfer process and photophysical properties for benzoxazole isothiocyanate fluorescent dyes by changing atomic electronegativity. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 331-337.	0.6	2
11276	Comparison of Nitrogen Activation on Trinuclear Niobium and Tungsten Sulfide Clusters Nb ₃ S _n and W ₃ S _n (n=0, 1, 2, 3): A DFT Study. <i>ChemPhysChem</i> , 2022, 23, e202200124.	1.0	4
11277	Synthesis, Experimental and Theoretical Study of Azidochromones. <i>Molecules</i> , 2022, 27, 2636.	1.7	1
11278	Structures, electronic and thermodynamic properties of NiB ₂ and their anions: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	1
11279	Construction of a Novel Closed-Loop Livestock Waste Valorization Paradigm: Bridging Manure and Ammonia Gas via Phosphate-Doped Hydrochar. <i>ACS ES&T Engineering</i> , 2022, 2, 1732-1744.	3.7	2
11280	Minoxidil Multi-Component Crystals with Aromatic Carboxylic Acids: Theoretical Calculation and Structural Analysis. <i>Crystal Growth and Design</i> , 2022, 22, 3941-3953.	1.4	6

#	ARTICLE	IF	CITATIONS
11281	Efficient recovery of aromatic compounds from the wastewater of styrene monomer and propylene oxide co-production plant via hypercrosslinked aryl-rich starch- β -cyclodextrin polymeric sorbent. Chinese Journal of Chemical Engineering, 2022, 49, 150-160.	1.7	6
11282	Synthesis and Crystal Structure of a New Hexavanadate Hybrid with Alkynyl Ligands. Journal of Chemical Crystallography, 0, , .	0.5	0
11283	The Stibium Bond or the Antimony-Centered Pnictogen Bond: The Covalently Bound Antimony Atom in Molecular Entities in Crystal Lattices as a Pnictogen Bond Donor. International Journal of Molecular Sciences, 2022, 23, 4674.	1.8	10
11284	Theoretical investigation and reconsideration of intramolecular proton-transfer-induced the twisted charge-transfer for the fluorescent sensor to detect the aluminum ion. Structural Chemistry, 2022, 33, 1355-1364.	1.0	3
11285	P π -Ru-Complexes with a Chelate-Bridge-Switch: A Comparison of 2-Picolyl and 2-Pyridyloxy Moieties as Bridging Ligands. Molecules, 2022, 27, 2778.	1.7	1
11286	Ion-Specific Effects on Vesicle-to-Micelle Transitions of an Amino Acid Surfactant Probed by Chemical Trapping. Langmuir, 2022, 38, 6295-6304.	1.6	6
11287	Palladium Catalysis Featuring Attractive Noncovalent Interactions Enabled Highly Enantioselective Access to β -Quaternary γ -Lactams. ACS Catalysis, 2022, 12, 5559-5564.	5.5	6
11288	Energy transfer processes in excited states of {[Ir(N ^C) ₂ (N ^N)] ⁺ Rhodamine} dyad; experimental and theoretical study. ChemPhotoChem, 0, , .	1.5	2
11289	Symmetrical end-capped molecular engineering of star-shaped triphenylamine-based derivatives having remarkable photovoltaic properties for efficient organic solar cells. Journal of Molecular Modeling, 2022, 28, 132.	0.8	2
11290	Aurophilic Interactions in Cationic Three-Coordinate Gold(I) Bipyridyl/Isocyanide Complex. Crystals, 2022, 12, 613.	1.0	7
11291	Disrupting bonding in azoles through beryllium bonds: Unexpected coordination patterns and acidity enhancement. Journal of Chemical Physics, 0, , .	1.2	2
11292	Ionic Liquid-Based Redox Active Electrolytes for Supercapacitors. Advanced Functional Materials, 2022, 32, .	7.8	40
11293	Solution-Processed Yellow Organic Light-Emitting Diodes Based on Two New Ionic Ir (III) Complexes. Molecules, 2022, 27, 2840.	1.7	6
11294	Small molecule activation and dehydrogenation of an amine-borane system using frustrated Lewis pairs. Structural Chemistry, 2022, 33, 1853-1865.	1.0	9
11295	Synthesis, Theoretical Calculation, and Biological Studies of Mono- and Diphenyltin(IV) Complexes of N-Methyl-N-hydroxyethylthiocarbamate. Molecules, 2022, 27, 2947.	1.7	3
11296	Theoretical Insights on the Two-Dimensional Transitional Metal Trihydroxytriaminophenalenyl for Highly Efficient Carbon Dioxide Electroreduction. Journal of the Electrochemical Society, 2022, 169, 056512.	1.3	0
11297	High-Voltage Organic Cathodes for Zinc-Ion Batteries through Electron Cloud and Solvation Structure Regulation. Angewandte Chemie - International Edition, 2022, 61, .	7.2	60
11298	Molecular simulations of the effects of substitutions on the dissolution properties of amorphous cellulose acetate. Carbohydrate Polymers, 2022, 291, 119610.	5.1	7

#	ARTICLE	IF	CITATIONS
11299	Static, dynamic nonlinear optical (NLO) response and electride characteristics of superalkalis doped star like C6S6Li6. <i>Surfaces and Interfaces</i> , 2022, 31, 102044.	1.5	9
11300	Photo-thermo semi-hydrogenation of acetylene on Pd1/TiO2 single-atom catalyst. <i>Nature Communications</i> , 2022, 13, 2648.	5.8	61
11301	Influence of an Oriented External Electric Field on the Mechanism of Double Proton Transfer between Pyrazole and Guanidine: from an Asynchronous Plateau Transition State to a Synchronous or Stepwise Mechanism. <i>Journal of Physical Chemistry A</i> , 2022, , .	1.1	2
11302	Heteroanionic Melilite Oxysulfide: A Promising Infrared Nonlinear Optical Candidate with a Strong Second-Harmonic Generation Response, Sufficient Birefringence, and Wide Bandgap. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 23645-23652.	4.0	33
11303	Crystal Growth, Structural, Vibrational, Effects of Hydrogen Bonding (C-Hâ€¦O and C-Hâ€¦N), Chemical Reactivity, Antimicrobial Activity, Inhibitory Effects and Molecular Dynamic Simulation of 4-Methoxy-N-(Nitrobenzylidene)-Aniline. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 2690-2744.	1.4	9
11304	Mechanisms and Kinetics Studies of Butylated Hydroxytoluene Degradation to Isobutene. <i>Journal of Physical Chemistry A</i> , 2022, , .	1.1	2
11305	Quantum Chemistry Study on the Structures and Electronic Properties of Bimetallic Ca2-Doped Magnesium Ca2Mgn (n = 1â€“15) Clusters. <i>Nanomaterials</i> , 2022, 12, 1654.	1.9	5
11306	Cobalt(III)/Chiral Carboxylic Acidâ€Catalyzed Enantioselective Synthesis of Benzothiadiazineâ€1â€xides via CâˆH Activation. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	6
11307	ESIPT and AIE characteristics of three Schiff base derivatives and the relevant photophysical mechanism analyses. <i>Journal of Luminescence</i> , 2022, 248, 118951.	1.5	8
11308	Reaction mechanism study on transesterification in synthesis of thermotropic liquid crystalline polymer catalyzed by zinc(II) carboxylate: A combination of DFT and kinetics analyses. <i>Chemical Engineering Journal</i> , 2022, 446, 136848.	6.6	9
11309	Theoretical study on aggregation-induced emission of new multi-layer 3D chiral molecules. <i>Molecular Simulation</i> , 0, , 1-10.	0.9	0
11310	Integrating Bi@C Nanospheres in Porous Hard Carbon Frameworks for Ultrafast Sodium Storage. <i>Advanced Materials</i> , 2022, 34, e2202673.	11.1	93
11311	Synthesis, Characterization and Photophysical Properties of Mesoionic <i>N</i>-â€Heterocyclic Imines. <i>Chemistry - an Asian Journal</i> , 2022, 17, e202200281.	1.7	6
11312	Variation in electrophilicity on electronic excitation. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	9
11313	3Dâ€QSAR, Molecular Docking and Molecular Dynamics Analysis of 1,2,3,4â€Tetrahydroquinoxalines as BRD4/BD2 Inhibitors. <i>ChemistrySelect</i> , 2022, 7, .	0.7	3
11314	Redox Properties of <i>N,Nâ€2</i>-Disubstituted Dihydrophenazine and Dihydrodibenzo[<i>a,c</i>]phenazine: The First Isolation of Their Crystalline Radical Cations and Dications. <i>Crystal Growth and Design</i> , 2022, 22, 3587-3593.	1.4	8
11315	Harnessing Greenhouse Gases Absorption by Doped Fullerenes with Externally Oriented Electric Field. <i>Molecules</i> , 2022, 27, 2968.	1.7	3
11316	Substantially Promoted Energy Density of Li CF_x Primary Battery Enabled by Li⁺-DMP Coordinated Structure. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 6217-6229.	3.2	9

#	ARTICLE	IF	CITATIONS
11317	A DFT investigation on theranostic potential of alkaline earth metal doped phosphorenes for ifosfamide anti-cancer drug. <i>Applied Surface Science</i> , 2022, 596, 153618.	3.1	14
11318	Copper(II) Monomer Bearing Phenolate-Based Ligand: Theoretical and Experimental Visions. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 3489-3501.	1.4	5
11319	Highly-selective CO ₂ conversion through single oxide CuO enhanced NiFe ₂ O ₄ thermal catalytic activity. <i>Sustainable Materials and Technologies</i> , 2022, 32, e00441.	1.7	4
11320	Unlocking Air- and Water-Stable Technetium Acetylides and Other Organometallic Complexes. <i>Inorganic Chemistry</i> , 2022, , .	1.9	6
11321	The effect of intramolecular and intermolecular charge transfers on the third order nonlinear optical properties of the self-assembled chromophores. <i>Journal of Luminescence</i> , 2022, , 118991.	1.5	1
11322	Efficient removal of organophosphate esters by ligand functionalized MIL-101 (Fe): Modulated adsorption and DFT calculations. <i>Chemosphere</i> , 2022, 302, 134881.	4.2	21
11323	Efficient degradation of atrazine through in-situ anchoring NiCo ₂ O ₄ nanosheets on biochar to activate sulfite under neutral condition. <i>Journal of Environmental Sciences</i> , 2023, 126, 81-94.	3.2	9
11324	Cobalt(III)/Chiral Carboxylic Acid-Catalyzed Enantioselective Synthesis of Benzothiadiazine Oxides via C-H Activation. <i>Angewandte Chemie - International Edition</i> , 2022, 61, e202205341.	7.2	51
11325	Structural Engineering of Anthracene Diimide Polymers for Molecular Ordering Manipulation. <i>Macromolecules</i> , 2022, 55, 4102-4110.	2.2	4
11326	A Silylene-Stabilized Germanium Analogue of Alkynylaluminum. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	2
11327	A Silylene-Stabilized Germanium Analogue of Alkynylaluminum. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	7
11328	Understanding the Role of Sulfonyl Amine Donors in Propylene Polymerization Using MgCl ₂ -Supported Ziegler-Natta Catalyst. <i>Journal of Physical Chemistry C</i> , 2022, 126, 8655-8666.	1.5	8
11329	Theoretical Insights into Enantioselective [3 + 2] Cycloaddition between Cinnamaldehyde and Cyclic N-Sulfonyl Trifluoromethylated Ketimine Catalyzed by N-Heterocyclic Carbene. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3124-3134.	1.1	1
11330	Effects of Organic Acids on the Release of Fruity Esters in Water: An Insight at the Molecular Level. <i>Molecules</i> , 2022, 27, 2942.	1.7	5
11331	A systematic study on Zn(II)-Iminocarboxyl complexation applied in supramolecular PDMS networks. <i>Polymer</i> , 2022, 250, 124896.	1.8	6
11332	Transition orbital projection approach for excited state tracking. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	2
11333	Integrating coral-like morphology into cyano-containing carbon nitride towards efficient photocatalytic H ₂ evolution and Cr(III) reduction. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 20803-20815.	3.8	6
11334	Interaction of the Serine Amino Acid with BNNT, BNAINT, and BC2NNT. <i>Arabian Journal for Science and Engineering</i> , 0, , .	1.7	1

#	ARTICLE	IF	CITATIONS
11335	The determinants of effective defluorination by the LiAl-LDHs. <i>Journal of Environmental Sciences</i> , 2023, 126, 153-162.	3.2	3
11336	Enhancing Transition Dipole Moments of Heterocyclic Semiconductors via Rational Nitrogen-Substitution for Sensitive Near Infrared Detection. <i>Advanced Materials</i> , 2022, 34, e2201600.	11.1	19
11337	Chemical bonds and weak interactions of methoxysalicylic acid isomers investigated by terahertz spectroscopy and density functional theory. <i>AIP Advances</i> , 2022, 12, .	0.6	2
11338	Unveiling the reactivity of truxillic and truxinic acids (TXAs): deprotonation, anion- π and cation- π interactions in TXA π -Y $^+$ and TXA π -Z $^+$ complexes (Y = Li, Na, K; Z = F, Cl). <i>TJ ET</i>		
11339	Ab Initio Wavefunction Analysis of Electron Removal Quasi-Particle State of NdNiO ₂ With Fully Correlated Quantum Chemical Methods. <i>Frontiers in Physics</i> , 2022, 10, .	1.0	0
11340	The role of weak intermolecular interactions in photophysical behavior of isocoumarins on the example of their interaction with cyclic trinuclear silver(I) pyrazolate. <i>Inorganica Chimica Acta</i> , 2022, 539, 121004.	1.2	4
11341	Design of Rational JAK3 Inhibitors Based on the Parent Core Structure of 1,7-Dihydro-Dipyrrolo [2,3-b:3'-b':2'-e] Pyridine. <i>International Journal of Molecular Sciences</i> , 2022, 23, 5437.	1.8	3
11342	S-scheme Cs ₂ AgBiBr ₆ /Ag ₃ PO ₄ heterojunction with efficient photocatalysis performance for H ₂ production and organic pollutant degradation under visible light. <i>Separation and Purification Technology</i> , 2022, 295, 121250.	3.9	38
11343	Novel fluorescent chemosensor sensitively detect copper (II) through the collaboration of quinoline and coumarin groups. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	1.7	6
11344	Tuning the optoelectronic properties of cross conjugated small molecules using benzodithiophene as a core unit with favorable photovoltaic parameters: a DFT study. <i>Journal Physics D: Applied Physics</i> , 2022, 55, 295106.	1.3	3
11345	DFT Explorations on the Spectral, Non-Covalent Interactions and the invitro analysis of a synthesized Anti-Bacterial Nanocomposite Pure Hydroxyapatite. <i>Journal of Molecular Structure</i> , 2022, , 133270.	1.8	0
11346	Comparative Research on Promising Energetic 1,3-Diazinane and 1,3-Oxazinane Structures. <i>Arabian Journal of Chemistry</i> , 2022, , 103947.	2.3	0
11347	Endohedral $\dot{\pi}$ -Diradical Nitrogen-Vacancy Diamond Nanoclusters with a Confined Magnetic Space and Strong Electronic Spin Couplings. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3174-3184.	1.1	3
11348	Unexplored $\dot{\pi}$ -hole and $\dot{\pi}$ -hole interactions in (X ₂ CY) ₂ complexes (X = F, Cl; Y = O, S). <i>Journal of Molecular Structure</i> , 2022, 1265, 133232.	1.8	4
11349	Remote Effect from Boron Cluster: Tunable Photophysical Properties of $\langle i \rangle \langle /i \rangle$ Carborane-Based Luminogens. <i>Chemistry - A European Journal</i> , 2022, , e202200303.	1.7	2
11350	Chitin-Based Carbon Dots with Tunable Photoluminescence for Fe ³⁺ Detection. <i>ACS Applied Nano Materials</i> , 2022, 5, 7502-7511.	2.4	14
11351	Ortho-halogen effects: π - π^* interactions, halogen bonding, and deciphering chiral attributes in N-aryl glycine peptoid foldamers. <i>Journal of Molecular Structure</i> , 2022, 1264, 133276.	1.8	2
11352	Vanadium(IV) coordination complexes with excellent biological activities: a synthetic, characterization, and density functional theory approach. <i>Journal of Coordination Chemistry</i> , 2022, 75, 689-706.	0.8	1

#	ARTICLE	IF	CITATIONS
11353	Mild Catalytic Mechanism of the Mannich Reaction for Synthesizing Methylacrolein by <i>sec</i> -Amine Short-Chain Aliphatic Acid Ionic Liquid Catalysts. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 6687-6698.	3.2	4
11354	Salt-Enhanced Oxidative Addition of Iodobenzene to Pd: An Interplay Between Cation, Anion, and Pd-Pd Cooperative Effects. <i>Inorganic Chemistry</i> , 2022, 61, 7935-7944.	1.9	6
11355	Precisely modulated electrostatic attraction to the recognition site for on-site ultrafast visualization of trace hydrazine. <i>Cell Reports Physical Science</i> , 2022, 3, 100878.	2.8	5
11356	Conformational Landscape of the Hydrogen-Bonded 1-Phenyl-2,2,2-Trifluoroethanol-1,4-Dioxane Complex: Dispersion Interactions and Conformational Conversion. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2942-2949.	1.1	4
11357	Theoretical evaluation of poly(amidoamine) dendrimers with different peripheral groups as a purinethol drug delivery system in aqueous medium. <i>Colloids and Surfaces B: Biointerfaces</i> , 2022, 216, 112534.	2.5	5
11358	Efficient Xe/Kr Separation Based on a Lanthanide-Organic Framework with One-Dimensional Local Positively Charged Rhomboid Channels. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 22233-22241.	4.0	18
11359	Sigmatropic [1,5] carbon shift of transient C3 ammonium enolates. <i>Angewandte Chemie</i> , 0, , .	1.6	0
11360	Extra contribution to the crystal stability of insensitive explosive TATB: The cooperativity of intermolecular interactions. <i>Defence Technology</i> , 2023, 25, 88-98.	2.1	4
11361	Cubic Nanogrids for Counterbalance Contradiction among Reorganization Energy, Strain Energy, and Wide Bandgap. <i>Journal of Physical Chemistry Letters</i> , 2022, , 4297-4308.	2.1	3
11362	Preparation and characterization of non-aromatic ether self-assemblies on a HOPG surface. <i>Nanotechnology</i> , 2022, 33, 355603.	1.3	3
11363	Sigmatropic [1,5] Carbon Shift of Transient C3 Ammonium Enolates. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	5
11364	A facile synthesis of ibandronate modified hydroxyapatite renewable nanomaterials for simultaneous removal of Cu ²⁺ /Pb ²⁺ and chlortetracycline: Experimental design and adsorption mechanism study. <i>Journal of Cleaner Production</i> , 2022, 361, 132173.	4.6	11
11365	The interaction between H and CH ₃ of adsorption on the diamond (100)-2×1 surface based on DFT Calculations. <i>Journal of Molecular Modeling</i> , 2022, 28, 147.	0.8	0
11366	Molecular-level nucleation mechanism of iodic acid and methanesulfonic acid. <i>Atmospheric Chemistry and Physics</i> , 2022, 22, 6103-6114.	1.9	8
11367	Molecular Dynamics Study on Properties of Hydration Layers above Polymer Antifouling Membranes. <i>Molecules</i> , 2022, 27, 3074.	1.7	6
11368	The second derivative of the electronic energy with respect to the compression scaling factor in the <i>XP-PCM</i> model: Theory and applications to compression response functions of atoms. <i>Journal of Computational Chemistry</i> , 2022, 43, 1176-1185.	1.5	2
11369	The adsorption of Tenofovir in aqueous solution on activated carbon produced from maize cobs: Insights from experimental, molecular dynamics simulation, and DFT calculations. <i>Chemical Physics Letters</i> , 2022, 801, 139676.	1.2	26
11370	High-Voltage Organic Cathodes for Zinc-Ion Batteries through Electron Cloud and Solvation Structure Regulation. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	20

#	ARTICLE	IF	CITATIONS
11371	Retaining Hückel Aromaticity in the Triplet Excited State of Azobenzene. <i>ChemPhysChem</i> , 2022, 23, e202200045.	1.0	3
11372	Theoretical insights of the drug-drug interaction between favipiravir and ibuprofen: a DFT, QTAIM and drug-likeness investigation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 4313-4320.	2.0	8
11373	External Electric Field Effect on the Strength of π -Hole Interactions: A Theoretical Perspective in Like-Unlike Carbon-Containing Complexes. <i>Molecules</i> , 2022, 27, 2963.	1.7	4
11374	Structure and Electronic Properties of Neutral and Anionic X-Doped Medium-Sized Mg ₁₆ (X = Co, Fe, Ni) Clusters. <i>Journal of Cluster Science</i> , 0, , 1.	1.7	1
11375	Weaving a 2D net of hydrogen and halogen bonds: cocrystal of a pyrazolium bromide with tetrafluorodiodobenzene. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 324-331.	0.2	0
11376	Bonding properties of molecular cerium oxides tuned by the 4 <i>f</i> -block from <i>ab initio</i> perspective. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	7
11377	AIE mechanism of 2-(2-hydroxyphenyl) benzothiazole derivatives: CASPT2 and spin-flip study. <i>Dyes and Pigments</i> , 2022, 204, 110396.	2.0	2
11378	NHC Catalyzed α -Carbon functionalization of carboxylic esters towards formation of β -Lactams: A mechanistic study. <i>Molecular Catalysis</i> , 2022, 524, 112311.	1.0	0
11379	Triarylamidazole-ZnII, CdII, and HgII Complexes: Structures, Photophysics, and Antibacterial Properties. <i>Crystals</i> , 2022, 12, 680.	1.0	3
11380	Efficient degradation of sulfamethoxazole using peracetic acid activated by zero-valent cobalt. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 107783.	3.3	22
11381	Hydrogen-Bonded Aggregates Featuring π - π^* Electronic Transition for Efficient Visible-Light-Responsive Photocatalysis. <i>ACS Catalysis</i> , 2022, 12, 6276-6284.	5.5	11
11382	Chalcogen and Hydrogen Bonds at the Periphery of Arylhydrazone Metal Complexes. <i>Crystal Growth and Design</i> , 2022, 22, 3932-3940.	1.4	12
11383	A DFT approach towards therapeutic potential of phosphorene as a novel carrier for the delivery of felodipine (cardiovascular drug). <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113724.	1.1	7
11384	The structures and properties of Mo ($n=2$) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 232 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"). <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113720.	1.1	3
11385	Study of ultrafast nonlinear optical response and transient dynamics of pyrene derivatives with intramolecular charge transfer characteristics. <i>Optical Materials</i> , 2022, 128, 112378.	1.7	3
11386	Mechanism evaluation of the interactions between bisphenol AP and bovine serum albumin based on multi-spectroscopy, wavefunction analysis, and molecular docking. <i>Chinese Journal of Analytical Chemistry</i> , 2022, 50, 100099.	0.9	2
11387	Analysis of Geometric Structure, Electronic Charge Density and Absorption Spectrum of Germanium Sulfide (GeS) under an External Electric Field: A DFT calculation. <i>International Journal of Electrochemical Science</i> , 0, , ArticleID:220679.	0.5	0
11388	Unravelling functions of halogen substituents in the enantioseparation of halogenated planar chiral ferrocenes on polysaccharide-based chiral stationary phases: experimental and electrostatic potential analyses. <i>Journal of Chromatography A</i> , 2022, 1673, 463097.	1.8	7

#	ARTICLE	IF	CITATIONS
11389	Nitrogen reduction to ammonia triggered by heterobimetallic uranium-group 10 metal complexes of phosphinoaryl oxides: A relativistic DFT study. <i>Molecular Catalysis</i> , 2022, 525, 112345.	1.0	1
11390	Effect of electrical stimulation on red meat Neu5Gc content reduction: a combined experimental and DFT study. <i>Food Science and Human Wellness</i> , 2022, 11, 982-991.	2.2	2
11391	Experimental and computational insights into self-assembly sodium oleate on anodized aluminum interface in electric field. <i>Corrosion Science</i> , 2022, 203, 110334.	3.0	5
11392	Donor acceptor groups effect, polar protic solvents influence on electronic properties and reactivity of 2-Chloropyridine-4-carboxylic acid. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100478.	1.3	10
11393	Wangzaozin A, a potent novel microtubule stabilizer, targets both the taxane and laulimalide sites on β -tubulin through molecular dynamics simulations. <i>Life Sciences</i> , 2022, 301, 120583.	2.0	1
11394	Removal of tetracycline by aerobic granular sludge from marine aquaculture wastewater: A molecular dynamics investigation. <i>Bioresource Technology</i> , 2022, 355, 127286.	4.8	23
11395	Zwitterionic interface engineering enables ultrathin composite membrane for high-rate vanadium flow battery. <i>Energy Storage Materials</i> , 2022, 49, 471-480.	9.5	12
11396	Designing new donors organic compounds with IDIC core for photovoltaic application. <i>Optik</i> , 2022, 262, 169174.	1.4	2
11397	Origin of the unexpected attractive interactions between positive σ -holes and positive σ -lumps. <i>Computational and Theoretical Chemistry</i> , 2022, 1213, 113736.	1.1	1
11398	Covalent-anion-driven self-assembled cadmium/ molybdenum sulfide hybrids for efficient nitenpyram degradation. <i>Journal of Environmental Management</i> , 2022, 316, 115269.	3.8	3
11399	The oxalic acid-assisted fast pyrolysis of biomass for the sustainable production of furfural. <i>Fuel</i> , 2022, 322, 124279.	3.4	11
11400	New insights into the excited state intramolecular proton transfer (ESIPT) competition mechanism for different intramolecular hydrogen bonds of Kaempferol and Quercetin in solution. <i>Journal of Luminescence</i> , 2022, 248, 118914.	1.5	5
11401	Lithium selectivity of crown ethers: The effect of heteroatoms and cavity size. <i>Separation and Purification Technology</i> , 2022, 294, 121142.	3.9	20
11402	Origin of metabolites diversity and selectivity of P450 catalyzed benzo[a]pyrene metabolic activation. <i>Journal of Hazardous Materials</i> , 2022, 435, 129008.	6.5	9
11403	The heteroaggregation and deposition behavior of nanoplastics on Al ₂ O ₃ in aquatic environments. <i>Journal of Hazardous Materials</i> , 2022, 435, 128964.	6.5	15
11404	Theoretical insights into the uptake of sulfonamides onto phospholipid bilayers: Mechanisms, interaction and toxicity evaluation. <i>Journal of Hazardous Materials</i> , 2022, 435, 129033.	6.5	10
11405	Remarkable non-linear optical properties of gold cluster doped graphyne (GY): A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 114, 108204.	1.3	9
11406	An ultra-sensitive kaempferol electrochemical sensor based on flower-like ZIF-8 pyrolysis-derived ZnWO ₄ /porous nanocarbon composites. <i>Microchemical Journal</i> , 2022, 179, 107519.	2.3	5

#	ARTICLE	IF	CITATIONS
11407	Ultrafast dynamics of dual fluorescence of 2-(2-hydroxyphenyl) benzothiazole and its derivatives by femtosecond transient absorption spectroscopy. <i>Journal of Luminescence</i> , 2022, 248, 118922.	1.5	11
11408	Molecular structure adjustment enhanced anti-oxidation ability of polymer electrolyte for solid-state lithium metal battery. <i>Nano Energy</i> , 2022, 98, 107330.	8.2	32
11409	Evidence of significant non-covalent interactions in the solution of Levetiracetam in water and methanol. <i>Journal of Molecular Liquids</i> , 2022, 359, 119289.	2.3	12
11410	FeC ₂ O ₄ ·2H ₂ O enables sustainable conversion of hydrogen peroxide to hydroxyl radical for promoted mineralization and detoxification of sulfadimidine. <i>Journal of Hazardous Materials</i> , 2022, 436, 129049.	6.5	12
11411	Computational investigation into structural, topological, electronic properties, and biological evaluation of spiro[1H-indole-3,2'-3H-1,3-benzothiazole]-2-one. <i>Journal of Molecular Liquids</i> , 2022, 359, 119234.	2.3	18
11412	In-depth insight into the mechanism on photocatalytic synergistic removal of antibiotics and Cr (VI): The decisive effect of antibiotic molecular structure. <i>Applied Catalysis B: Environmental</i> , 2022, 313, 121443.	10.8	60
11413	Developing a molecularly imprinted channels catalyst based on template effect for targeted removal of organic micropollutants from wastewaters. <i>Chemical Engineering Journal</i> , 2022, 445, 136755.	6.6	11
11414	Lithium difluoro(bisoxalato) phosphate-based multi-salt low concentration electrolytes for wide-temperature lithium metal batteries: Experiments and theoretical calculations. <i>Chemical Engineering Journal</i> , 2022, 445, 136802.	6.6	17
11415	Selective detection of F ⁺ ion and SO ₂ molecule: An experimental and DFT study. <i>Journal of Molecular Liquids</i> , 2022, 359, 119329.	2.3	16
11416	Photophysical characteristics of Phenylimidazo(4,5-f)1,10-phenanthroline Rhenium(I) complexes - A theoretical approach to their potential applications in lighting devices. <i>Materials Science in Semiconductor Processing</i> , 2022, 147, 106733.	1.9	0
11417	Characteristics of nitrogen oxide emissions from combustion synthesis of a CuO oxygen carrier. <i>Fuel Processing Technology</i> , 2022, 233, 107295.	3.7	7
11418	Computational redox chemistry of functionalized Polycaprolactone as electrolytes for lithium batteries. <i>Journal of Electroanalytical Chemistry</i> , 2022, 916, 116377.	1.9	2
11419	Synergistic adsorption-photocatalysis for dyes removal by a novel biochar-based Z-scheme heterojunction BC/2ZIS/WO ₃ : Mechanistic investigation and degradation pathways. <i>Chemical Engineering Journal</i> , 2022, 445, 136677.	6.6	48
11420	Unraveling the direct effect of hydrogen bonding on density and thermostability of energetic materials through isomerism. <i>Chemical Engineering Journal</i> , 2022, 444, 136539.	6.6	15
11421	H ₂ storage capacity of Li-doped five member aromatic heterocyclic superalkali complexes; an in silico study. <i>Sustainable Energy Technologies and Assessments</i> , 2022, 52, 102235.	1.7	3
11422	Assembling high nitrogen isomeric energetic molecules via a lithium-mediated concerted [2+3] reaction of two diazo compounds. <i>Chemical Engineering Journal</i> , 2022, 444, 136596.	6.6	7
11423	Diketone-mediated photochemical reduction of selenite to elemental selenium: Role of carbon-centered radicals and complexation. <i>Chemical Engineering Journal</i> , 2022, 445, 136831.	6.6	5
11424	Insights on isomeric emitters with thermally activated delayed fluorescence: Comparison between solvent and crystal state. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 278, 121328.	2.0	4

#	ARTICLE	IF	CITATIONS
11425	Substituent control of dynamical process for excited state intramolecular proton transfer of benzothiazole derivatives. <i>Chemical Physics</i> , 2022, 560, 111568.	0.9	3
11426	A novel Schiff base sensor through "off-on-off" fluorescence behavior for sequentially monitoring Al ³⁺ and Cu ²⁺ . <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 430, 113990.	2.0	9
11427	Electronic structure modulation of g-C ₃ N ₄ by Hydroxyl-grafting for enhanced photocatalytic peroxymonosulfate Activation: Combined experimental and theoretical analysis. <i>Separation and Purification Technology</i> , 2022, 294, 121246.	3.9	8
11428	Highly efficient photocatalytic hydrogen production via porphyrin-fullerene supramolecular photocatalyst with donor-acceptor structure. <i>Chemical Engineering Journal</i> , 2022, 444, 136621.	6.6	22
11429	Structural, spectral inspection, electronic properties in different solvents, Fukui functions, 6-acetyl-2H-1,4-benzoxazin-3(4H)-one " Multiple sclerosis and auto immune disorders therapeutics. <i>Journal of Molecular Liquids</i> , 2022, 359, 119248.	2.3	11
11430	Horizontal planetary mechanochemical method for rapid and efficient remediation of high-concentration lindane-contaminated soils in an alkaline environment. <i>Journal of Hazardous Materials</i> , 2022, 436, 129078.	6.5	6
11431	Study of O-H...O bonded-cyclic dimer for 2,5-Dihydroxyterephthalic acid as aided by MD, DFT calculations and IR, Raman, NMR spectroscopy. <i>Journal of Molecular Structure</i> , 2022, 1264, 133174.	1.8	5
11432	Density functional studies and spectroscopic analysis (FT-IR, FT-Raman, UV-vis, and NMR) with molecular docking approach on an anticancer and antifungal drug 4-hydroxy-3-methoxybenzaldehyde. <i>Journal of Molecular Structure</i> , 2022, 1264, 133134.	1.8	2
11433	Spectroscopic and molecular electronic property investigation of 2-phenylpyrimidine-4, 6-diamine via ¹ H NMR, UV-vis, FT-Raman, FT-IR, and DFT approach. <i>Journal of Molecular Structure</i> , 2022, 1263, 133195.	1.8	29
11434	The comparison researches of cis/trans-butenedioic acids in regulating solid crystalline forms and improving pharmaceutical properties of antifungal drug econazole. <i>Journal of Molecular Structure</i> , 2022, 1263, 133183.	1.8	1
11435	Electrochemical sensing of heptazine graphitic C ₃ N ₄ quantum dot for chemical warfare agents; a quantum chemical approach. <i>Materials Science in Semiconductor Processing</i> , 2022, 148, 106753.	1.9	18
11436	Preparation of graphene-supported-metal-phthalocyanine and mechanistic understanding of its catalytic nature at molecular level. <i>Journal of Colloid and Interface Science</i> , 2022, 622, 708-718.	5.0	0
11437	Spectral investigation on single molecular optoelectronics of ladder phenylenes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 278, 121283.	2.0	3
11438	Computational study of Brønsted acidity in the metal-organic framework UiO-66. <i>Chemical Physics Letters</i> , 2022, 800, 139658.	1.2	2
11439	Structural and mechanistic study of antimonite complexation with organic ligands at the goethite-water interface. <i>Chemosphere</i> , 2022, 301, 134682.	4.2	5
11440	A new class of deep blue emitting four-coordinate NHC-Cu(I) complexes bearing nonconjugated triazolyl-imidazolylidene-type ligand: Synthesis, photophysical properties and theoretical investigations. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 431, 114008.	2.0	3
11441	Physicochemical properties and formation mechanism of whey protein isolate-sodium alginate complexes: Experimental and computational study. <i>Food Hydrocolloids</i> , 2022, 131, 107786.	5.6	22
11442	±-(1,2,3-Triazolyl)-acetophenone: Synthesis and theoretical studies of crystal and 2,4-dinitrophenylhydrazine cocrystal structures. <i>Journal of Molecular Structure</i> , 2022, 1264, 133225.	1.8	4

#	ARTICLE	IF	CITATIONS
11443	Estimation of the ability of the π -system of pseudohalides (azide and thiocyanate) to participate in CH π - π interactions in cyclic hetero-tetranuclear cobalt(III)/sodium and linear trinuclear mixed valence cobalt(III/II/III) complexes. <i>Polyhedron</i> , 2022, 222, 115862.	1.0	4
11444	Performance and mechanism of lignin and quercetin as bio-based anti-aging agents for asphalt binder: A combined experimental and ab initio study. <i>Journal of Molecular Liquids</i> , 2022, 359, 119310.	2.3	21
11445	Computational molecular-level prediction of heterocyclic compound-metal surface interfacial behavior. <i>Journal of Colloid and Interface Science</i> , 2022, 622, 452-468.	5.0	16
11446	Detection of excited triplet species from photolysis of carbonyls: Direct evidence for single oxygen formation in atmospheric environment. <i>Science of the Total Environment</i> , 2022, 837, 155464.	3.9	0
11447	Dependence between luminescence properties of Cu(III) complexes and electronic/structural parameters derived from steric effects. <i>New Journal of Chemistry</i> , 2022, 46, 10584-10593.	1.4	2
11448	Theoretical investigation of electronic structures, second-order NLO responses of cyclometalated Ir(III) and Rh(III) counterpart complexes: effect of metal centers. <i>New Journal of Chemistry</i> , 2022, 46, 10652-10661.	1.4	7
11449	Fast photostimulus-responsive ultralong room-temperature phosphorescence behaviour of benzoic acid derivatives@boric acid. <i>Journal of Materials Chemistry C</i> , 2022, 10, 8806-8814.	2.7	6
11450	Nucleophilicity of the boron atom in compounds R-B, (R = F, Cl, Br, I, CN, NC, CH ₃ , SiH ₃ , CF ₃ , H): a new look at the inductive effects of the groups R. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	1.3	3
11451	Screening of Biocompatible MOFs for the Clearance of Indoxyl Sulfate Using GCMC Simulations. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 6618-6627.	1.8	1
11452	Concise Synthesis of BN-Dibenzo[<i>f,k</i>]tetraphenes with Different BN Substitution Positions and Direct Comparison with Their Carbonaceous Analogue. <i>Journal of Organic Chemistry</i> , 2022, 87, 6630-6637.	1.7	2
11453	Priority Separation of Phenols with Deep Eutectic Solvents from an Acetonitrile-Extractable Portion of a Shale Oil: Experimental and Computational. <i>Energy & Fuels</i> , 2022, 36, 5657-5665.	2.5	3
11454	Upgrading the peroxi-coagulation treatment of complex water matrices using a magnetically assembled mZVI/DNA anode: Insights into the importance of ClO radical. <i>Chemosphere</i> , 2022, 303, 134948.	4.2	10
11455	Efficient and selective capture of xenon over krypton by a window-cage metal-organic framework with parallel aromatic rings. <i>Separation and Purification Technology</i> , 2022, 295, 121281.	3.9	14
11456	Novel NIR-Phosphorescent Ir(III) Complexes: Synthesis, Characterization and Their Exploration as Lifetime-Based O ₂ Sensors in Living Cells. <i>Molecules</i> , 2022, 27, 3156.	1.7	12
11457	Aucubin as a natural potential anti-acute hepatitis candidate: Inhibitory potency and hepatoprotective mechanism. <i>Phytomedicine</i> , 2022, 102, 154170.	2.3	5
11458	Correlation between Excited-State Intramolecular Proton Transfer and Electron Population on Proton Donor/Acceptor in 2-(2-Hydroxyphenyl)oxazole Derivatives. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4486-4494.	2.1	7
11459	Bridging H ₂ O and H ₂ S homomeric clusters via H ₂ O-H ₂ S mixed clusters: Impact of the changing ratio of H ₂ O and H ₂ S moieties. <i>Computational and Theoretical Chemistry</i> , 2022, 1213, 113740.	1.1	2
11460	Electric field modulated water permeation through laminar Ti ₃ C ₂ T _x MXene membrane. <i>Water Research</i> , 2022, 219, 118598.	5.3	26

#	ARTICLE	IF	CITATIONS
11461	Cation- π interaction: A strategy for enhancing the performance of graphene-based drug delivery systems. <i>Inorganic Chemistry Communication</i> , 2022, 141, 109542.	1.8	6
11462	Synthesis, characterization, DFT studies, and molecular modeling of azo dye derivatives as potential candidate for trypanosomiasis treatment. <i>Chemical Physics Impact</i> , 2022, 4, 100076.	1.7	57
11463	Novel insights into formation mechanism of organic chloramines from pre-oxidized algae-laden water: Multiple roles of dissolved organic nitrogen. <i>Science of the Total Environment</i> , 2022, 838, 155894.	3.9	3
11464	Antimalarial potential of naphthalene-sulfonic acid derivatives: Molecular electronic properties, vibrational assignments, and in-silico molecular docking studies. <i>Journal of Molecular Structure</i> , 2022, 1264, 133298.	1.8	76
11465	Mixed-Linker Isoreticular Zn(II) Metal-Organic Frameworks as Brønsted Acid-Base Bifunctional Catalysts for Knoevenagel Condensation Reactions. <i>Inorganic Chemistry</i> , 2022, 61, 8339-8348.	1.9	27
11466	Antimicrobial activities of 1-phenyl-3-methyl-4-trichloroacetyl-pyrazolone: Experimental, DFT studies, and molecular docking investigation. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100524.	1.3	62
11467	Novel La _{1-x} CaxTi _{1-y} TayO _{3-δ} perovskites with enhanced conductivity for Solid Oxide Fuel Cell electrodes. <i>Journal of Alloys and Compounds</i> , 2022, , 165370.	2.8	4
11468	Bioisosteric-Replacement-Driven Lead Optimization of Tyclopyrazoflor. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 11123-11137.	2.4	7
11469	Study on the fire extinguishing efficiency and mechanism of composite superfine dry powder containing ferrocene. <i>Fire Safety Journal</i> , 2022, 130, 103606.	1.4	5
11470	Defective MWCNT Enabled Dual Interface Coupling for Carbon-Based Perovskite Solar Cells with Efficiency Exceeding 22%. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	35
11471	Molecular simulation investigations on the coating of Al-alloy surface by nano-SiO ₂ -epoxy composite. <i>Current Applied Physics</i> , 2022, 39, 263-271.	1.1	1
11472	New mechanistic insights into direct ethylene glycol synthesis from syngas over modified Rh carbonyl catalysts. <i>Fuel</i> , 2022, 324, 124500.	3.4	0
11473	Theoretical insights into molecular design of hot-exciton based thermally activated delayed fluorescence molecules. <i>Materials Advances</i> , 2022, 3, 4954-4963.	2.6	12
11474	Unravelling conformational and crystal packing preferences of cyclohexane-5-spirohydantoin derivatives incorporating a halogenated benzoyl group. <i>CrystEngComm</i> , 0, , .	1.3	1
11475	Enhanced C-H bond activation by tuning the local environment of surface lattice oxygen of MoO ₃ . <i>Chemical Science</i> , 2022, 13, 7468-7474.	3.7	3
11476	2D phosphorus carbide as promising anode materials for Na/K-ion batteries from first-principles study. <i>Journal of Molecular Modeling</i> , 2022, 28, 152.	0.8	2
11477	Enantioselective (8+3) Cycloadditions by Activation of Donor-Acceptor Cyclopropanes Employing Chiral Brønsted Base Catalysis. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	15
11478	Halogen-Bonded Cocrystals of 1,3,5-Triiodo-2,4,6-trifluorobenzene and Structural Isomers of Benzoylpyridine. <i>Crystal Growth and Design</i> , 2022, 22, 3981-3989.	1.4	6

#	ARTICLE	IF	CITATIONS
11479	Asymmetric Coordination Mode of Phenanthroline-like Ligands in Gold(I) Complexes: A Case of the Antichelate Effect. <i>Crystal Growth and Design</i> , 2022, 22, 3882-3895.	1.4	3
11480	One-step removal of all pollutants to produce clean water: Construct a novel dual-functional aramid nanofibre membrane for simultaneous oil-in-water separation and single-ring aromatic compound removal. <i>Journal of Cleaner Production</i> , 2022, 361, 132259.	4.6	6
11481	Controllable Sensitivity Mechanism in an Energetic Compound of [FeII(Rtrz)6] as a molecular switch. <i>Chemical Physics Letters</i> , 2022, , 139682.	1.2	1
11482	Enantioselective synthesis of amino acids from ammonia. <i>Nature Catalysis</i> , 2022, 5, 571-577.	16.1	42
11483	Enantioselective (8+3) Cycloadditions by Activation of Donor-Acceptor Cyclopropanes Employing Chiral Brønsted Base Catalysis. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	2
11484	Effect of fluorine substitution on properties of hole-transporting materials for perovskite solar cells. <i>Dyes and Pigments</i> , 2022, 204, 110370.	2.0	4
11485	Acidified glycerol as a one-step efficient green extraction and preservation strategy for anthocyanin from blueberry pomace: New insights into extraction and stability protection mechanism with molecular dynamic simulation. <i>Food Chemistry</i> , 2022, 390, 133226.	4.2	6
11486	Electron-Induced Decomposition of Different Silver(I) Complexes: Implications for the Design of Precursors for Focused Electron Beam Induced Deposition. <i>Nanomaterials</i> , 2022, 12, 1687.	1.9	3
11487	Machine Learning Screening of Efficient Ionic Liquids for Targeted Cleavage of the C-O-C Bond of Lignin. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3693-3704.	1.2	6
11488	Hirshfeld surface and electrostatic potential surface analysis of clozapine and its solubility and molecular interactions in aqueous blends. <i>Journal of Molecular Liquids</i> , 2022, 360, 119328.	2.3	12
11489	Theoretical Study of Rhodium-Catalyzed Dual C-H Activation to Synthesize C-N Axially Chiral <i>N</i> -Aryloxindoles: Origin of Axial Chirality. <i>Organometallics</i> , 2022, 41, 1275-1283.	1.1	0
11490	In silico exploration of disulfide derivatives of <i>Ferula foetida</i> oleo-gum (Covexir®) as promising therapeutics against SARS-CoV-2. <i>Computers in Biology and Medicine</i> , 2022, , 105566.	3.9	1
11491	Syntheses, Structures, and Properties of Polynitro-Substituted 5,6-Dihydroimidazo[1,2- <i>a</i>]pyrazine Energetic Compounds. <i>Crystal Growth and Design</i> , 2022, 22, 3914-3923.	1.4	10
11492	A DFT study on the structure activity relationship of the natural xanthotoxin-based pharmaceutical cocrystals. <i>Journal of Molecular Modeling</i> , 2022, 28, 155.	0.8	1
11493	A DFT study on the adsorption behavior of antiviral Favipiravir drug on B N (n=12, 16, 20, and 24) nanocages: The size effect. <i>Journal of Molecular Liquids</i> , 2022, 360, 119388.	2.3	14
11494	Metal-Ligand Bonds in Rare Earth Metal-Biphenyl Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 8135-8143.	1.9	4
11495	Electrochemical Deoxygenative Barbier-Type Reaction. <i>Organic Letters</i> , 2022, 24, 3668-3673.	2.4	11
11496	Catalytic Enantioselective Synthesis of β -Lactams with α -Quaternary Centers via Merging of C-C Activation and Sulfonyl Radical Migration. <i>Journal of the American Chemical Society</i> , 2022, 144, 9222-9228.	6.6	16

#	ARTICLE	IF	CITATIONS
11497	Exploring the excited-state charge transfer fluorescence profile of 7-hydroxycoumarin and 2-methylimidazole – a combined X-ray diffraction and theoretical approach. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	1.3	0
11498	λ^{6+} -Coordinated ruthenabenzenes from three-component assembly on a diruthenium λ^4 -allenyl scaffold. <i>Dalton Transactions</i> , 2022, 51, 8390-8400.	1.6	8
11499	Recombinant Antibody-Based and Computer-Aided Comprehensive Analysis of Antibody's Equivalent Recognition Mechanism of Alternariol and Alternariol Monomethyl Ether. <i>Frontiers in Chemistry</i> , 2022, 10, 871659.	1.8	0
11500	Ultrafast study of substituted-position-dependent excited-state evolution in benzophenone-carbazole dyads. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14623-14630.	1.3	6
11501	Tunable 1,2,3-triazole- <i>N</i> -oxides towards high energy density materials: theoretical insight into structure-property correlations. <i>New Journal of Chemistry</i> , 2022, 46, 11741-11750.	1.4	5
11502	Synthesis of asymmetric indolonaphthyridines with enhanced excited state charge-transfer character. <i>Journal of Materials Chemistry C</i> , 2022, 10, 10742-10747.	2.7	10
11503	Resonance-assisted intramolecular triel bonds. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 15015-15024.	1.3	6
11504	B_{96} : a complete core-shell structure with high symmetry. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 15687-15690.	1.3	12
11505	<i>Ab initio</i> molecular dynamics simulations on the adsorption of 1-hydroxyethane-1,1-diphosphonic acid on the iron (100) surface. <i>New Journal of Chemistry</i> , 2022, 46, 11797-11803.	1.4	1
11506	Red aqueous room-temperature phosphorescence modulated by anion and intermolecular electronic coupling interactions. <i>Chemical Science</i> , 2022, 13, 7247-7255.	3.7	13
11507	A π -orbital model to study substituent effects in organic room-temperature phosphorescent materials. <i>Journal of Materials Chemistry C</i> , 2022, 10, 9319-9325.	2.7	1
11508	Theoretical study of the NO_3 radical reaction with CH_2ClBr , CH_2ClI , CH_2BrI , $CHCl_2Br$, and $CHCl_2I$. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14365-14374.	1.3	3
11509	Shearing bridge bonds in carbon nitride vesicles with enhanced hot carrier utilization for photocatalytic hydrogen production. <i>Catalysis Science and Technology</i> , 2022, 12, 4193-4200.	2.1	24
11510	Small practical cluster models for perovskites based on the similarity criterion of central location environment and their applications. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14375-14389.	1.3	6
11511	Theoretical mechanistic insights into the polar hydrohalogenation of olefins. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 4976-4985.	1.5	2
11512	Predicting dinitrogen activation by borenium and borinium cations. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14651-14657.	1.3	5
11513	Donor-acceptor interactions of gold(III) porphyrins with cobalt(II) phthalocyanine: chemical structure of products, their spectral characterization and DFT study. <i>Dalton Transactions</i> , 0, , .	1.6	0
11514	A Sustainable Route for the Synthesis of Alkyl Arylacetates via Halogen and Base Free Carbonylation of Benzyl Acetates. <i>Catalysis Science and Technology</i> , 0, , .	2.1	3

#	ARTICLE	IF	CITATIONS
11515	Interplay between chalcogen bonds and dynamic covalent bonds. <i>Organic Chemistry Frontiers</i> , 2022, 9, 3966-3975.	2.3	5
11516	Quantitative analysis of molecular surface: systematic application on sodiation mechanism of benzoquinone-based pillared compound as cathode. <i>Inorganic Chemistry Frontiers</i> , 0, , .	3.0	3
11517	Dyeing Thermodynamics and Supramolecular Structure of Lac Red on Protein Fibers. <i>Journal of Textile Science and Technology</i> , 2022, 08, 89-106.	0.2	0
11518	Visible-light-induced cross-coupling of aryl iodides with hydrazones <i>via</i> an EDA-complex. <i>Chemical Science</i> , 2022, 13, 7165-7171.	3.7	15
11519	Unraveling the role of the electron-pair density symmetry in reaction mechanism patterns: the Newman–Kwart rearrangement. <i>New Journal of Chemistry</i> , 2022, 46, 12002-12009.	1.4	4
11520	Potential-Dependent Free Energy Relationship in Interpreting the Electrochemical Performance of CO ₂ Reduction on Single Atom Catalysts. <i>ACS Catalysis</i> , 2022, 12, 6606-6617.	5.5	34
11521	Spontaneous exciton dissociation in organic photocatalyst under ambient conditions for highly efficient synthesis of hydrogen peroxide. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	17
11522	Structure-based model of fucoxanthin–chlorophyll protein complex: Calculations of chlorophyll electronic couplings. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	7
11523	Anion chemistry enabled positive valence conversion to achieve a record high-voltage organic cathode for zinc batteries. <i>CheM</i> , 2022, 8, 2204-2216.	5.8	65
11524	4-Phenyl-1,2,3-triazoles as Versatile Ligands for Cationic Cyclometalated Iridium(III) Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 8509-8520.	1.9	6
11525	Excited-State Properties of Some Thermally Activated Delayed Fluorescence Emitters: Quest for an Accurate and Reliable Computational Method. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3452-3462.	1.1	4
11526	A Theoretical Study of the Sensing Mechanism of a Schiff-Based Sensor for Fluoride. <i>Sensors</i> , 2022, 22, 3958.	2.1	1
11527	Influence of the anion base X (X=F ⁻ , Cl ⁻ , Br ⁻ , NO ₃ ⁻ and SO ₄ ²⁻) on the formation of Chalcogen bonds in Chalcogenodiazoles C_4N_4X (Ch=S, Se and Te). <i>Journal of Molecular Structure</i> , 2022, 1265, 133371.	1.8	3
11528	Persistent prevalence of non-covalent interaction in pyrimidine containing sulfonamide derivative: A quantum computational analysis. <i>Journal of Molecular Structure</i> , 2022, 1266, 133378.	1.8	18
11529	Atomic mechanisms of separation failure at the asphalt–aggregate interface and its dependence on aging and rejuvenation: Insights from molecular dynamics simulations and DFT calculations. <i>Applied Surface Science</i> , 2022, 598, 153775.	3.1	23
11530	A Theoretical Study on the Medicinal Properties and Electronic Structures of Platinum(IV) Anticancer Agents With Cl Substituents. <i>Frontiers in Oncology</i> , 2022, 12, .	1.3	0
11531	Hydrogen bonding between 1-ethyl-3-methyl-imidazolium dicyanamide ionic liquid and selected co-solvents with varying polarity: A DFT study. <i>Journal of Molecular Liquids</i> , 2022, , 119418.	2.3	5
11532	Improved volume variable cluster model method for crystal-lattice optimization: effect on isotope fractionation factor. <i>Geochemical Transactions</i> , 2022, 23, .	1.8	0

#	ARTICLE	IF	CITATIONS
11533	Electrochromic and photovoltaic properties of benzothiadiazole-based donor-acceptor conjugated polymers with oligo(ethylene glycol) side chains. <i>Dyes and Pigments</i> , 2022, 204, 110432.	2.0	14
11534	Influence of the leaving group on the mechanism of hydrolysis of organophosphorus compounds by phosphotriesterase from bacterium <i>Pseudomonas diminuta</i> . <i>Russian Chemical Bulletin</i> , 2022, 71, 921-926.	0.4	1
11535	Theoretical Studies on the Role of Guest in $\text{I}^{\pm}\text{-CL-20/Guest}$ Crystals. <i>Molecules</i> , 2022, 27, 3266.	1.7	1
11536	Quantum Chemical Calculation on the Decomposition Mechanism of Na_3AlF_6 . <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 1035-1043.	0.1	2
11537	Fabricating binary cathode interface layer by effective molecular electrostatic potential and interfacial dipole to optimize electron transport and improve organic solar cell. <i>Chemical Engineering Journal</i> , 2022, 446, 137209.	6.6	16
11538	Mechanism and conformation changes for the whole regeneration process of cellulose in pyridinium-based ionic liquids. <i>Cellulose</i> , 2022, 29, 5479-5492.	2.4	7
11539	Mimicking DNA Periodic Docking Grooves for Adaptive Identification of L -Tryptophan in a Biological Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2022, 144, 9559-9563.	6.6	19
11540	Exploration of noncovalent interactions in the solid state structures of carboxylate bridged trinuclear mixed valence cobalt complexes using computational tools based on the topological analysis of the electron density. <i>Polyhedron</i> , 2022, 223, 115910.	1.0	5
11541	Guerbet coupling of methanol catalysed by titanium clusters. <i>Chemical Physics Letters</i> , 2022, 802, 139719.	1.2	5
11542	Signature of Au as a Halogen. <i>Journal of Physical Chemistry Letters</i> , 0, , 4721-4728.	2.1	4
11543	Effect of CO_2 on the As_2O_3 adsorption over carbonaceous surface: Experiment and quantum chemistry study. <i>Chemical Engineering Journal</i> , 2022, 446, 137156.	6.6	5
11544	Efficient circularly polarized photoluminescence and electroluminescence of chiral spiro-skeleton based thermally activated delayed fluorescence molecules. <i>Science China Chemistry</i> , 2022, 65, 1347-1355.	4.2	23
11545	The antioxidant capacity of myricetin. A molecular electrostatic potential analysis based on DFT calculations. <i>Chemical Physics Letters</i> , 2022, 801, 139708.	1.2	15
11546	Liquid-liquid extraction and mechanism exploration for separation of mixture 2,2,3,3-Tetrafluoro-1-propanol and water using pyridine-based ionic liquids. <i>Journal of Molecular Liquids</i> , 2022, 360, 119468.	2.3	7
11547	Insights into the Mechanism of Ozone Activation and Singlet Oxygen Generation on N-Doped Defective Nanocarbons: A DFT and Machine Learning Study. <i>Environmental Science & Technology</i> , 2022, 56, 7853-7863.	4.6	27
11548	DFT study of the therapeutic potential of borospherene and metalloborospherenes as a new drug-delivery system for the 5-fluorouracil anticancer drug. <i>Journal of Molecular Liquids</i> , 2022, 360, 119457.	2.3	8
11549	Theoretical study on the formation of Criegee intermediates from ozonolysis of pentenal: An example of trans-2-pentalen. <i>Chemosphere</i> , 2022, 303, 135142.	4.2	5
11550	Synthesis, X-ray diffraction analysis, quantum chemical studies and I^{\pm} -amylase inhibition of probenecid derived <i>S</i> -alkylphthalimide-oxadiazole-benzenesulfonamide hybrids. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022, 37, 1464-1478.	2.5	24

#	ARTICLE	IF	CITATIONS
11551	Unique Oâ•N...O Pnicogen Interactions in Nitromethane Dimers: Evidence Using Matrix Isolation Infrared Spectroscopy and Computational Methodology. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3511-3520.	1.1	5
11552	High-Throughput Computational Exploration of MOFs with Open Cu Sites for Adsorptive Separation of Hydrogen Isotopes. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 24980-24991.	4.0	10
11553	Isosorbide-based cyclomatrix polyphosphazene for high-efficient and selective adsorption of cationic dyes: Experimental and computational studies. <i>Applied Surface Science</i> , 2022, 598, 153689.	3.1	11
11554	Part per trillion level DMMP gas sensor based on calixarene modified organic thin film transistor. <i>Chemical Engineering Journal</i> , 2022, 446, 137097.	6.6	6
11555	Construction of the Largest Metal-Centered Double-Ring Tubular Boron Clusters Based on Actinide Metal Doping. <i>Journal of Physical Chemistry A</i> , 0, , .	1.1	3
11556	Synthesis, Structure, and Biologic Activity of Some Copper, Nickel, Cobalt, and Zinc Complexes with 2-Formylpyridine N4-Allylthiosemicarbazone. <i>Bioinorganic Chemistry and Applications</i> , 2022, 2022, 1-18.	1.8	6
11557	Unraveling the multiple roles of VUV mediated hydroxyl radical in VUV/UV/chlorine process: Kinetic simulation, mechanistic consideration and byproducts formation. <i>Chemical Engineering Journal</i> , 2022, 446, 137066.	6.6	14
11558	Molecular modeling of ceftriaxone activation in the active sites of penicillin-binding proteins 2. <i>Russian Chemical Bulletin</i> , 2022, 71, 915-920.	0.4	1
11559	Synthesis, XRD, spectral, structural, quantum mechanical and anticancer studies of di(p-chlorobenzyl) (dibromo) (1, 10-phenanthroline) tin (IV) complex. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100540.	1.3	8
11560	Impact of side-chain engineering on the A-ï€-D-ï€-A type SM-BF1 donor molecule for bulk heterojunction and their photovoltaic performance: A DFT approach. <i>Solar Energy</i> , 2022, 240, 38-56.	2.9	25
11561	Strategies toward the end-group modifications of indacenodithiophene based non-fullerene small molecule acceptor to improve the efficiency of organic solar cells; a DFT study. <i>Computational and Theoretical Chemistry</i> , 2022, 1213, 113747.	1.1	9
11562	Efficient removal of micropollutants from low-conductance surface water using an electrochemical Janus ceramic membrane filtration system. <i>Water Research</i> , 2022, 220, 118627.	5.3	26
11563	Axial g-C3N4 coordinated iron(III) phthalocyanine mediated ultra-efficient peroxymonosulfate activation for high-valent iron species generation. <i>Applied Catalysis A: General</i> , 2022, 641, 118679.	2.2	9
11564	2D boron nitride material as a sensor for H2SiCl2. <i>Computational and Theoretical Chemistry</i> , 2022, 1213, 113742.	1.1	29
11565	Theoretical discussion on the Hydrogen Bond Interactions between Acrylic Acid dimer and dibutyl ether Monomer. <i>Computational and Theoretical Chemistry</i> , 2022, 1213, 113746.	1.1	2
11566	Probing the structural evolution, electronic and vibrational properties of neutral and anionic calcium-doped magnesium clusters. <i>Results in Physics</i> , 2022, 38, 105635.	2.0	2
11567	Effects of different halogen and chalcogen substitutions on the ESIPT process of benzoxazole derivatives: Theoretical research. <i>Chemical Physics Letters</i> , 2022, 801, 139706.	1.2	4
11568	Effect of aromatic linkers on thermally activated delayed fluorescence of selected organic molecules. <i>Chemical Physics Letters</i> , 2022, 801, 139711.	1.2	2

#	ARTICLE	IF	CITATIONS
11569	Construction of dual transfer channels in graphitic carbon nitride photocatalyst for high-efficiency environmental pollution remediation: Enhanced exciton dissociation and carrier migration. <i>Journal of Hazardous Materials</i> , 2022, 436, 129171.	6.5	13
11570	A quantum-chemistry and molecular-dynamics study of non-covalent interactions between tri-n-butyl phosphate and 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. <i>Journal of Molecular Liquids</i> , 2022, 360, 119430.	2.3	8
11571	Capturing low-carbon alcohols from CO ₂ gas with ionic liquids. <i>Chemical Engineering Science</i> , 2022, 258, 117745.	1.9	6
11572	Rational tuning of intermolecular and intramolecular interactions enabling high-efficiency indoor organic photovoltaics. <i>Nano Energy</i> , 2022, 99, 107414.	8.2	14
11573	B8C10: A C _{2v} planar polycyclic structure bridged by the central strong C C bond and strengthened by the aromaticity. <i>Chemical Physics Letters</i> , 2022, 801, 139715.	1.2	0
11574	Coordinatively Unsaturated Reduced Iron Sites Enable Hemin-Catalyzed Electrochemical Dechlorination of Trichloroethylene. <i>Journal of Environmental Engineering, ASCE</i> , 2022, 148, .	0.7	0
11575	Mutual effects of <i>Shewanella putrefaciens</i> -montmorillonite and their impact on uranium immobilization. <i>Chemosphere</i> , 2022, 303, 135096.	4.2	4
11576	Kill two birds with one stone: A near-infrared ratiometric fluorescent probe for simultaneous detection of β -galactosidase in senescent and cancer cells. <i>Sensors and Actuators B: Chemical</i> , 2022, 367, 132061.	4.0	15
11577	Acetamidiprid in several binary aqueous solutions: Solubility, intermolecular interactions and solvation behavior. <i>Journal of Chemical Thermodynamics</i> , 2022, 172, 106828.	1.0	6
11578	Computational and experimental study of different brines in temperature swing solvent extraction desalination with amine solvents. <i>Desalination</i> , 2022, 537, 115863.	4.0	12
11579	Influence of alkali metal Na on coal-based soot production. <i>Fuel</i> , 2022, 323, 124327.	3.4	5
11580	Identification of potential inhibitors against FemX of <i>Staphylococcus aureus</i> : A hierarchical in-silico drug repurposing approach. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 115, 108215.	1.3	5
11581	Intramolecular copigmentation in malvidin-3-O-(6-O-p-coumaryl)-glucoside: Insights from experimental and theoretical study. <i>Food Chemistry</i> , 2022, 391, 133255.	4.2	1
11582	Importance of R-CH ₃ â€¯O tetrel bonding and vinylâ€¯aryl stacking interactions in stabilizing the crystal packing of 2â€™,4â€™-dihydroxy-3â€™-methoxychalcone: Exploration of antileishmanial activity and molecular docking studies. <i>Journal of Molecular Structure</i> , 2022, 1265, 133357.	1.8	1
11583	Two-Dimensional Activated Carbon Nanosheets from Natural Corn Straw Piths and its Rapid Removal of Tetracycline Via Strongâ€¯Electron Donor Receptor Interactions. <i>SSRN Electronic Journal</i> , 0, , .	0.4	1
11584	New Cadmium(II) Porphyrin-Based Coordination Dimer: Experimental and Theoretic Studies. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11585	1-(4-Hydroxyphenyl)-2 <i>H</i> -tetrazole-5-thione as a leveler for acid copper electroplating of microvia. <i>RSC Advances</i> , 2022, 12, 16153-16164.	1.7	5
11586	Highly Efficient Removal of Organic Contaminant with Wide Concentration Range by a Novel Self-Cleaning Hydrogel: Mechanism, Degradation Pathway and Dft Calculation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
11587	An unexpected all-metal aromatic tetranuclear silver cluster in human copper chaperone Atox1. <i>Chemical Science</i> , 2022, 13, 7269-7275.	3.7	5
11588	Synthesis, Crystal Structure, Hirshfeld Surface Analysis, Energy Frameworks and Computational Studies of Schiff Base Derivative. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11589	Molecular Structure and Excitation Characteristics of Dhr Under Different External Electric Fields. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11590	Theoretical studies on the excited-state properties of thermally activated delayed fluorescence molecules with aggregation induced emission. <i>Journal of Materials Chemistry C</i> , 2022, 10, 9377-9390.	2.7	7
11591	A Super Stable Near-Infrared Garnet Phosphor Resistant to Thermal Quenching, Thermal Degradation and Hydrolysis. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11592	<i>N</i> -Hydroxy- <i>N</i> -oxide photoinduced tautomerization and excitation wavelength dependent luminescence of ES IPT-capable zinc(II) complexes with a rationally designed 1-hydroxy-2,4-di(pyridin-2-yl)-1 <i>H</i> -imidazole ES IPT-ligand. <i>Dalton Transactions</i> , 2022, 51, 9818-9835.	1.6	13
11593	Copper Oxide Modified Activated Carbon for Enhanced Adsorption Performance of Siloxane: An Experimental and Dft Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11594	2,2,3,3,3-Pentafluoro-1-propanol and its dimer: structural diversity, conformational conversion, and tunnelling motion. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14975-14984.	1.3	6
11595	Competitor Hydrogen-Bond Acceptors in the Sp(Nh) ₃ -Based Structures: Similarity/Differences of Structural Features Completed with Database Survey and Chemical Calculation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11596	Understanding the interaction of N-doped graphene and sulfur compounds in a lithium-sulfur battery – a density functional theory investigation. <i>New Journal of Chemistry</i> , 0, , .	1.4	4
11597	Insight into understanding magnetic transition quite sensitive to nonmagnetic impurity in a one-dimensional <i>S</i> = 1/2 regular linear chain system. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 3709-3718.	3.0	2
11598	X-ray absorption near-edge spectroscopy of antimony complexed with organic molecules: a theoretical interpretation. <i>Journal of Analytical Atomic Spectrometry</i> , 2022, 37, 1578-1586.	1.6	1
11599	Persistent Free Radicals on Carbon Nanotubes and Their Catalytic Effect on Benzoyl Peroxide Decomposition. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11600	In Situ Prepared All-Fluorinated Polymer Electrolyte for Energy-Dense High-Voltage Lithium-Metal Batteries. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11601	In Silico Package Solutions for Deriving Values of Solute Parameters in Linear Solvation Energy Relationships. <i>SSRN Electronic Journal</i> , 0, , .	0.4	1
11602	A new krypton complex – experimental and computational investigation of the krypton sulphur pentafluoride cation, [KrSF ₅] ⁺ , in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14631-14639.	1.3	2
11603	Improved Photovoltaic Performances of Coumarin Derivatives by Forming D-A ² -A Structure Using Diketopyrrolopyrrole as Auxiliary Acceptor. <i>SSRN Electronic Journal</i> , 0, , .	0.4	1
11604	Characterizing the n ⁺ π* interaction of pyridine with small ketones: a rotational study of pyridine-acetone and pyridine-2-butanone. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 15484-15493.	1.3	5

#	ARTICLE	IF	CITATIONS
11605	Insight into the nucleoside transport and inhibition of human ENT1. <i>Current Research in Structural Biology</i> , 2022, 4, 192-205.	1.1	1
11606	Diversity-Oriented Synthesis of Functional Polymers with Multisubstituted Small Heterocycles by Facile Stereoselective Multicomponent Polymerizations. <i>Macromolecules</i> , 2022, 55, 4389-4401.	2.2	4
11607	Enhancing CH ₄ Capture from Coalbed Methane through Tuning van der Waals Affinity within Isoreticular Al-Based Metal-Organic Frameworks. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 25374-25384.	4.0	32
11608	Cis-Trans Isomerism Inducing Cocrystal Polymorphism with Thermally Activated Delayed Fluorescence and Two-Photon Absorption. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	6
11609	Synthesis of dielectric polystyrene via one-step nitration reaction for large-scale energy storage. <i>Chemical Engineering Journal</i> , 2022, 446, 137281.	6.6	38
11610	Evaluating the conformational space of the active site of D_2 dopamine receptor. Scope and limitations of the standard docking methods. <i>Journal of Computational Chemistry</i> , 2022, 43, 1298-1312.	1.5	2
11611	The mechanisms and molecular properties about isomerization of resin acids, synthesis of acrylopinaric acid based on DFT Calculation. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	0
11612	The Pnictogen Bond: The Covalently Bound Arsenic Atom in Molecular Entities in Crystals as a Pnictogen Bond Donor. <i>Molecules</i> , 2022, 27, 3421.	1.7	13
11613	Targeted preparation and recognition mechanism of broad-spectrum antibody specific to Aconitum alkaloids based on molecular modeling and its application in immunoassay. <i>Analytica Chimica Acta</i> , 2022, 1222, 340011.	2.6	2
11614	A DFT Study of the Hydrogen Bonded Structures of Pyruvic Acid-Water Complexes. <i>Frontiers in Physics</i> , 0, 10, .	1.0	4
11615	Phase Splitting Rules of the Primary/Secondary Amine-Tertiary Amine Systems: Experimental Rapid Screening and Corrected Quasi-Activity Coefficient Model. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 7709-7717.	1.8	3
11616	Carbon nitride coupled with Fe-based MOFs as an efficient photoelectrocatalyst for boosted degradation of ciprofloxacin: Mechanism, pathway and fate. <i>Separation and Purification Technology</i> , 2022, 296, 121325.	3.9	13
11617	Singlet Spin State Drives [V]-Carbene To Catalyze Olefin Metathesis: A Computational Analysis . <i>Organometallics</i> , 2022, 41, 1295-1303.	1.1	4
11618	Desensitizing high energy materials HMX and CL-20 by the smallest all carbon compound cyclo[18]carbon: a DFT study. <i>Journal of Materials Science</i> , 2022, 57, 10197-10212.	1.7	9
11619	Temperature-Independent Ultralong Organic Phosphorescence with a Symmetrical Butterfly-Type Structure. <i>Crystal Growth and Design</i> , 0, , .	1.4	0
11620	Synthesis, crystal structure, and a molecular modeling approach to identify effective antiviral hydrazide derivative against the main protease of SARS-CoV-2. <i>Journal of Molecular Structure</i> , 2022, 1265, 133391.	1.8	6
11621	Adsorption of Industrial Gases (CH ₄ , CO ₂ , and CO) on Olympicene: A DFT and CCSD(T) Investigation. <i>ACS Omega</i> , 2022, 7, 18852-18860.	1.6	14
11622	Synthesis, Structure and Bonding in Pentagonal Bipyramidal Cluster Compounds Containing a cyclo-Sn ₅ Ring, [(CO) ₃ MSn ₅ (CO) ₃] ₄ ²⁺ (M = Cr, Mo). <i>Inorganics</i> , 2022, 10, 75.	1.2	5

#	ARTICLE	IF	CITATIONS
11623	Green Synthesis and Biological Activity Investigation of New Thiazinotriazines: A Combined Experimental and Theoretical Investigation. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 3613-3639.	1.4	0
11624	Deep Eutectic Solvents or Eutectic Mixtures? Characterization of Tetrabutylammonium Bromide and Nonanoic Acid Mixtures. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3889-3896.	1.2	22
11625	New insights in the hydrolysis mechanism of carbon disulfide (CS ₂): a density functional study. <i>Structural Chemistry</i> , 2023, 34, 71-82.	1.0	2
11626	Chain-Length- and Concentration-Dependent Isomerization of Bithiophenyl-Based Diaminotriazine Derivatives in Two-Dimensional Polymorphic Self-Assembly. <i>Langmuir</i> , 2022, 38, 7005-7012.	1.6	10
11627	First principle study on the structures and properties of Ag _m (Ag ₂ S) ₆ (m = 3, 12) clusters. <i>Journal of Nanoparticle Research</i> , 2022, 24, .	0.8	4
11628	Interaction of Cysteine with Li ⁺ and LiF in the Presence of (H ₂ O) _n (n = 6) Clusters. <i>ACS Omega</i> , 2022, 7, 18646-18659.	1.6	2
11629	Computer-Aided Rational Construction of Mediated Bioelectrocatalysis with π -Conjugated (Hetero)cyclic Molecules: Toward Promoted Distant Electron Tunneling and Improved Biosensing. <i>Analytical Chemistry</i> , 2022, 94, 8033-8040.	3.2	5
11630	Photoinduced manganese-catalysed hydrofluorocarbofunctionalization of alkenes. , 2022, 1, 475-486.		36
11631	Interactions and spectroscopic characteristics of propidium dication on soluble graphene oxides. <i>Journal of Molecular Structure</i> , 2022, 1265, 133402.	1.8	6
11632	The Key Role of Competition between Orbital and Electrostatic Interactions in the Adsorption on Transition Metal Single-Atom Catalysts Anchored by N-doped Graphene. <i>ChemCatChem</i> , 2022, 14, .	1.8	12
11633	Theoretical study of electronic and nonlinear optical properties of novel graphenylene-based materials with donor-acceptor frameworks. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	0
11634	Study of Intermolecular Interaction between Small Molecules and Carbon Nanobelt: Electrostatic, Exchange, Dispersive and Inductive Forces. <i>Catalysts</i> , 2022, 12, 561.	1.6	4
11635	Coumarinolignans with Reactive Oxygen Species (ROS) and NF- κ B Inhibitory Activities from the Roots of <i>Waltheria indica</i> . <i>Molecules</i> , 2022, 27, 3270.	1.7	3
11636	Quantum computational, spectroscopic (FT-IR, NMR and UV-Vis) profiling, Hirshfeld surface, molecular docking and dynamics simulation studies on pyridine-2,6-dicarbonyl dichloride. <i>Journal of Molecular Structure</i> , 2022, 1265, 133374.	1.8	26
11637	Molecules with a TEMPO-based head group as high-performance organic friction modifiers. <i>Friction</i> , 2023, 11, 316-332.	3.4	6
11638	Nickel and Palladium Complexes of a PP(O)P Pincer Ligand Based upon a <i>peri</i> -Substituted Acenaphthyl Scaffold and a Secondary Phosphine Oxide. <i>Inorganic Chemistry</i> , 2022, 61, 8406-8418.	1.9	3
11639	A study on monoterpene-based natural deep eutectic solvents. <i>Green Chemical Engineering</i> , 2023, 4, 99-114.	3.3	7
11640	Ab initio study for superior sensitivity of graphyne nanoflake towards nitrogen halides over ammonia. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	5

#	ARTICLE	IF	CITATIONS
11641	DFT study of transition metals doped calix-4-pyrrole with excellent electronic and non-linear optical properties. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113767.	1.1	29
11642	Composition-selective full inclusion host-guest interaction of azobenzene-containing photoresponsive nanoring with fullerene C ₆₀ . <i>Journal of Computational Chemistry</i> , 0, .	1.5	3
11643	New hydrate cocrystal of l-proline with 4-acetylphenylboronic acid obtained via mechanochemistry and solvent evaporation: An experimental and theoretical study. <i>Journal of Solid State Chemistry</i> , 2022, , 123282.	1.4	2
11644	Synthesis, structural and electrochemical properties of a new family of amino-acid-based coordination complexes. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2022, 78, 520-536.	0.5	1
11645	Pyran-based derivative: non-conventional organogel and tri-colored high-contrast mechanochromism. <i>Tetrahedron Letters</i> , 2022, 100, 153888.	0.7	5
11646	Structures of 18-crown-6/Cs ⁺ complexes in aqueous solutions by wide angle X-ray scattering and density functional theory. <i>Journal of Molecular Liquids</i> , 2022, 360, 119477.	2.3	1
11647	Mesoporous Polyimide-Linked Covalent Organic Framework with Multiple Redox-Active Sites for High-Performance Cathodic Li Storage. <i>Angewandte Chemie</i> , 0, , .	1.6	3
11648	Computational study of 2N-atom functionalized corannulene by alkali metals doping: Towards the development of highly efficient nonlinear optical materials. <i>Physica B: Condensed Matter</i> , 2022, 640, 414041.	1.3	14
11649	Conversion of SeS ₂ to Organoselenosulfides Enables High-Performance Rechargeable Lithium Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 7526-7535.	3.2	1
11650	Expanded Azaporphyrins Consisting of Multiple BODIPY Units: Global Aromaticity and High Affinities Towards Alkali Metal Ions. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	9
11651	Self-aggregating behavior of poly(4-vinyl pyridine) and the potential in mitigating sand production based on I-I stacking interaction. <i>Petroleum Science</i> , 2022, 19, 2165-2174.	2.4	1
11652	A supramolecular photosensitizer derived from an Arene-Ru(II) complex self-assembly for NIR activated photodynamic and photothermal therapy. <i>Nature Communications</i> , 2022, 13, .	5.8	58
11653	Effect of starch-catechin interaction on regulation of starch digestibility during hot-extrusion 3D printing: Structural analysis and simulation study. <i>Food Chemistry</i> , 2022, 393, 133394.	4.2	31
11654	DFT investigation of graphene quantum dot-Ixora floral natural dye (GQD-NDIX) nanocomposites as visible light harvesters in dye-sensitized solar cells. <i>Journal of Molecular Liquids</i> , 2022, 360, 119531.	2.3	15
11655	A Theoretical Study of Unsupported Uranium-Ruthenium Bonds Based on Tripodal Ligands. <i>Organometallics</i> , 2022, 41, 1304-1313.	1.1	0
11656	Highly Emissive Platinum(II) Complexes Bearing Bulky Phenyltriazolate Ligands: Synthesis, Structure, and Photophysics. <i>Organometallics</i> , 2022, 41, 1381-1390.	1.1	3
11657	A lysosome-targeted near-infrared fluorescent probe for cell imaging of Cu ²⁺ . <i>Dyes and Pigments</i> , 2022, 204, 110472.	2.0	17
11658	Guest-induced amorphous-to-crystalline transformation enables sorting of haloalkane isomers with near-perfect selectivity. <i>Science Advances</i> , 2022, 8, .	4.7	29

#	ARTICLE	IF	CITATIONS
11659	Revisiting the Role of Charge Transfer in the Emission Properties of Carborane-Fluorophore Systems: A TDDFT Investigation. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4199-4210.	1.1	5
11660	Hydrogen bonding interactions on molecular properties of pesticidal compound 4-nitrophthalic acid: experimental density functional theory computations, electron localized function, localized orbital locator analysis and molecular docking scrutiny. <i>Spectroscopy Letters</i> , 2022, 55, 362-372.	0.5	6
11661	Sterically Hindered Tellurium(IV) Catecholate as a Lewis Acid. <i>Inorganic Chemistry</i> , 0, , .	1.9	6
11662	Boosting faradaic efficiency of CO ₂ electroreduction to CO for Fe-N-C single-site catalysts by stabilizing Fe ³⁺ sites via F-doping. <i>Nano Research</i> , 2022, 15, 7896-7902.	5.8	27
11663	Computational study of furosemide-piperazine (FS-PZ) and 2,3,5,6-tetramethylpyrazine (FS-TP) co-crystals. <i>Journal of Molecular Liquids</i> , 2022, 360, 119537.	2.3	9
11664	Theoretical insights into the linear relationship between $\epsilon_{\text{mml}}^{\text{math}}$ values and vibrational frequencies. <i>Chemical Physics Letters</i> , 2022, 803, 139746.	1.2	10
11665	Real-Time Fluorescence Imaging of the Abscisic Acid Receptor Allows Nondestructive Visualization of Plant Stress. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 28489-28500.	4.0	7
11666	Molecular Orientation-Induced Second-Harmonic Generation: Deciphering Different Contributions Apart. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3732-3738.	1.1	5
11667	Theoretical studies on 2,3,5,6-Tetra(1H-tetrazol-5-yl)pyrazine and 1,1-diamino-2,2-Dinitroethylene blending system. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108235.	1.3	3
11668	Expanded Azaporphyrins Consisting of Multiple BODIPY Units: Global Aromaticity and High Affinities Towards Alkali Metal Ions. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	2
11669	Synthesis, characterization, vibrational analysis and computational studies of a new Schiff base from pentafluoro benzaldehyde and sulfanilamide. <i>Journal of Molecular Structure</i> , 2022, 1265, 133445.	1.8	45
11670	A multicolor fluorescent sensor array based on curcumin and its analogs as a shrimp freshness indicator. <i>Sensors and Actuators B: Chemical</i> , 2022, 367, 132153.	4.0	14
11671	Effect of Annulation Mode of Twistarene on the Physical Property and Self-Assembly Behavior of Functionalized Curved Aromatic Molecules. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	8
11672	Theoretical investigation of the structural, optoelectronic, and the application of waste graphene oxide/polymer nanocomposite as a photosensitizer. <i>Materials Research Express</i> , 2022, 9, 065301.	0.8	3
11673	A new quinolinone-chalcone hybrid with potential antibacterial and herbicidal properties using in silico approaches. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	5
11674	Dissociation of Bipyridine and Coordination with Nitrosyl: Cyclometalated Ruthenium Nitrosyl Complex. <i>Inorganic Chemistry</i> , 2022, 61, 8997-9011.	1.9	5
11675	Control and Modulation of Photoinduced Charge Transfer in a Rigid Donor-Bridge-Acceptor System by Electric Fields. <i>Journal of Physical Chemistry A</i> , 0, , .	1.1	3
11676	Large steric hindrance amide modified benzothiadiazole: High contrast mechanochromic luminescence and volatile acid vapor response. <i>Dyes and Pigments</i> , 2022, 204, 110471.	2.0	7

#	ARTICLE	IF	CITATIONS
11677	Study of Cyclozaprid Co-crystals: Characterization, Theory Calculation, Solubility, and Stability. <i>Crystal Growth and Design</i> , 2022, 22, 4437-4452.	1.4	8
11678	Experimental and theoretical studies of novel Schiff base based on diammino benzophenone with formyl chromone "BPAMC. <i>Journal of Molecular Structure</i> , 2022, 1265, 133450.	1.8	7
11679	Excited-state regulated electroluminescence performance from thermally-activated delayed fluorescence (TADF) to hybridized local and charge-transfer (HLCT) emission. <i>Dyes and Pigments</i> , 2022, 205, 110463.	2.0	11
11680	A hybrid of tetrazolium and pentazolate: An energetic salt with ultrahigh nitrogen content and energy. <i>Energetic Materials Frontiers</i> , 2023, 4, 63-67.	1.3	4
11681	Molecular Structure Design, Crystal Growth, and Characterization of New Types of Organic Nonlinear Optical Chalcone Crystals. <i>Crystal Growth and Design</i> , 2022, 22, 4210-4220.	1.4	12
11682	Molecular Dynamics Simulation of CO ₂ Hydrate Growth and Intermolecular Weak Interaction Analysis. <i>Chemistry and Technology of Fuels and Oils</i> , 2022, 58, 410-421.	0.2	5
11683	Modulation of the Naked-Eye and Fluorescence Color of a Protonated Boron-doped Thiazolothiazole by Anion-dependent Hydrogen Bonding. <i>Chemistry - A European Journal</i> , 0, , .	1.7	5
11684	Coordination of Azobisisobutyronitrile with Cobalt Complexes in Cobalt-Mediated Radical Polymerization Disclosed by Linear Correlation between the Equilibrium Constant and Half-Wave Potential. <i>Macromolecules</i> , 0, , .	2.2	3
11685	Electronic structure and interaction in CH ₄ @C ₆₀ : a first-principle investigation. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	2
11686	[6,6]CNB with controllable external electric field deformation: a theoretical study of the structure-function relationship. <i>Materials Research Express</i> , 2022, 9, 064001.	0.8	3
11687	Enhanced steric effect and desolvation process on organic solvent nanofiltration: A mechanism study for removing anionic dyes. <i>Chemical Engineering Journal</i> , 2022, 446, 137360.	6.6	4
11688	Silver-Catalyzed Asymmetric Aldol Reaction of Isocyanoacetic Acid Derivatives Enabled by Cooperative Participation of Classical and Nonclassical Hydrogen Bonds. <i>Advanced Synthesis and Catalysis</i> , 2022, 364, 2333-2339.	2.1	9
11689	Predicting Dinitrogen Activation by Carborane-Based Frustrated Lewis Pairs. <i>Organometallics</i> , 2022, 41, 1480-1487.	1.1	8
11690	Photo- and Electroluminescent Neutral Iridium(III) Complexes Bearing Imidoamidinate Ligands. <i>Inorganic Chemistry</i> , 2022, 61, 8670-8684.	1.9	5
11691	Synthesis, characterization, and theoretical investigation of potential SARS-CoV-2 agent. <i>ChemistrySelect</i> , 2023, 8, 4839-4857.	0.7	4
11692	Photovoltaic properties of novel reactive azobenzoquinolines: experimental and theoretical investigations. <i>ChemistrySelect</i> , 2022, .	0.7	8
11693	Metallated porphyrinic metal-organic frameworks for CO ₂ conversion to HCOOH: A computational screening and mechanistic study. <i>Molecular Catalysis</i> , 2022, 527, 112407.	1.0	9
11694	The passage of alkali metal cations through the pores in phenine and N-doped phenine nanotubes. <i>Surfaces and Interfaces</i> , 2022, 31, 102083.	1.5	1

#	ARTICLE	IF	CITATIONS
11695	QSAR model and mechanism research on color removal efficiency of dying wastewater by FeCl ₃ coagulation. <i>Ecotoxicology and Environmental Safety</i> , 2022, 240, 113693.	2.9	5
11696	Effect of methyl substituents, ring size, and oxygen on bond dissociation energies and ring-opening kinetics of five- and six-membered cyclic acetals. <i>Combustion and Flame</i> , 2022, 242, 112211.	2.8	7
11697	The inhibition efficiencies of some organic corrosion inhibitors of iron: An insight from density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113759.	1.1	5
11698	Theoretical studies on the photophysical property of 3DPyM-pDTC in solution and in the solid phase. <i>Chemical Physics Letters</i> , 2022, 801, 139727.	1.2	0
11699	Milrinone solubility in aqueous cosolvent solutions revisited: Inter/intra-molecular interactions, enthalpy-entropy compensation, and preferential solvation. <i>Journal of Molecular Liquids</i> , 2022, 360, 119452.	2.3	1
11700	Ultrasensitive and rapid colorimetric detection of urotropin boosted by effective electrostatic probing and non-covalent sampling. <i>Journal of Hazardous Materials</i> , 2022, 436, 129263.	6.5	6
11701	Phenol-cyclohexanol eutectic mixtures: Phase diagram and microscopic structure by experimental and computational studies. <i>Journal of Molecular Liquids</i> , 2022, 360, 119492.	2.3	6
11702	Recovery of chromium (VI) from hazardous APV wastewater using a novel synergistic extraction system. <i>Science of the Total Environment</i> , 2022, 839, 156278.	3.9	8
11703	A mussel-pearl side chain interaction in mercury(II) and phenol removal by sulfur-functionalized covalent organic frameworks: A DFT study. <i>Science of the Total Environment</i> , 2022, 838, 156082.	3.9	6
11704	Tunable fluorescence of Imidazo[1,2-a]pyridine derivatives with additional proton transfer sites Harnessing excited-state intramolecular double proton transfer: Theoretical insight. <i>Journal of Luminescence</i> , 2022, 249, 119016.	1.5	0
11705	Theoretical enhancement of the electronic and optical properties of a new D- π -A- π -D synthesized donor molecule for a new generation of fullerene-based bulk heterojunction (BHJ) for new organic solar cells devices. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 115, 108226.	1.3	4
11706	Magnetic powdery acrylic polymer with ultrahigh adsorption capacity for atenolol removal: Preparation, characterization, and microscopic adsorption mechanism. <i>Chemical Engineering Journal</i> , 2022, 446, 137175.	6.6	16
11707	The combination of terahertz spectroscopy and density functional theory for vibrational modes and weak interactions analysis of vanillin derivatives. <i>Journal of Molecular Structure</i> , 2022, 1265, 133404.	1.8	9
11708	Sulfamic acid/water complexes (SAA-H ₂ O(1-8)) intermolecular hydrogen bond interactions: FTIR, X-ray, DFT and AIM analysis. <i>Journal of Molecular Structure</i> , 2022, 1265, 133394.	1.8	38
11709	Structural-property relationship in halogen-bonded Schiff base derivative: Crystal structure, computational and SARS-CoV-2 docking studies. <i>Journal of Molecular Structure</i> , 2022, 1265, 133409.	1.8	6
11710	Understanding the mechanism of thioguanine's binding to Ag ₆ and bimetallic (Ag ₃ @Au ₃ and Ag ₃ @Cu ₃) clusters. <i>Journal of Molecular Structure</i> , 2022, 1265, 133415.	1.8	16
11711	Characterization of degradation behaviors of PLA biodegradable plastics by infrared spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 279, 121376.	2.0	10
11712	Substituent derivatives of benzothiazole-based fluorescence probes for hydrazine with conspicuous luminescence properties: A theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 279, 121449.	2.0	6

#	ARTICLE	IF	CITATIONS
11713	Atomically dispersed cobalt on carbon nitride for peroxydisulfate activation: Switchable catalysis enabled by light irradiation. <i>Chemical Engineering Journal</i> , 2022, 446, 137277.	6.6	19
11714	Substitution-independent proton transfer in hydroxychromones. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 431, 114024.	2.0	6
11715	Effect of the R126C mutation on the structure and function of the glucose transporter GLUT1: A molecular dynamics simulation study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108227.	1.3	2
11716	A theoretical analysis on the electron and energy transfer between host and guest materials in phosphor-doped OLED. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 432, 114058.	2.0	2
11717	Synthesis and investigations of reactive properties, photophysical properties and biological activities of a pyrazole-triazole hybrid molecule. <i>Journal of Molecular Structure</i> , 2022, 1265, 133363.	1.8	11
11718	Formation of persistent free radicals and reactive chlorine species during photochemical processes of Polychlorophenols: Effect of temperature, humidity and particles. <i>Chemical Engineering Journal</i> , 2022, 446, 137149.	6.6	4
11719	Spectroscopic (UV-vis, FT-IR, FT-Raman, and NMR) analysis, structural benchmarking, molecular properties, and the in-silico cerebral anti-ischemic activity of 2-amino-6-ethoxybenzothiazole. <i>Journal of Molecular Structure</i> , 2022, 1265, 133318.	1.8	28
11720	A molecular electron density theory study on the Chichibabin reaction: The origin of regioselectivity. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108240.	1.3	7
11721	Study on regulation effect of external electric field on energetic material 1-methyl-2,4,5-Trinitroimidazole. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108237.	1.3	2
11722	Quantification of the interactions in halide-anion-based imidazolium ionic liquids. <i>Journal of Ionic Liquids</i> , 2022, 2, 100032.	1.0	11
11723	[Pt ₁ Ag ₃₇ (SAdm) ₂₁ (Dppp) ₃ Cl ₆] ²⁺ : intercluster transformation and photochemical properties. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 3907-3914.	3.0	6
11724	Theoretical Study on Geometric Structures and Hydrogen Storage in Anionic Cehnâ” Â(N=2-20). <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11725	Metal Chelation Ability of Protocatechuic Acid Anion with Radioactive 210po84; a Theoretical Insight. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11726	Solvent Controlled Excited State Intramolecular Proton Transfer (Esipt) Behavior and Luminescent Property of a Novel Phthalimide-Based Fluorophore: A Td-Dft Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11727	Experimental and Theoretical Study on the Evolution of Functional Groups in Cellulose Char During Oxidative Pyrolysis. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11728	Design of potential singlet fission chromophores based on diketofurofuran: an alternative to diketopyrrolopyrrole. <i>Journal of Materials Chemistry C</i> , 2022, 10, 10404-10411.	2.7	3
11729	Three-Photon-Induced Singlet Excited-State Absorption for the Tunable Ultrafast Optical-Limiting in Distyrylbenzene: A First-Principles Study. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	2
11730	Theoretical investigation on structure and optoelectronic performance of two-dimensional fluorbenzidine perovskites. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2022, 71, 208801.	0.2	2

#	ARTICLE	IF	CITATIONS
11731	The regioselectivity of the sulfonylation of tetrazoles: a theoretical view. <i>Organic Chemistry Frontiers</i> , 2022, 9, 4009-4015.	2.3	6
11732	Molecular origins of the multi-donor strategy in inducing bathochromic shifts and enlarging Stokes shifts of fluorescent proteins. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 15937-15944.	1.3	5
11733	An atomically precise silver nanocluster for artificial light-harvesting system through supramolecular functionalization. <i>Chemical Science</i> , 2022, 13, 8355-8364.	3.7	21
11734	Insights into the energetic performance from structures: a density functional theory study on N_6 . <i>New Journal of Chemistry</i> , 2022, 46, 14170-14176.	1.4	1
11735	A theoretical study on the on-off phosphorescence of novel Pt(II)/Pt(IV)-bisphenylpyridinylmethane complexes. <i>RSC Advances</i> , 2022, 12, 18238-18244.	1.7	2
11736	Catalytic Activity Enhancement by P and S Co-Doping of a Single-Atom Fe Catalyst for Peroxymonosulfate-Based Oxidation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11737	Detection of volatile organic compounds, water in organic solvents, and anions using all-in-one type fluorescent emitters, and their data protection applications. <i>Journal of Materials Chemistry C</i> , 2022, 10, 10595-10608.	2.7	6
11738	Organic-conjugated polyanthraquinonylimide cathodes for rechargeable magnesium batteries. <i>Journal of Materials Chemistry A</i> , 2022, 10, 14111-14120.	5.2	15
11739	Insight on noncovalent interactions and orbital constructs in low-dimensional antimony halide perovskites. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 15305-15320.	1.3	1
11740	Structures, and electronic and spectral properties of single-atom transition metal-doped boron clusters MB_{24}^+ ($M = Sc, Ti, V, Cr, Mn, Fe, Co, \text{ and } Ni$). <i>RSC Advances</i> , 2022, 12, 16706-16716.	1.7	7
11741	Decoupling of Thermoelectric Parameters in Two-Dimensional Hyperbranched Platinum Acetylides. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11742	Insights from molecular dynamics simulations for interaction between cellulose microfibrils and hemicellulose. <i>Journal of Materials Chemistry A</i> , 2022, 10, 14451-14459.	5.2	9
11743	Selectivity mechanism of BCL-XL/2 inhibition through in silico investigation. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	2
11744	Robust formation of discrete non-covalent pyrene dimers in an amorphous film by strong π - π interaction. <i>Chemical Communications</i> , 2022, 58, 8250-8253.	2.2	5
11745	Competing on the same stage: Ru-based catalysts modified by basic ligands and organic chlorine salts for acetylene hydrochlorination. <i>Catalysis Science and Technology</i> , 2022, 12, 5086-5096.	2.1	5
11746	Engineering bistetrazoles: (E)-5,5-(ethene-1,2-diyl)bis(1H-tetrazol-1-ol) as a new planar high-energy-density material. <i>Materials Advances</i> , 2022, 3, 6062-6068.	2.6	7
11747	Metal-ligand bonding in tricarbonyliron(0) complexes bearing thiochalcone ligands. <i>New Journal of Chemistry</i> , 2022, 46, 12924-12933.	1.4	1
11748	Novel carbazole- and dioxino[2,3-b]pyrazine-based bipolar hosts for red PhOLEDs with a high brightness. <i>New Journal of Chemistry</i> , 0, , .	1.4	2

#	ARTICLE	IF	CITATIONS
11749	Theoretical study on the mechanism, chemo- and enantioselectivity of the Ag- vs. Rh-catalyzed intramolecular carbene transfer reaction of diazoacetamides. <i>RSC Advances</i> , 2022, 12, 18197-18208.	1.7	1
11750	Effect of Alkyl Chain Length on High-Temperature Corrosion Inhibition Behavior and Mechanism of Imidazole Ionic Liquids: An Experimental, Density Functional Theory and Molecular Dynamics Simulation Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11751	CSi _n Ge _{4-n} ²⁺ ($n = 1-3$): prospective systems containing planar tetracoordinate carbon (ptC). <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16701-16711.	1.3	17
11752	Construction of Carbon Dots with Color-Tunable Electrochemiluminescence and Enhanced Efficiency Enabled by Shadow Trapping States and Intramolecular Charge Transfer. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11753	Intermolecular Adsorption-Pairing Synergy for Accelerated Polysulfide Redox Reactions Towards Lithium-Sulfur Battery with High Stability. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11754	Synthesis and characterization of Pd/NHC _F complexes with fluorinated aryl groups. <i>Dalton Transactions</i> , 2022, 51, 9843-9856.	1.6	3
11755	Comment on "Realization of the Zn ³⁺ oxidation state" by H. Fang, H. Banjade, Deepika and P. Jena, <i>Nanoscale</i> , 2021, 13, 14041-14048. <i>Nanoscale</i> , 2022, 14, 8875-8880.	2.8	2
11756	Metal Chelation Ability of Protocatechuic Acid Anion with Radioactive ²¹⁰ Po84; a Theoretical Insight. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11757	Study on the Non-Thermal Microwave Effect of Organic Sulfur Removal from Coal by Microwave with Peroxyacetic Acid. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11758	A theoretical perspective of the relationship between the structures and luminescence properties of red thermally activated delayed fluorescence molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17140-17154.	1.3	6
11759	Modulating singlet fission through interchromophoric rotation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16193-16199.	1.3	1
11760	Nhc-Catalyzed [3+4] Annulation between 2-Dromoenal and Aryl 1,2-Diamine: Insights into Mechanisms, Chemo and Stereoselectivities. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11761	Dual functional amphiphilic sugar-coated AIE-active fluorescent organic nanoparticles for the monitoring and inhibition of insulin amyloid fibrillation based on carbohydrate-protein interactions. <i>Journal of Materials Chemistry B</i> , 2022, 10, 5602-5611.	2.9	3
11762	HYDROGEN BONDING IN THE CRYSTAL OF 1,1'-((1E,1'E)-(PYRIDINE-3,4-DIYL)BIS(Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 22) EXPERIMENTAL AND THEORETICAL STUDY. <i>Journal of Structural Chemistry</i> , 2022, 63, 626-633.	0.3	1
11763	The microwave spectra and molecular structures of the chiral and achiral rotamers of 2,3,3-trifluoropropene and their gas-phase heterodimers with the argon atom. <i>Journal of Molecular Spectroscopy</i> , 2022, 387, 111656.	0.4	2
11764	Recovery of lithium from salt lake brine with high Na/Li ratio using solvent extraction. <i>Journal of Molecular Liquids</i> , 2022, 362, 119667.	2.3	18
11765	Reconstruction of Electronic Structure of MOF-525 via Metalloporphyrin for Enhanced Photoelectro-Fenton Process. <i>Catalysts</i> , 2022, 12, 671.	1.6	3
11766	Understanding the solvation dynamics of metformin in water using theoretical tools. <i>Journal of Molecular Liquids</i> , 2022, 362, 119678.	2.3	8

#	ARTICLE	IF	CITATIONS
11767	Towards Anion Recognition and Precipitation with Water-Soluble 1,2,4-Selenodiazolium Salts: Combined Structural and Theoretical Study. <i>International Journal of Molecular Sciences</i> , 2022, 23, 6372.	1.8	16
11768	Packing Density-Promoted Emission Strategy toward Tunable Photoluminescence and Room-Temperature Phosphorescence. <i>ACS Sustainable Chemistry and Engineering</i> , 0, , .	3.2	5
11769	D-Ï€-A Dual-Mode Probe Design for the Detection of nM-Level Typical Oxidants. <i>Analytical Chemistry</i> , 2022, 94, 9184-9192.	3.2	9
11770	Influence of Aliphatic Chain Length on Structural, Thermal and Electrochemical Properties of n-alkylene Benzyl Alcohols: A Study of the Odd-Even Effect. <i>Molecules</i> , 2022, 27, 3781.	1.7	2
11771	Local Phonon Environment as a Design Element for Long-Lived Excitonic Coherence: Dithia-anthracenophane Revisited. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3765-3773.	1.1	0
11772	Theoretical studies on <sc>excited-state</sc> properties and luminescence mechanism of a <sc>Carbene-Metal-Amide</sc> Au(I) complex with thermally activated delayed fluorescence. <i>Journal of the Chinese Chemical Society</i> , 2023, 70, 680-688.	0.8	1
11773	PTSA-catalyzed selective synthesis and antibacterial evaluation of 1,2-disubstituted benzimidazoles. <i>Molecular Diversity</i> , 2023, 27, 873-887.	2.1	7
11774	Synergistic surface oxygen defect and bulk Ti3+ defect engineering on SrTiO3 for enhancing photocatalytic overall water splitting. <i>Journal of Colloid and Interface Science</i> , 2022, 626, 662-673.	5.0	23
11775	Enhanced Fluorescence with Tunable Color in Doped Diphosphine-Protected Gold Nanoclusters. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5873-5880.	2.1	10
11776	A trefoil knot self-templated through imination in water. <i>Nature Communications</i> , 2022, 13, , .	5.8	13
11777	Theoretical Studies of a Silica Functionalized Acrylamide for Calcium Scale Inhibition. <i>Polymers</i> , 2022, 14, 2333.	2.0	2
11778	Significant Ï€ Bonding in Coinage Metal Complexes OCTMCCO⁻ from Infrared Photodissociation Spectroscopy and Theoretical Calculations. <i>Journal of Chemical Physics</i> , 0, , .	1.2	0
11779	Photocatalytic Superoxide Radical Generator that Induces Pyroptosis in Cancer Cells. <i>Journal of the American Chemical Society</i> , 2022, 144, 11326-11337.	6.6	90
11780	Leveraging Nitrogen Linkages in the Formation of a Porous Thorium-Organic Nanotube Suitable for Iodine Capture. <i>Inorganic Chemistry</i> , 2022, 61, 9480-9492.	1.9	14
11781	Synthesis of adjustable {312}/{004} facet heterojunction MWCNTs/Bi5O7I photocatalyst for ofloxacin degradation: Novel insights into the charge carriers transport. <i>Journal of Hazardous Materials</i> , 2022, 437, 129374.	6.5	12
11782	Resonance and Electrostatics Making the Difference in Boron- and Aluminum-Halide Structures and Exchange Reactivity. <i>Journal of Chemical Physics</i> , 0, , .	1.2	2
11783	Investigation on the Solvent Effect in Vanillin Habit Evolution. <i>Crystal Growth and Design</i> , 2022, 22, 4086-4093.	1.4	2
11784	Fused Hybrids of a [22]Smaragdyrin BF2-Complex with a Nill Porphyrin. <i>Angewandte Chemie</i> , 0, , .	1.6	0

#	ARTICLE	IF	CITATIONS
11785	Theoretical investigation on the interactions of microplastics with a SARS-CoV-2 RNA fragment and their potential impacts on viral transport and exposure. <i>Science of the Total Environment</i> , 2022, 842, 156812.	3.9	17
11786	Unveil the quantum chemical descriptors determining direct photodegradation of antibiotics under simulated sunlight: Batch experiments and model development. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108086.	3.3	10
11787	Understanding of Photoinduced Reversible Rearrangement from Borepin to Borirane. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	4
11788	Nonlinear optical properties and optimization strategies of D- π -A type phenylamine derivatives in the near-infrared region. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 280, 121539.	2.0	6
11789	Alkaline earth metals doped C ₂ N with enhanced non-linear optical properties. <i>Optik</i> , 2022, 265, 169514.	1.4	3
11790	A high-voltage and stable zinc-air battery enabled by dual-hydrophobic-induced proton shuttle shielding. <i>Joule</i> , 2022, 6, 1617-1631.	11.7	28
11791	Enhanced non-linear optical response of alkali metal-doped nitrogenated holey graphene (C ₂ N). <i>Journal of Molecular Structure</i> , 2022, 1267, 133580.	1.8	3
11792	In silico drug repurposing for coronavirus (COVID-19): screening known HCV drugs against the SARS-CoV-2 spike protein bound to angiotensin-converting enzyme 2 (ACE2) (6M0J). <i>Molecular Diversity</i> , 2023, 27, 1087-1099.	2.1	1
11793	Periphery-Core Strategy to Access a Bowl-Shaped Molecule Bearing Multiple Heteroatoms. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	10
11794	Metal-rich clusters: synthesis, structure and bonding of metallaboranes featuring μ -5-boride and triply bridging borylene units. <i>Inorganica Chimica Acta</i> , 2022, 540, 121045.	1.2	1
11795	Planar Octacoordinate Aluminium in Dual Aromatic AlBe ₄ N ₄ Cluster. <i>Journal of Cluster Science</i> , 0, , .	1.7	0
11796	Synthesis, Crystal Structures, Lipophilic Properties and Antimicrobial Activity of 5-Pyridylmethylidene-3-rhodanine-carboxyalkyl Acids Derivatives. <i>Molecules</i> , 2022, 27, 3975.	1.7	4
11797	Unveiling the <i>cb</i> -type Intramolecular [3+2] Cycloaddition Reactions of Fluorinated Azomethine Ylides to Ester Carbonyls with a Molecular Electron Density Theory Perspective. <i>ChemistrySelect</i> , 2022, 7, .	0.7	1
11798	Experimental and theoretical investigations of lithium isotopes separation using 10-hydroxybenzoquinoline. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2022, 331, 3155-3165.	0.7	2
11799	Effect of pH and Cl ⁻ concentration on the electrochemical oxidation of pyridine in low-salinity reverse osmosis concentrate: Kinetics, mechanism, and toxicity assessment. <i>Chemical Engineering Journal</i> , 2022, 449, 137669.	6.6	11
11800	Exploring the influence of intermolecular hydrogen bonding on the fluorescence properties of HQCT and HQPH fluorescent chemosensors. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 280, 121537.	2.0	1
11801	Combination of FTIR and DFT to study the regulation law of [EMIM][OAc] on the microstructure of the acetone-methanol azeotrope system. <i>Journal of Molecular Liquids</i> , 2022, 362, 119601.	2.3	6
11802	Solvent-Induced Isomeric Cu ₁₃ Nanoclusters: Chlorine to Copper Charge Transfer Boosting Molecular Oxygen Activation in Sulfide Selective Oxidation. <i>ACS Nano</i> , 2022, 16, 9598-9607.	7.3	28

#	ARTICLE	IF	CITATIONS
11803	Reactivityâ€Tunable Palladium Precatalysts with Favorable Catalytic Properties in Suzukiâ€Miyaura Crossâ€Coupling Reactions. <i>ChemCatChem</i> , 2022, 14, .	1.8	1
11804	Noncovalent Interactions and Crystal Structure Prediction of Energetic Materials. <i>Molecules</i> , 2022, 27, 3755.	1.7	5
11805	Do certain imidazolium-based ionic liquid ion pairs/mordenite capture H ₂ S by conformational traps? An ONIOM-DFT study. <i>Microporous and Mesoporous Materials</i> , 2022, , 112053.	2.2	0
11806	UV-Vis Spectroscopy, Electrochemical and DFT Study of Tris(Î²-diketonato)iron(III) Complexes with Application in DSSC: Role of Aromatic Thienyl Groups. <i>Molecules</i> , 2022, 27, 3743.	1.7	3
11807	Aromaticity Concepts Derived from Experiments. <i>Sci</i> , 2022, 4, 24.	1.8	2
11808	Comparative investigation of diclofenac degradation by Fe ²⁺ /chlorine and Fe ²⁺ /PMS processes. <i>Separation and Purification Technology</i> , 2022, 297, 121555.	3.9	20
11809	Virtual Experiments on Real Asphaltenes: Predicting Properties Using Quantum Chemical Simulations of Structures from Non-contact Atomic Force Microscopy. <i>Energy & Fuels</i> , 2022, 36, 8714-8724.	2.5	6
11810	Domination of H-Bond Interactions in the Solvent-Triggering Gelation Process. <i>Langmuir</i> , 0, , .	1.6	1
11811	Boron based intramolecular heterocyclic frustrated Lewis pairs as organocatalysts for <sc>CO</sc> adsorption and activation. <i>Journal of Computational Chemistry</i> , 2022, 43, 1474-1483.	1.5	10
11812	De-scaling, experimental, DFT, and MD-simulation studies of unwanted growing plant as natural corrosion inhibitor for SS-410 in acid medium. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 649, 129333.	2.3	19
11813	Mixed-Orbital Charge Transport in N-Shaped Benzene- and Pyrazine-Fused Organic Semiconductors. <i>Journal of the American Chemical Society</i> , 2022, 144, 11159-11167.	6.6	14
11814	Resonating B, N Covalent Bond and Coordination Bond in Aromatic Compounds and Conjugated Polymers. <i>Angewandte Chemie</i> , 0, , .	1.6	2
11815	Inverse molecular design of alkoxides and phenoxides for aqueous direct air capture of CO ₂ . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	8
11816	A Steroidal Molecular Rotor with Fast Solidâ€State Dynamics Obtained by Crystal Engineering: Role of the Polarity of the Stator. <i>European Journal of Organic Chemistry</i> , 0, , .	1.2	5
11817	Missing Recipe in the Naâ€B Bond in NaBH ₃ ⁺ Cluster. <i>ChemistrySelect</i> , 2022, 7, .	0.7	1
11818	Experimental and Computational Studies on Octyl Hydroxamic Acid as an Environmentally Friendly Inhibitor of Cobalt Chemical Mechanical Polishing. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 28321-28336.	4.0	19
11819	Hydrazone-based Materials; DFT, TD-DFT, NBO Analysis, Fukui Function, MESP Analysis, and Solar Cell Applications. <i>Journal of Fluorescence</i> , 0, , .	1.3	25
11820	Auâ€Au Chemical Bonding in Nitronyl Nitroxide Gold(I) Derivatives. <i>Organometallics</i> , 2022, 41, 1710-1720.	1.1	2

#	ARTICLE	IF	CITATIONS
11821	The effect of anchoring group on the performances of metal-free phthalocyanine and metallophthalocyanine dye/titanium dioxide interface for dye-sensitized solar cells. <i>Surfaces and Interfaces</i> , 2022, 32, 102089.	1.5	7
11822	Highly Retentive, Anti-Interference, and Covert Individual Marking Taggant with Exceptional Skin Penetration. <i>Advanced Science</i> , 2022, 9, .	5.6	4
11823	Spectroscopic studies, TD/DFT calculations, electrochemical, antibacterial, and Hirshfeld surface analysis of Ni(II) and Co(III) complexes based on 3-ethoxy salicylaldehyde. <i>Journal of Molecular Structure</i> , 2022, 1266, 133554.	1.8	14
11824	Synthesis, XRD, Hirshfeld surface analysis, DFT studies, cytotoxicity and anticancer activity of di(m-chlorobenzyl) (dichloro) (4, 7-diphenyl-1,10-phenanthroline) tin (IV) complex. <i>Journal of Molecular Structure</i> , 2022, 1267, 133542.	1.8	23
11825	Fine-tuning the ð bridge of organic dye molecules with triaryl amino as an electron donor by using electron-rich/deficient groups for more efficient dye-sensitized solar cells. <i>Molecular Physics</i> , 2022, 120, .	0.8	2
11826	Fully Bio-Based and Supertough PLA Blends via a Novel Interlocking Strategy Combining Strong Dipolar Interactions and Stereocomplexation. <i>Macromolecules</i> , 2022, 55, 5864-5878.	2.2	18
11827	Cellulose polymers with ð ² -amino ester pendant group: design, synthesis, molecular docking and application in adsorption of toxic metals from wastewater. <i>BMC Chemistry</i> , 2022, 16, .	1.6	17
11828	Enhanced adsorption of fluoroquinolone antibiotic on the surface of the Mg-, Ca-, Fe- and Zn-doped C60 fullerenes: DFT and TD-DFT approach. <i>Materials Today Communications</i> , 2022, 31, 103798.	0.9	10
11829	Study on antibody adsorption and elution performance of carboxyl and hydrophobic groups on mixed-mode ligands. <i>Journal of Separation Science</i> , 2022, 45, 2946-2955.	1.3	2
11830	Experimental and Mechanistic Study of Synergistic Removal of Hg by Evaporation from Desulfurization Wastewater. <i>Energies</i> , 2022, 15, 4541.	1.6	0
11831	General Designing Strategy of Anti-Aromatic Porphyrinoids. <i>Chemistry - A European Journal</i> , 0, , .	1.7	2
11832	Tailoring electric dipole of hole-transporting material p-dopants for perovskite solar cells. <i>Joule</i> , 2022, 6, 1689-1709.	11.7	38
11833	A Resonating B, N Covalent Bond and Coordination Bond in Aromatic Compounds and Conjugated Polymers. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	20
11834	Aggregation Modes of Chiral Diketopyrrolo[3,4- <i>bc</i>]pyrrole Dyes in Solution and Thin Films. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	10
11835	Adsorption of a thione derivative on carbon, AlN, and BN nanotubes: a detailed DFT and MD investigation. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	12
11836	Effect of Molecular Shape on the Properties of Indolo[3,2,1- <i>ijk</i>]carbazole-Based Compounds. <i>European Journal of Organic Chemistry</i> , 2022, 2022, .	1.2	4
11837	Structural evolution and electronic properties of germanium-doped boron clusters and their anions: GeBnO/ ⁻ (n = 6-20). <i>Journal of Nanoparticle Research</i> , 2022, 24, .	0.8	0
11838	Effects of non-covalent interactions between pectin and volatile compounds on the flavor release of tomato paste. <i>Food Hydrocolloids</i> , 2022, 133, 107886.	5.6	6

#	ARTICLE	IF	CITATIONS
11839	Tetramethylammonium Cation: Directionality and Covalency in Its Interactions with Halide Ions. <i>Inorganic Chemistry</i> , 2022, 61, 9082-9095.	1.9	8
11840	Bismuth Coordinates with Iodine Atoms to Form Chemical Bonds for Existing Stabilization in Boron Class. <i>Inorganic Chemistry</i> , 2022, 61, 9860-9867.	1.9	4
11841	Green and Facile Fabrication of Metal Oxide/Red Phosphorus Composite Catalysts for CO ₂ Photoreduction. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 8658-8668.	3.2	8
11842	Through-Bond-Driven Through-Space Interactions in a Fullerene C ₆₀ Noncovalent Dyad: An Unusual Strong Binding between Spherical and Planar π Electron Clouds and Culmination of Dyadic Fractals. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3629-3641.	1.1	4
11843	Direct Spectroscopic Evidence for Charge-Assisted Hydrogen-Bond Formation between Ionizable Organic Chemicals and Carbonaceous Materials. <i>Environmental Science & Technology</i> , 2022, 56, 9356-9366.	4.6	19
11844	Selective Removal of Iron, Lead, and Copper Metal Ions from Industrial Wastewater by a Novel Cross-Linked Carbazole-Piperazine Copolymer. <i>Polymers</i> , 2022, 14, 2486.	2.0	3
11845	Synthesis, characterization and anticancer activities of cationic η^6 -p-cymene ruthenium(II) complexes containing phosphine and nitrogenous ligands. <i>Polyhedron</i> , 2022, 224, 115980.	1.0	2
11846	Various Sorts of Chalcogen Bonds Formed by an Aromatic System. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4025-4035.	1.1	9
11847	Mechanisms of ionic liquids on the enhancement of interfacial transport of lithium ions in crown ether system. <i>Journal of Cleaner Production</i> , 2022, 366, 132782.	4.6	10
11848	Simulation Studies on Signature Interactions between Cancer DNA and Cysteamine-Decorated AuNPs for Universal Cancer Screening. <i>ACS Applied Nano Materials</i> , 2022, 5, 9042-9052.	2.4	8
11849	Role of methoxy and C -based substituents in electrochemical oxidation mechanisms and bond cleavage selectivity of β^2 -O-4 lignin model compounds. <i>Green Energy and Environment</i> , 2024, 9, 114-125.	4.7	6
11850	Insight into the Clustering-Triggered Emission and Aggregation-Induced Emission Exhibited by an Adamantane-Based Molecular System. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5358-5364.	2.1	7
11851	Theoretical Investigation of Switch Effect on the Efficiency and Adaptivity of Molecular Optoelectronic Conversion Devices. <i>Chemistry - an Asian Journal</i> , 0, , .	1.7	0
11852	Metal-Rich Phosphides Obtained from the Lead Flux: Synthesis, Crystal, and Electronic Structure of Sr ₅ Pt ₁₂ P ₉ and BaPt ₃ P ₂ . <i>Inorganic Chemistry</i> , 2022, 61, 9173-9183.	1.9	3
11853	Impact of Graphene Quantum Dot Edge Morphologies on Their Optical Properties. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5801-5807.	2.1	5
11854	Design, Synthesis, and Fungicidal Evaluation of Novel 1,3-Benzodioxole-Pyrimidine Derivatives as Potential Succinate Dehydrogenase Inhibitors. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 7360-7374.	2.4	15
11855	Evaluation of Slight Changes in Aromaticity through Electronic and Density Functional Reactivity Theory-Based Descriptors. <i>ACS Omega</i> , 2022, 7, 21939-21945.	1.6	9
11856	Fluorinated copper phthalocyanine as an electron transport material in perovskite solar cell. <i>International Journal of Energy Research</i> , 2022, 46, 15127-15142.	2.2	15

#	ARTICLE	IF	CITATIONS
11894	Design of frustrated Lewis pair in defective TiO ₂ for photocatalytic non-oxidative methane coupling. <i>Chem Catalysis</i> , 2022, 2, 1775-1792.	2.9	12
11895	Binding Modes and Origins of Enantioselectivity in the Phase-Transfer-Catalyzed Conjugate Cyanation of <i>p</i> -Trifluoromethylated Chalcones. <i>ACS Catalysis</i> , 2022, 12, 8185-8194.	5.5	5
11896	Effects of solvents on the excited-state intramolecular proton transfer in 3- <i>H</i> TC. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, .	0.9	2
11897	Efficient synthesis of the promising energetic material precursor 4-azido-3,5-dinitro-1 <i>H</i> -pyrazole with high detonation performance. <i>Journal of Molecular Structure</i> , 2022, 1267, 133526.	1.8	4
11898	Synthesis, Characterization, and Properties of BN-Fluoranthenes. <i>Organic Letters</i> , 0, , .	2.4	2
11899	Experimental and Theoretical Study of N ₂ Adsorption on Hydrogenated Y ₂ C ₄ H ⁺ and Dehydrogenated Y ₂ C ₄ H ⁻ Cluster Anions at Room Temperature. <i>International Journal of Molecular Sciences</i> , 2022, 23, 6976.	1.8	2
11900	Advanced prediction of organic-metal interactions through DFT study and electrochemical displacement approach. <i>Journal of Magnesium and Alloys</i> , 2023, 11, 301-316.	5.5	6
11901	Important Routes for Methanediol Formation by Formaldehyde Hydrolysis Catalyzed by Iodic Acid and for the Contribution to an Iodic Acid Sink by the Reaction of Formaldehyde with Iodic Acid Catalyzed by Atmospheric Water. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 1890-1898.	1.2	4
11902	Impact of end-capped modification of MO-IDT based non-fullerene small molecule acceptors to improve the photovoltaic properties of organic solar cells. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108255.	1.3	37
11903	Banana-shaped electron acceptors with an electron-rich core fragment and 3D packing capability. , 2023, 5, .		22
11904	Microsolvated Ion-Molecule S _N 2 Reactions with Dual Nucleophiles Induced by Solvent Molecules. <i>ChemPhysChem</i> , 2022, 23, .	1.0	4
11905	Theoretical Studies on the Structure and Intramolecular Interactions of Fagopyrins Natural Photosensitizers of Fagopyrum. <i>Molecules</i> , 2022, 27, 3689.	1.7	6
11906	Mesoporous Polyimide-Linked Covalent Organic Framework with Multiple Redox-Active Sites for High-Performance Cathodic Li Storage. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	79
11907	Unraveling the Key Role of the Benzyl Group in the Synthesis of CL-20 Precursor HBIW. <i>ACS Omega</i> , 2022, 7, 21912-21924.	1.6	3
11908	Direct assembly between closed-shell coinage metal superatoms. <i>Nano Research</i> , 2022, 15, 8665-8672.	5.8	6
11909	Mechanistic Insights into Palladium(II)-Catalyzed Carboxylation of Thiophene and Carbon Dioxide. <i>Catalysts</i> , 2022, 12, 654.	1.6	2
11910	Inverse Design of Hybrid Organic-Inorganic Perovskites with Suitable Bandgaps via Proactive Searching Progress. <i>ACS Omega</i> , 2022, 7, 21583-21594.	1.6	14
11911	Strain-boosted hyperoxic graphene oxide efficiently loading and improving performances of microcystinase. <i>IScience</i> , 2022, 25, 104611.	1.9	2

#	ARTICLE	IF	CITATIONS
11912	Hydroxy-safflower yellow A composites: An effective strategy to enhance anti-myocardial ischemia by improving intestinal permeability. <i>International Journal of Pharmaceutics</i> , 2022, 623, 121918.	2.6	2
11913	Effects of additional π -bridges on a terpolymer based on the second acceptor unit of DTBT and the performance of organic solar cells. <i>Polymer</i> , 2022, 254, 125089.	1.8	0
11914	Hydroxyl-ionic liquid functionalized metalloporphyrin as an efficient heterogeneous catalyst for cooperative cycloaddition of CO ₂ with epoxides. <i>Journal of CO₂ Utilization</i> , 2022, 62, 102107.	3.3	9
11915	Tuning the photovoltaic parameters of spiro[fluorenehexanthenes]-diol (SFX-OH)-based crosslinked donor materials for efficient organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113778.	1.1	1
11916	DFT study on the mechanism of the CO ₂ -to-CO conversion by Co-quaterpyridine complexes. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113794.	1.1	2
11917	Adsorption properties of seaweed-based biochar with the greenhouse gases (CO ₂ , CH ₄ , N ₂ O) through density functional theory (DFT). <i>Biomass and Bioenergy</i> , 2022, 163, 106519.	2.9	20
11918	Synthesis, structural features, excited state properties, fluorescence spectra, and quantum chemical modeling of (E)-2-hydroxy-5-(((4-sulfamoylphenyl)imino) methyl)benzoic acid. <i>Journal of Molecular Liquids</i> , 2022, 360, 119557.	2.3	30
11919	A TD-DFT study on photoswitchable chloride salts receptor based on acylhydrazone and crown ether embedded Macrocyclic molecule. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113785.	1.1	0
11920	Computational modeling for the design of new fluorescent organic compounds based on both diketopyrrolopyrrole and nitrobenzofurazan moieties. <i>Journal of Molecular Liquids</i> , 2022, 360, 119550.	2.3	13
11921	Comparative study on organic solvents and green solvents in separation of aromatic hydrocarbons/low-carbon alcohols azeotrope by structure-activity relationship. <i>Separation and Purification Technology</i> , 2022, 297, 121498.	3.9	7
11922	Insights into solvation effects, spectroscopic, Hirshfeld surface Analysis, reactivity analysis and anti-Covid-19 ability of doxylamine succinate: Experimental, DFT, MD and docking simulations. <i>Journal of Molecular Liquids</i> , 2022, 361, 119609.	2.3	11
11923	Combustion kinetics of $\text{C}_3\text{H}_7\text{N}$ -propylamine: Theoretical calculations and ignition delay time measurements. <i>Fuel</i> , 2022, 324, 124710.	3.4	3
11924	Discovery of dearomatized isoprenylated acylphloroglucinols with colon tumor suppressive activities in mice via inhibiting NF- κ B-FAT1-PDCD4 signaling activation. <i>European Journal of Medicinal Chemistry</i> , 2022, 239, 114532.	2.6	3
11925	Terephthalato and succinato bridged Mn(II) and Zn(II) coordination polymers involving structure-guiding H-bonded tetrameric assemblies: Antiproliferative evaluation and theoretical studies. <i>Polyhedron</i> , 2022, 224, 115982.	1.0	3
11926	Weak antiferromagnetic interaction in Cu(II) complex with semi-coordination exchange pathway. <i>Polyhedron</i> , 2022, 223, 115962.	1.0	6
11927	Enol or keto? Interplay between solvents and substituents as a factor controlling ESIPT. <i>Journal of Molecular Liquids</i> , 2022, 361, 119611.	2.3	9
11928	Structural and theoretical exploring of noncovalent interactions in Chlorido- and Nitrito-rhenium(I) tricarbonyl complexes bearing 2,3-Butadiene-bis(2-nitrobenzylidene)hydrazine Ligand: Intramolecular Re-endo-ONO(lone pair)- π *(C O) interaction. <i>Inorganica Chimica Acta</i> , 2022, 540, 121049.	1.2	0
11929	Geometric and electronic structure analyses on three Au ₄₂ (SR) ₂₆ isomers. <i>Chemical Physics Letters</i> , 2022, 802, 139804.	1.2	2

#	ARTICLE	IF	CITATIONS
11930	Influence of intermolecular hydrogen bond interaction on fluorescence mechanism for ESIPT characteristic o-Hydroxybenzaldehyde. <i>Chemical Physics</i> , 2022, 561, 111622.	0.9	2
11931	A dinuclear cuprous chloride coordination polymer with grinding triggered luminescence enhancement and temperature dependent luminescent properties. <i>Journal of Solid State Chemistry</i> , 2022, 313, 123331.	1.4	0
11932	Inter-/intra-molecular interactions, preferential solvation, and dissolution and transfer property for tirofiban in aqueous co-solvent mixtures. <i>Journal of Molecular Liquids</i> , 2022, 361, 119665.	2.3	2
11933	Molecular-dynamics study on the thermodynamic properties of nano-SiO ₂ particle-doped silicone rubber composites. <i>Computational Materials Science</i> , 2022, 212, 111571.	1.4	8
11934	Design anion regulated layered double hydroxide and explore its theoretical mechanism of immobilizing uranium. <i>Journal of Hazardous Materials</i> , 2022, 437, 129352.	6.5	6
11935	Effect of intermolecular hydrogen bonds on the proton transfer and fluorescence characteristics of 1-hydroxy-2-acetonaphthone. <i>Journal of Molecular Liquids</i> , 2022, 361, 119555.	2.3	7
11936	Cinnamoylformate derivatives photoinitiators with excellent photobleaching ability and cytocompatibility for visible LED photopolymerization. <i>Progress in Organic Coatings</i> , 2022, 170, 106969.	1.9	10
11937	Molecular dynamics study on adsorption and desorption of lysozyme above polymer antifouling membranes. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 649, 129466.	2.3	8
11938	Enhancement on the degradation of naproxen in CuO activated peroxymonosulfate system by complexing reagents. <i>Journal of Hazardous Materials</i> , 2022, 437, 129416.	6.5	8
11939	Modulating the nanoscale morphology on carboxylate-pyrazine containing terpolymer toward 17.8% efficiency organic solar cells with enhanced thermal stability. <i>Chemical Engineering Journal</i> , 2022, 446, 137424.	6.6	14
11940	Synthesis, spectral, structural features, electronic properties, biological activities, computational, wave function properties, and molecular docking studies of (E)-4-(((pentafluorophenyl) methylene)) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5		
11941	Research on the gamma irradiation decomposition products of 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105). <i>Radiation Physics and Chemistry</i> , 2022, 199, 110352.	1.4	1
11942	Hybridizing electron-mediated H5PMo10V2O40 with CdS/g-C ₃ N ₄ for efficient photocatalytic performance of Z-scheme heterojunction in wastewater treatment. <i>Chemosphere</i> , 2022, 305, 135315.	4.2	9
11943	Structure and hydrogen-bond properties of N-alkyl-N-methyl-pyrrolidinium bis(trifluoromethylsulfonyl)imide and ethanol: A combination of FTIR and theoretical studies. <i>Journal of Molecular Structure</i> , 2022, 1265, 133488.	1.8	2
11944	Probing the mechanism of green solvent solubilization of hemicellulose based on molecular dynamics simulations. <i>Industrial Crops and Products</i> , 2022, 186, 115159.	2.5	9
11945	Doping of superalkali and superhalogen on graphene quantum dot surfaces to enhance nonlinear optical response: An efficient strategy for fabricating novel electro-optical materials. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 169, 110859.	1.9	16
11946	Structural characterization and computational investigations of three fluorine-containing ligands with a terphenyl core. <i>Journal of Molecular Structure</i> , 2022, 1266, 133474.	1.8	0
11947	A WS ₂ /sepiolite composite with highly dispersed WS ₂ nanosheets for photocatalytic wastewater treatment. <i>Applied Clay Science</i> , 2022, 228, 106576.	2.6	7

#	ARTICLE	IF	CITATIONS
11948	Benzothiazole-Isatin Hybrids: Synthesis, Characterization, Computational and Cytotoxic Activity Studies. <i>Journal of Molecular Structure</i> , 2022, 1266, 133517.	1.8	5
11949	Revealing the nature of interaction between C1 chemical molecules and flat nano-carbon graphene/graphyne: Direct picture and quantitative description based on first-principles. <i>Surface Science</i> , 2022, 724, 122133.	0.8	0
11950	Removal of O-containing functional groups during hydrothermal treatment dewatering: A combined experimental and theoretical theory study. <i>Fuel</i> , 2022, 326, 124971.	3.4	8
11951	Exploring competitive inhibition of a family 10 xylanase derived from Hu sheep rumen microbiota by <i>Oryza sativa</i> xylanase inhibitor protein: In vitro and in silico perspectives. <i>Enzyme and Microbial Technology</i> , 2022, 160, 110082.	1.6	5
11952	Investigation of optical, TD-DFT calculation and electrical conductivity in semiconducting [(CH ₃)NH ₃] ₂ ZnBr ₄ . <i>Journal of Molecular Structure</i> , 2022, 1266, 133495.	1.8	0
11953	Boosting hydrogen peroxide accumulation by a novel air-breathing gas diffusion electrode in electro-Fenton system. <i>Applied Catalysis B: Environmental</i> , 2022, 316, 121617.	10.8	25
11954	Mechanism of MnSOD removing peroxy radical for inhibiting coal spontaneous combustion. <i>Fuel</i> , 2022, 325, 124967.	3.4	7
11955	Characteristics of graphite oxide membranes with different thickness by low temperature thermal reduction for aqueous EDLC electrodes and hot activation phenomenon. <i>Materials Research Bulletin</i> , 2022, 154, 111927.	2.7	2
11956	Maximally exploiting active sites on Yolk@shell nanoreactor: Nearly 100% PMS activation efficiency and outstanding performance over full pH range in Fenton-like reaction. <i>Applied Catalysis B: Environmental</i> , 2022, 316, 121594.	10.8	73
11957	Nitronium salts as mild and inexpensive oxidizing reagents toward designing efficient strategies in organic syntheses; A mechanistic investigation based on the DFT insights. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108253.	1.3	2
11958	Deciphering the non-covalent binding patterns of three whey proteins with rosmarinic acid by multi-spectroscopic, molecular docking and molecular dynamics simulation approaches. <i>Food Hydrocolloids</i> , 2022, 132, 107895.	5.6	36
11959	Rational design of freestanding and high-performance thick electrode from carbon foam modified with polypyrrole/polydopamine for supercapacitors. <i>Chemical Engineering Journal</i> , 2022, 447, 137562.	6.6	28
11960	Computational analysis of substituent effect on indole derivatives as potential antibacterial agents. <i>Chemical Physics Impact</i> , 2022, 5, 100088.	1.7	3
11961	Ultrafast Förster resonance energy transfer between tyrosine and tryptophan: potential contributions to protein-water dynamics measurements. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18055-18066.	1.3	4
11962	Binary mono-anions with unprecedented anti-aromatic planar tetracoordinate carbon and nitrogen atoms. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17956-17960.	1.3	7
11963	Simple methods for the introduction of nitrate ester, amino and diazo-oxide substituents into dinitromethylpyrazole. <i>New Journal of Chemistry</i> , 2022, 46, 14186-14191.	1.4	2
11964	A Gd ³⁺ -Doped Blue TiO ₂ Nanotube Array Anode for Efficient Electrocatalytic Degradation of Iohexol. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11965	Rational design of small molecule hole-transporting materials with a linear ĩ€-bridge for highly efficient perovskite solar cells. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18793-18804.	1.3	2

#	ARTICLE	IF	CITATIONS
11966	Hot-exciton harvesting <i>via</i> through-space single-molecule based white-light emission and optical waveguides. <i>Chemical Science</i> , 2022, 13, 9004-9015.	3.7	12
11967	Size-Controllable Crown Ether-Embedded 2d Nanosheets for the Host-Guest Ion Segregation and Recovery: Insights from Dft Simulations. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11968	Janus Dione Derivatives: Novel High-Mobility Hole Transport Materials for Perovskite Solar Cells. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11969	Non-covalent interactions in the glutathione peroxidase active center and their influence on the enzyme activity. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 5551-5557.	1.5	3
11970	A DFT study of the second-order nonlinear optical properties of Ru(<i>ii</i>) polypyridine complexes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18217-18226.	1.3	4
11971	Design and synthesis of piezochromic materials exploring intermolecular charge transfer: chalconoids bound to the <i>p</i> -sulfonatocalix[6]arene macrocycle. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1
11972	Anion photoelectron spectroscopy and density functional theory study of TM ₂ Si _n (TM = V, Cr; <i>n</i> = 14–20) clusters. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18321-18330.	1.3	12
11973	Organocatalytic Synthesis of Chiral Allene Catalyzed by Chiral Phosphoric Acid Via Asymmetric 1,8-Addition of Indole Imine Methide: Mechanism and Origin of Enantioselectivity. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11974	A general approach to S-rhodamines from diaryl thioethers and their application in constructing pH probes. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 5694-5698.	1.5	2
11975	Exploring halogen–halogen interactions in supramolecular self-assemblies of BODIPY networks. <i>CrystEngComm</i> , 2022, 24, 5630-5641.	1.3	6
11976	Constructing high-performance TADF polymers from non-TADF monomers: a computational investigation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17686-17694.	1.3	6
11977	Machine learning with quantum chemistry descriptors: predicting the solubility of small-molecule optoelectronic materials for organic solar cells. <i>Journal of Materials Chemistry A</i> , 2022, 10, 15999-16006.	5.2	5
11978	Mechanism of the Fe(<i>iii</i>)-catalyzed synthesis of hexahydropyrimidine with $\hat{\pm}$ -phenylstyrene: a DFT study. <i>RSC Advances</i> , 2022, 12, 20523-20529.	1.7	0
11979	Theoretical Studies on the Interaction of Uranyl with Carboxylic Acids and Oxime Ligands. <i>Acta Chimica Sinica</i> , 2022, 80, 708.	0.5	0
11980	Conceptual density functional theory under pressure: Part I. XP-PCM method applied to atoms. <i>Chemical Science</i> , 2022, 13, 9329-9350.	3.7	7
11981	Planarization of a Bowl-Shaped Molecule by Triple-Decker Stacking. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11982	Reduction of Np(<i>vi</i>) with hydrazinopropionitrile <i>via</i> water-mediated proton transfer. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	3
11983	Theoretical Study on the Isomerization Mechanism of Azobenzene Derivatives under Electric Field. <i>Acta Chimica Sinica</i> , 2022, 80, 781.	0.5	1

#	ARTICLE	IF	CITATIONS
11984	An experimental and modeling study on the catalytic effects of select metals on the fast pyrolysis of hardwood and softwood lignin. <i>Green Chemistry</i> , 2022, 24, 6189-6199.	4.6	7
11985	Silver-catalyzed [4 + 3] cycloaddition of 1,3-dienes with alkenyl-N-trifosylhydrazones: a practical approach to 1,4-cycloheptadienes. <i>Organic Chemistry Frontiers</i> , 2022, 9, 4426-4434.	2.3	5
11986	The Zintl phase compounds $AEIn_2As_2$ (AE = Ca, Sr, Ba): topological phase transition under pressure. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17337-17347.	1.3	8
11987	Symmetry and spacing controls in periodic covalent functionalization of graphite surfaces templated by self-assembled molecular networks. <i>Nanoscale</i> , 2022, 14, 12595-12609.	2.8	2
11988	The chiral pyridoxal-catalyzed biomimetic Mannich reaction: the mechanism and origin of stereoselectivity. <i>Organic Chemistry Frontiers</i> , 0, , .	2.3	6
11989	Adsorption of Glyphosate on Graphene and Functionalized Graphenes: A Dft Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11990	Substituent Effects on the Photocatalytic Properties of A Symmetric Covalent Organic Framework. <i>Chinese Journal of Chemical Physics</i> , 0, , .	0.6	0
11991	Pyridine-di-phosphonates as chelators for trivalent f-elements: kinetics, thermodynamic and interfacial study of $Am(III)/Eu(III)$ solvent extraction. <i>Dalton Transactions</i> , 2022, 51, 11180-11192.	1.6	7
11992	Coordination mode and stability of the tetrahydroborate ligand in group 10 metal pincer complexes. <i>Dalton Transactions</i> , 0, , .	1.6	3
11993	On the Influence of Pnictogen Bonding on Acidity Declaration of Interests. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11994	Chalcogen-bonded donor-acceptor complexes of 5,6-dicyano[1,2,5]selenadiazolo[3,4-b]pyrazine with halide ions. <i>New Journal of Chemistry</i> , 2022, 46, 14490-14501.	1.4	6
11995	Tuning the dielectric response by co-crystallisation of sumanene and its fluorinated derivative. <i>Chemical Communications</i> , 2022, 58, 8950-8953.	2.2	8
11996	Theoretical insights into selective extraction of uranium from seawater with tetradentate N,O-mixed donor ligands. <i>Dalton Transactions</i> , 2022, 51, 11381-11389.	1.6	6
11997	Evolution of microstructures and hydrogen bond interactions within choline amino acid ionic liquid and water mixtures. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17792-17808.	1.3	4
11998	Excited-state geometry relaxation of pyrene-modified cellulose nanocrystals under UV-light excitation for detecting Fe^{3+} . <i>Nanotechnology Reviews</i> , 2022, 11, 2526-2534.	2.6	2
11999	Activation of Molecular Oxygen by Tenorite and Ascorbic Acid: Generation of High-Valent Copper Species for Organic Compound Oxidation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12000	Molecular modeling and nonlinear optical properties of new isostructural halogenated dihydroquinolinones. <i>New Journal of Chemistry</i> , 2022, 46, 14192-14204.	1.4	2
12001	Möbius-aromatic interlocked $Mn_2B_{10}H_{10}$ wheel to metal-doped boranaphthalene $M_2@B_{10}H_8$ and M_2B_5 2D-sheets (M = Mn and Fe): A Molecules to Materials continuum using DFT Study. <i>Chemical Science</i> , 0, , .	3.7	1

#	ARTICLE	IF	CITATIONS
12002	Mechanistic insights into Ag ⁺ induced size-growth from [Au ₆ (DPPP) ₄] ²⁺ to [Au ₇ (DPPP) ₄] ²⁺ clusters. <i>Nanoscale Advances</i> , 0, , .	2.2	0
12003	Tailoring benzo[<i>a</i>]phenoxazine moiety for efficient photosensitizers in dye sensitized solar cells via the DFT/TD-DFT method. <i>New Journal of Chemistry</i> , 2022, 46, 15155-15167.	1.4	6
12004	A Metal-Free Catalyst of Montmorillonite-Supported Hydrochar for Activating Peroxymonosulfate to Effectively Degrade Dicamba: Mechanism and Dft Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12005	Can an alkalide act as a perfect Lewis base?. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18144-18149.	1.3	2
12006	Theoretically investigating the ability of phenanthroline derivatives to separate transuranic elements and their bonding properties. <i>New Journal of Chemistry</i> , 2022, 46, 14532-14542.	1.4	4
12007	Morphology Constraint of $\hat{\Gamma}$ -Hmx in Polymeric Carbon Nitrides Towards Hybrid Energetic Materials. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12008	Magnetic couplings and applied electric field regulation in diradical SiC defect diamond-like nanoclusters. <i>New Journal of Chemistry</i> , 2022, 46, 14676-14689.	1.4	1
12009	Antibacterial silver and gold complexes of imidazole and 1,2,4-triazole derived N-heterocyclic carbenes. <i>Dalton Transactions</i> , 2022, 51, 12056-12070.	1.6	6
12010	Theoretical study on the mechanism of hot excitons combined with aggregation-induced emission in efficient red fluorescent molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17632-17640.	1.3	5
12011	Unravelling a New Conformer of Psilocin Through Computational Methods. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12012	Simultaneous Removal of Tetracycline and Arsenic(III) Using Copper-Manganese Composite Oxide: Competition Behaviors and Removal Mechanisms. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12013	Multi-scale structure optimization of boron-doped hard carbon nanospheres boosting the plateau capacity for high performance sodium ion batteries. <i>Journal of Materials Chemistry A</i> , 2022, 10, 17225-17236.	5.2	32
12014	Acid catalysis through N-protonation in undistorted carboxamides: improvement of amide proton sponge acylating ability. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
12015	Mechanism and Origin of Regioselectivity in Rh-Catalyzed Desymmetric [2+2+2] Cycloaddition: Charge versus π - π Stacking Interaction. <i>Organic Chemistry Frontiers</i> , 0, , .	2.3	1
12016	A universal bipolar host based on isonicotinonitrile and carbazole for efficient red, green and blue PhOLEDs. <i>New Journal of Chemistry</i> , 2022, 46, 15344-15350.	1.4	3
12017	New insight into the electronic structure of SiF ₄ : synergistic back-donation and the eighteen-electron rule. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17679-17685.	1.3	3
12018	Achieving Simultaneous Hydrogen Evolution and Organic Pollutants Degradation Through the Modification of Ag ₃ PO ₄ Using Cs ₂ AgBiBr ₆ Quantum Dots and Graphene Hydrogel. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12019	As(V) Removal from Aqueous Environments Using Quaternary Ammonium Modified Zif-8/Chitosan Composite Adsorbent. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
12020	Tailoring defect-type and ligand-vacancies in Zr(<i>iv</i>) frameworks for CO ₂ photoreduction. <i>Journal of Materials Chemistry A</i> , 2022, 10, 16396-16402.	5.2	25
12021	Reasons of Low Formaldehyde Adsorption Capacity on Activated Carbon: Multi-Scale Simulation of Dynamic Interaction between Pore Size and Functional Groups. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12022	Thermodynamic properties of temozolomide in crystalline and gaseous aggregate states. <i>Journal of the Belarusian State University Chemistry</i> , 2022, , 18-30.	0.1	0
12023	Cooperative pentavalent pnictogen bonding versus dominant hydrogen bonding in POCl ₃ -diethylether dimer characterized using matrix isolation infrared spectroscopy and ab initio computations. <i>Journal of Molecular Spectroscopy</i> , 2022, 387, 111672.	0.4	1
12024	Molecular insights into the complex formation between dodecamethylcucurbit[6]uril and phenylenediamine isomers. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2022, 102, 637-651.	0.9	2
12025	Understanding the Regioselectivity of Ion-Pair-Assisted Meta-Selective C(sp ²)-H Activation in Conformationally Flexible Arylammonium Salts. <i>Journal of Organic Chemistry</i> , 2022, 87, 9222-9231.	1.7	2
12026	Interlayer spacing control of boron nitride sheets with hydrated cations. <i>Molecular Physics</i> , 2022, 120, .	0.8	1
12027	Interaction of Uracil with LiF and Water Studied by Density Functional Theory Study on Anionic Complexes. <i>Journal of Cluster Science</i> , 2023, 34, 1249-1258.	1.7	1
12028	Self-Assembly Metal Chelate as Ultraviolet Filterable Interface Layer for Efficient Organic Solar Cells. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	7
12029	Through-Space Charge Transfer: A New Way to Develop High-Performance Fluorescence Sensing Film towards Opto-Electronically Inert Alkanes. <i>Angewandte Chemie</i> , 0, , .	1.6	1
12030	Rational Design of Alkynyl-Based Linear Donor-Acceptor Conjugated Polymers with Accelerated Exciton Dissociation for Photocatalysis. <i>Macromolecules</i> , 2022, 55, 5412-5421.	2.2	17
12031	Prediction of the Mechanism of Sodium Butyrate against Radiation-Induced Lung Injury in Non-Small Cell Lung Cancer Based on Network Pharmacology and Molecular Dynamic Simulations. <i>Frontiers in Oncology</i> , 0, 12, .	1.3	5
12032	Molecular Docking, Dynamic Simulation and DFT Approach to Noble α -2-Hydrazinobenzothiazole Compound. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 4271-4298.	1.4	2
12033	NIR Photodetectors with Highly Efficient Detectivity Enabled by 2D Fluorinated Dithienopicenocarbazole-Based Ultra-Narrow Bandgap Acceptors. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	24
12034	Qualitative and quantitative study of intermolecular weak interactions for aminosalicic acid isomers by terahertz spectroscopy. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	1
12035	Plasma-Assisted Dinitrogen Activation on Small Cobalt Clusters: Co ₄ N ₉ ⁺ with Enhanced Stability. <i>ChemPhysChem</i> , 2022, 23, .	1.0	6
12036	From the Free Ligand to the Transition Metal Complex: FeEDTA ⁴⁻ Formation Seen at Ligand K-Edges. <i>Inorganic Chemistry</i> , 2022, 61, 10321-10328.	1.9	5
12037	Interplay between the Enamine and Imine Forms of the Hydrolyzed Imipenem in the Active Sites of Metallo- β -lactamases and in Water Solution. <i>Journal of Chemical Information and Modeling</i> , 0, , .	2.5	3

#	ARTICLE	IF	CITATIONS
12038	Guignardones Yâ€“Z, Antiviral Meroterpenes from <i>Penicillium</i> sp. NBUF154 Associated with a <i>Crella</i> Sponge from the Marine Mesophotic Zone. <i>Chemistry and Biodiversity</i> , 2022, 19, .	1.0	3
12039	Xenon Derivatives as Aerogen Bond-Donating Catalysts for Organic Transformations: A Theoretical Study on the Metaphorical “Spherical Cow in a Vacuum” Provides Insights into Noncovalent Organocatalysis. <i>Journal of Organic Chemistry</i> , 0, , .	1.7	8
12040	Two Novel Co-Crystals of Naproxen: Comparison of Stability, Solubility and Intermolecular Interaction. <i>Pharmaceuticals</i> , 2022, 15, 807.	1.7	5
12041	Exploring the effect of complexant on remarkably high static and dynamic second hyperpolarizability of aziridine-based diffuse electron systems: a theoretical study. <i>Structural Chemistry</i> , 2023, 34, 539-551.	1.0	5
12042	Through Space Charge Transfer: A New Way to Develop a High Performance Fluorescence Sensing Film towards Optoelectronically Inert Alkanes. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	19
12043	Sequence-Dependent Tyrosine-Containing Peptide Nanoassemblies for Sensing Tyrosinase and Melanoma. <i>ACS Macro Letters</i> , 2022, 11, 875-881.	2.3	3
12044	A DFT and TD-DFT study of charge transport and non-linear optical properties of N-(4- Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 507 Td (me complexes. <i>Journal of Chemical Sciences</i> , 2022, 134, .	0.7	2
12045	Oriented External Electric Fields Regulating the Reaction Mechanism of CH ₄ Oxidation Catalyzed by Fe(IV)-Oxo-Corrolazine: Insight from Density Functional Calculations. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	3
12046	Synthesis and Structure Elucidation of Novel Spirooxindole Linked to Ferrocene and Triazole Systems via [3 + 2] Cycloaddition Reaction. <i>Molecules</i> , 2022, 27, 4095.	1.7	4
12047	Structure-Property Relationships in Amorphous Thieno[3,2- <i>b</i>]thiophene-Diketopyrrolopyrrole Thiophene-Containing Polymers. <i>Journal of Physical Chemistry C</i> , 2022, 126, 10842-10854.	1.5	5
12048	Comparison of B ₂ bond and luminescence behavior of group 11/12 metal diborene complexes: Theoretical investigation. <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	0
12049	The role of weak H ⁺ ⋯O hydrogen bond in alcohol-water mixtures. <i>Journal of Raman Spectroscopy</i> , 2022, 53, 1551-1559.	1.2	3
12050	Electronic structure of substituted catecholate complexes of hexacoordinated silicon: a quantum chemical study. <i>Russian Chemical Bulletin</i> , 2022, 71, 1111-1122.	0.4	0
12051	Synthesis, characterisation, biological and theoretical studies of novel pyridine derivatives. <i>Molecular Physics</i> , 2022, 120, .	0.8	3
12052	Insights into the mechanism and stereoselectivity of the [3+2] cycloaddition reaction between N-methyl-C-(4-hydroxylphenyl) nitron and maleic anhydride with a molecular electron density theory perspective. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	7
12053	Quantum Chemical Calculations and Machine Learning Predictions Innovate Synthesis for High-Performance Optical Gold Nanorods. <i>Chemistry of Materials</i> , 2022, 34, 5928-5937.	3.2	4
12054	Rotational Spectroscopy of the 2,2,3,3-Pentafluoropropanol...Water Complex: Conformations and Large Amplitude Motions. <i>ChemPhysChem</i> , 2022, 23, .	1.0	3
12055	Bonding situations in tricoordinated beryllium phenyl complexes. <i>Journal of Computational Chemistry</i> , 2023, 44, 397-405.	1.5	7

#	ARTICLE	IF	CITATIONS
12056	On the Notation of Catastrophes in the Framework of Bonding Evolution Theory: Case of Normal and Inverse Electron Demand Diels-Alder Reactions. <i>ChemPhysChem</i> , 2022, 23, .	1.0	4
12057	How Ionic Structure Governs Bulk Properties: Charge Lever Moments of Alicyclic Ionic Liquids utilized in Lithium Metal Batteries. <i>Journal of the Electrochemical Society</i> , 0, , .	1.3	0
12058	A cycloruthenated complex: Detecting Hg ²⁺ by Hg ²⁺ -promoted coordination switch and Cu ²⁺ by coordination. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	1.7	3
12059	Developing Dawson-Type Polyoxometalates Used as Highly Efficient Catalysts for Lignocellulose Transformation. <i>ACS Catalysis</i> , 2022, 12, 9213-9225.	5.5	9
12060	Migration Mechanism of the B ^H Activation of Carboranes. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	0
12061	Reactions of Tc ^I (NO) and Tc ^V N Complexes with Alkynes and Alkynides. <i>Organometallics</i> , 2022, 41, 2011-2021.	1.1	4
12062	Highly efficient separation of benzene + cyclohexane mixtures by extraction combined extractive distillation using imidazolium-based dicationic ionic liquids. <i>Green Chemical Engineering</i> , 2023, 4, 312-323.	3.3	8
12063	A rapid classification method of tea products utilizing X-ray photoelectron spectroscopy: Relationship derived from correlation analysis, modeling, and quantum chemical calculation. <i>Food Research International</i> , 2022, 160, 111689.	2.9	7
12064	Extra-long C C single bonds via negative hyperconjugation in perfluoropinacolate complexes. <i>Polyhedron</i> , 2022, , 116040.	1.0	1
12065	What Determines the Drastic Reactivity of Nb _n ⁺ Clusters with Nitric Oxide under Thermalized Conditions?. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4801-4809.	1.1	3
12066	Site-Selective C ^H Arylation of Diverse Arenes Ortho to Small Alkyl Groups. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	6
12067	Elaborating the mechanism of a highly selective fluorescent "turn-on" probe to detect the group IIIA ions: a detailed time-dependent density functional theory study. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	0
12068	Fluorescence Enhancement of Dicyanomethylene-4H-Pyran Derivatives in Solid State for Visualization of Latent Fingerprints. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	3
12069	Antiparallel $\pi\cdots\pi$ and C ^H \cdots H \cdots C contacts in a novel Zn(II) coordination solid involving π -hole tetrel bonding interactions: A combined experimental and theoretical study, Hirshfeld surface analysis, molecular docking and potential drug property. <i>Journal of Molecular Structure</i> , 2022, 1268, 133686.	1.8	4
12070	Prediction of α -OH-Initiated and α -NO ₃ -Initiated Transformation Products of Polycyclic Aromatic Hydrocarbons by Electronic Structure Approaches. <i>ACS Omega</i> , 2022, 7, 24942-24950.	1.6	4
12071	Fluorescence emission modulation in cyanido-bridged Fe(II) spin crossover coordination polymers. <i>Science China Chemistry</i> , 2022, 65, 1569-1576.	4.2	13
12072	Basic Fluorescent Protonation-Type pH Probe Sensitive to Small pK_a of Methanol and Ethanol. <i>Analytical Chemistry</i> , 2022, 94, 10400-10407.	3.2	9
12073	Parallelized Raman Difference Spectroscopy for the Investigation of Chemical Interactions. <i>Analytical Chemistry</i> , 2022, 94, 10346-10354.	3.2	8

#	ARTICLE	IF	CITATIONS
12074	Structural Engineering of FDT toward Promising Spiro-Typed Hole-Transporting Materials: Promoting the Hole Transport and Stabilizing the HOMO Levels. <i>Journal of Physical Chemistry C</i> , 2022, 126, 11529-11536.	1.5	11
12075	Spatial Confinements Control the Multicolor Solid Fluorescence Based on the Dihydrophenazine Derivative. , 2022, 4, 1462-1467.		2
12076	Raman spectroscopy, AIM analysis, drug-likeness and molecular docking study of the hydrogen-bonded complex of Carmustine with Melatonin. <i>Materials Today: Proceedings</i> , 2022, , .	0.9	4
12077	Effect of methyl hydrogen sulfate on the formation of sulfuric acid-ammonia clusters: A theoretical study. <i>Journal of the Chinese Chemical Society</i> , 0, , .	0.8	0
12078	Large $B_{7\Delta}$ Triangles in Hollow Spherical Trihedral Metallo-borospherenes and Their Endohedral Complexes of $B_{20}TM_n$ ($TM = Sc, Y; n = 3, 4$): a Theoretical Characterization. <i>Inorganic Chemistry</i> , 2022, 61, 10652-10660.	1.9	5
12079	Tracking HOCl by an incredibly simple fluorescent probe with AIE plus ESPT in vitro and in vivo. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 281, 121649.	2.0	7
12080	2,15-Dibutoxy-6,11-dicyano[6]Helicene: Synthesis, electrochemical, photophysical properties and computational studies. <i>Journal of Molecular Structure</i> , 2022, , 133680.	1.8	0
12081	FTIR, NMR and UV-Visible Spectral Investigations, Theoretical Calculations, Topological Analysis, Chemical Stability, and Molecular Docking Study on Novel Bioactive Compound: The 5-(5-Nitro) Thiazolidin-4-One. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 4685-4706.	1.4	4
12082	Surface Complex and Nonradical Pathways Contributing to High-Efficiency Degradation of Perfluorooctanoic Acid on Oxygen-Deficient In_2O_3 Derived from an In-Based Metal Organic Framework. <i>ACS ES&T Water</i> , 2022, 2, 1344-1352.	2.3	7
12083	The sensitive detection and mechanism of Fe-3,5-dimethyl pyrazole fluorescent sensor to diethylenetriamine pentamethylene phosphonic acid: Experimental study and quantum chemical calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 281, 121623.	2.0	0
12084	Ferric oxide nanoclusters with low-spin Fe^{III} anchored g-C ₃ N ₄ rod for boosting photocatalytic activity and degradation of diclofenac in water under solar light. <i>Applied Catalysis B: Environmental</i> , 2022, 317, 121725.	10.8	35
12085	Molecular doped, color-tunable, high-mobility, emissive, organic semiconductors for light-emitting transistors. <i>Science Advances</i> , 2022, 8, .	4.7	31
12086	Experimental, DFT study, and in silico molecular docking investigations of dichlorodiphenyltrichloroethane against human estrogen receptor alpha. <i>Eletica Quimica</i> , 2022, 47, 39-52.	0.2	8
12087	External Electric Field-Induced Phase Transition of a Series of Energetic Pentazole Crystals: A First-Principles Study. <i>Crystal Growth and Design</i> , 0, , .	1.4	0
12088	Combination of 3-Aminofurazan-4-carboxylic Acid and Transition Metals to Prepare Functional Energetic Catalysts for Catalyzing the Decomposition of Ammonium Perchlorate. <i>Crystal Growth and Design</i> , 2022, 22, 5802-5813.	1.4	10
12089	Predicting the interaction between organic layer and metal substrate through DFTB and electrochemical approach for excellent corrosion protection. <i>Journal of Industrial and Engineering Chemistry</i> , 2022, 114, 190-204.	2.9	6
12090	Investigation into the structures and physicochemical properties of multi-component crystals of voriconazole. <i>Chinese Chemical Letters</i> , 2023, 34, 107668.	4.8	2
12091	Preparation and evaluation of a chitosan modified biochar as an efficient adsorbent for pipette tip-solid phase extraction of triazine herbicides from rice. <i>Food Chemistry</i> , 2022, 396, 133716.	4.2	10

#	ARTICLE	IF	CITATIONS
12092	Rational design of ZL003-based organic dyes for highly efficient dye-sensitized solar cells: Influence of alkynyl group and π -spacers on photovoltaic performance. <i>Journal of Molecular Structure</i> , 2022, 1269, 133728.	1.8	6
12093	Variation in the formation characteristics of PBDD/F, brominated PAH, and PBDE congeners along the secondary copper smelting processes. <i>Journal of Hazardous Materials</i> , 2022, 439, 129602.	6.5	0
12094	Degradation of metoprolol by UV/sulfite as an advanced oxidation or reduction process: The significant role of oxygen. <i>Journal of Environmental Sciences</i> , 2023, 128, 107-116.	3.2	2
12095	Atrazine adsorption by graphene-based materials: Interaction mechanism and application in real samples. <i>Environmental Technology and Innovation</i> , 2022, 28, 102823.	3.0	10
12096	Construction of biomass-based AIEgens with dehydroabiatic acid triarylamine and tetraphenylethene Moieties for non-doped OLEDs. <i>Tetrahedron</i> , 2022, 121, 132922.	1.0	1
12097	Structural, spectral characterization, and topological study of (E)-5-(diethylamino)-2-((3,5-dinitrophenylimino)methyl)phenol. <i>Structural Chemistry</i> , 2023, 34, 455-466.	1.0	1
12098	Pyrrrole – Best additional spacers for azo based dye sensitized solar cells: A computational study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 433, 114146.	2.0	7
12099	Molecular structure and excitation characteristics of DHR under different external electric fields. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113810.	1.1	3
12100	Piezo-enhanced photocatalytic performance of ZnO nanorod array for pollutants degradation in dynamic water: Insight into the effect of velocity and inner flow field. <i>Nano Energy</i> , 2022, 101, 107614.	8.2	49
12101	Understanding the Importance of Periodate Species in the pH-Dependent Degradation of Organic Contaminants in the H_2O_2 /Periodate Process. <i>Environmental Science & Technology</i> , 2022, 56, 10372-10380.	4.6	23
12102	Synthesis, characterization and self assembly of dinuclear zinc Schiff base complexes: A combined experimental and theoretical study. <i>Polyhedron</i> , 2022, 225, 116044.	1.0	5
12103	Thermodynamics, excess properties, spectra and computational chemistry of 1,2-propanediol+1,2-propane diamine binary system. <i>Arabian Journal of Chemistry</i> , 2022, 15, 104130.	2.3	6
12104	Influence of Alkali Metal Doping and BN Substitution on the Second-Order Nonlinear Optical Properties of Graphyne: A Theoretical Perspective. <i>Inorganic Chemistry</i> , 2022, 61, 10756-10767.	1.9	2
12105	Synthesis, X-ray crystallography, molecular electronic property investigation, and leukopoiesis activity of novel 4,6-dimethyl-1,6-dihydropyridin-2-amino nitrate hybrid material. <i>Journal of Molecular Structure</i> , 2022, 1268, 133733.	1.8	14
12106	Coordination Symmetry Breaking of Single-Atom Catalysts for Robust and Efficient Nitrate Electroreduction to Ammonia. <i>Advanced Materials</i> , 2022, 34, .	11.1	83
12107	Excited State Properties of Aggregation-Induced Delayed Fluorescence Molecules: A Microscopic Insight. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	2
12108	Automatized protocol and interface to simulate QM/MM time-resolved transient absorption at $TD-DFT$ level with $COBRAMM$. <i>Journal of Computational Chemistry</i> , 2022, 43, 1641-1655.	1.5	14
12109	Intermolecular interactions between cyclo[18]carbon and XCN ($X = H, F, Cl, Br, I$): a theoretical study. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	4

#	ARTICLE	IF	CITATIONS
12110	Disposing of excessive decomposition and destructive intercalation of solvated Li ⁺ in CNT-based flexible 3D Si anode of flexible battery. <i>Energy Storage Materials</i> , 2022, 51, 361-371.	9.5	6
12111	Excess properties, spectral analysis and computational chemistry of (1,3-propanediol+Ethylenediamine) ion-like liquids for CS ₂ capture. <i>Journal of Molecular Liquids</i> , 2022, 363, 119830.	2.3	9
12112	Imidazolate of 1-butyl-3-ethyl imidazole as corrosion inhibitor on API 5L X52 steel in NaCl saturated with CO ₂ . <i>Journal of Molecular Liquids</i> , 2022, 363, 119826.	2.3	8
12113	Catalytic Effect of Ferrocenyl Energetic Catalysts for <i>N</i> -Guanylurea Dinitramide (GUDN) or Tj ETQq1 1 0.784314 rgBT /Overlock	1.6	0
12114	Site-Selective C-H Arylation of Diverse Arenes Ortho to Small Alkyl Groups. <i>Angewandte Chemie</i> , 0, , .	1.6	0
12115	Ternary-Porous Conjugated <i>N</i> -Halamine Nanofibers/Graphene Aerogels for Rechargeable Degradation of Mustard Gas. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	13
12116	Impact of end capped modification on BT-CIC molecule for high-performance photovoltaic attributes: a DFT approach. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	10
12117	Preparation of D-A-D conjugated polymers based on [1,2,5]thiadiazolo[3,4-c]pyridine and thiophene derivatives and their electrochemical properties as anode materials for lithium-ion batteries. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 651, 129707.	2.3	8
12118	Dehydrochlorination of 1,1,1,3,3-Pentachloropropane promoted by fluoride. <i>Journal of Fluorine Chemistry</i> , 2022, 261-262, 110020.	0.9	1
12119	Propylene Epoxidation over Au/TS-1 Modified by Ammonium Salt: Enhancement of the Attractiveness of Gold Precursors and Supports. <i>Chemical Physics Letters</i> , 2022, , 139880.	1.2	2
12120	Copper oxide modified activated carbon for enhanced adsorption performance of siloxane: An experimental and DFT study. <i>Applied Surface Science</i> , 2022, 601, 154200.	3.1	5
12121	Molecular Simulation to Explore the Dissolution Behavior of Sulfur in Carbon Disulfide. <i>Molecules</i> , 2022, 27, 4402.	1.7	0
12122	Highly Regioselective Cobalt-Catalyzed Hydroboration of Internal Alkynes. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	14
12123	Photochemically Induced 1,3-Butadiene Ring-Closure from the Topological Analysis of the Electron Localization Function Viewpoint. <i>ChemPhysChem</i> , 2022, 23, .	1.0	5
12124	Conceptual DFT, QTAIM, and Molecular Docking Approaches to Characterize the T-Type Calcium Channel Blocker Anandamide. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	4
12125	The Excited State Calculation of Two-Dimensional MoSi ₂ N ₄ layered Material Doped with P Respectively for Visible Light Absorption by Gaussian. <i>ECS Journal of Solid State Science and Technology</i> , 2022, 11, 073009.	0.9	2
12126	Bowl-shaped CuB ₁₂ Cluster. A viable Global Minimum with Twofold Aromaticity. <i>ChemPhysChem</i> , 0, , .	1.0	3
12127	Structures and Photoluminescence Properties of Bis(aromatic amino)-Based Isomers with Biphenyl as Bridge. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0

#	ARTICLE	IF	CITATIONS
12128	Facile Synthesis of Multi-Emission Nitrogen/Boron Co-Doped Carbon Dots from Lignin for Anti-Counterfeiting Printing. <i>Polymers</i> , 2022, 14, 2779.	2.0	11
12129	Voltage-Dependent Emission Varying from Blue to Orangeâ€“Red from a Nondoped Organic Light-Emitting Diode with a Single Emitter. <i>Nanomaterials</i> , 2022, 12, 2333.	1.9	0
12130	Tuning Hybridized Local and Charge-Transfer Mixing for Efficient Hot-Exciton Emission with Improved Color Purity. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6664-6673.	2.1	5
12131	Hydrogen Bondâ€“Induced Cathode Engineering Enables Binary Allâ€“Smallâ€“Molecule Organic Solar Cells with 15.88% Efficiency and Enhanced Thermostability. <i>Solar Rrl</i> , 0, , .	3.1	1
12132	Silicon Carbide Based Nanotubes as a Sensing Material for Gaseous H ₂ SiCl ₂ . <i>Silicon</i> , 2023, 15, 177-186.	1.8	3
12133	Photophysical Properties of Donorâ€“Acceptorâ€“Î Bridgeâ€“Acceptor Sensitizers with a Naphthobisthiadiazole Auxiliary Acceptor: Toward Longer-Wavelength Access in Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2022, 126, 11875-11888.	1.5	8
12134	Photocatalystâ€“Free Lightâ€“Driven Dehydrogenation of Alcohols into Carbonyl Compounds under Mild Conditions. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	2
12135	Three-Dimensional Quantitative Structure and Activity Relationship of Flavones on Their Hypochlorite Scavenging Capacity. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 8799-8807.	2.4	3
12136	Molecular Engineering of Sulfurâ€“Bridged Polycyclic Emitters Towards Tunable TADF and RTP Electroluminescence. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	35
12137	Substitution Effects on the Reactivity and Thermostability of Five-Membered Ring Fluorides. <i>ACS Omega</i> , 2022, 7, 25476-25490.	1.6	2
12138	Firstâ€“Principles study of the adsorption of flavonoids on graphene oxide. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	1
12139	Angular shaped AIE generator based luminophores for mechanochromism: An explosive sensor. <i>Materials Today Communications</i> , 2022, 32, 104050.	0.9	0
12140	Combined Experimental and Computational Study on the Transformation of a Novel 1,3,4-Oxadiazole Thioether Nematicide in Aqueous Solutions. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 8963-8973.	2.4	3
12141	Î versus Î radical: Tuning the electronic nature of neutral carbon (I) compounds with three nonâ€“bonding electrons. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	0
12142	Molecular Engineering of Sulfurâ€“Bridged Polycyclic Emitters Towards Tunable TADF and RTP Electroluminescence. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	6
12143	<sc>Longâ€“bonding</sc> and effects of carbon hybridization on the bonding of <sc>M</sc> Î; <sc>Ng</sc> Î; <sc>C</sc> compounds (M=ACu, Ag, Au). <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	1
12144	Molecular dynamics study of water and ion behaviors of mixed salts solutions on extended quartz surface. <i>Journal of Applied Physics</i> , 2022, 132, 024701.	1.1	0
12145	Highly Regioselective Cobaltâ€“Catalyzed Hydroboration of Internal Alkynes. <i>Angewandte Chemie</i> , 0, , .	1.6	0

#	ARTICLE	IF	CITATIONS
12146	Side-Chain Engineering of Polystyrene Dielectrics Toward High-Performance Photon Memories and Artificial Synapses. <i>Chemistry of Materials</i> , 2022, 34, 6505-6517.	3.2	15
12147	Molecular structure, electronic properties, ESP map (polar aprotic and polar protic solvents), and topology investigations on 1-(tert-butylcarbonyl)-3-piperidinecarboxylic acid- Anticancer therapeutic agent. <i>Journal of Molecular Structure</i> , 2022, 1268, 133696.	1.8	9
12148	Mechanistic aspects of the Diels-Alder reaction between (E)-N-benzylidene-2,2-difluoro-1-phenylethenamine and 2-vinyl pyridine: A molecular electron density theory study. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113817.	1.1	4
12149	Size-effect on Ni electrocatalyst: The case of electrochemical benzyl alcohol oxidation. <i>Nano Research</i> , 2023, 16, 202-208.	5.8	7
12150	Density functional theory study of the hydrogen evolution reaction in haeckelite boron nitride quantum dots. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 41783-41794.	3.8	12
12151	The role of intramolecular interactions on the stability of the conformers of a spiropyran derivative. <i>Chemical Physics</i> , 2022, 562, 111654.	0.9	5
12152	Stability, Energetic, and Reactivity Properties of NiPd Alloy Clusters Deposited on Graphene with Defects: A Density Functional Theory Study. <i>Materials</i> , 2022, 15, 4710.	1.3	3
12153	Environment-Driven Coherent Population Transfer Governs the Ultrafast Photophysics of Tryptophan. <i>Journal of the American Chemical Society</i> , 2022, 144, 12884-12892.	6.6	8
12154	Host-guest binding selectivity of ethylated pillar[5]arene (EtP5A) towards octane, 1,7-octadiene, and 1,7-octadiyne: a computational investigation. <i>Structural Chemistry</i> , 0, , .	1.0	0
12155	Corrosion inhibition property and promotion of green basil leaves extract materials on Ti-Zr conversion composite coatings. <i>Advanced Composites and Hybrid Materials</i> , 2022, 5, 1922-1938.	9.9	16
12156	Desymmetrization of N-Cbz glutarimides through N-heterocyclic carbene organocatalysis. <i>Nature Communications</i> , 2022, 13, .	5.8	12
12157	Reductive Cross-Coupling of I^{\pm}Oxy Halides Enabled by Thermal Catalysis, Photocatalysis, Electrocatalysis, or Mechanochemistry. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	21
12158	Utilizing an Oxygen-Rich Interface by Hydroxyapatite to Regulate the Linear Diffusion for the Stable Solid-State Electrolytes. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 33392-33399.	4.0	6
12159	Hollow Covalent Organic Framework with $\text{Shell-Confined-Environment}$ for the Effective Removal of Anionic Per- and Polyfluoroalkyl Substances. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	18
12160	Experimental and theoretical insights into two fluorine-containing imidazoline Schiff base inhibitors for carbon steels in hydrochloric acid solution. <i>Journal of Molecular Structure</i> , 2022, 1268, 133737.	1.8	9
12161	Reductive Cross-Coupling of I^{\pm}Oxy Halides Enabled by Thermal Catalysis, Photocatalysis, Electrocatalysis, or Mechanochemistry. <i>Angewandte Chemie</i> , 0, , .	1.6	1
12162	The interaction of deep eutectic solvents with pristine carbon nanotubes and their associated defects: A density functional theory study. <i>Journal of Molecular Liquids</i> , 2022, 363, 119855.	2.3	5
12163	Preparation of hierarchically floral ZIF-8 derived carbon@polyaniline@Ni/Al layered double hydroxides composite with outstanding removal phenomenon for saccharin. <i>Chemical Engineering Journal</i> , 2022, 450, 138127.	6.6	34

#	ARTICLE	IF	CITATIONS
12164	Investigation of intramolecular hydrogen bonding in naphthoquinone derivatives by quantum chemical calculations. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	1
12165	Norfloracin Degradation by Persulfate Activated with Cu ₂ O@WO ₃ Composites: Efficiency, Stability, Mechanism, and Degradation Pathway. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 11237-11248.	1.8	2
12166	DFT study on CH ₃ O, CH ₃ SCN and S ₂ interaction energies in three dinuclear mixed valence cobalt(III/II) complexes with secondary diamine ligands having inner N ₂ O ₂ and outer O ₄ compartments. <i>Polyhedron</i> , 2022, , 116039.	1.0	1
12167	From Mosaic-Type to Heterojunction-Type SEI Films on the Li Anode: Decoupling Chemical and Electrochemical Degradation of the Electrolyte. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 9232-9241.	3.2	4
12168	Insight into substrate-assisted catalytic mechanism and stereoselectivity of bifunctional nocardicin thioesterase. <i>Proteins: Structure, Function and Bioinformatics</i> , 0, , .	1.5	0
12169	Preparation of the 1-Methylimidazole Borane/Tetrazole System for Hypergolic Fuels. <i>Molecules</i> , 2022, 27, 4466.	1.7	0
12170	Metal-Doped Al ₁₂ N ₁₂ X (X = Na, Mg, K) Nanoclusters as Nanosensors for Carboplatin: Insight from First-Principles Computation. <i>Journal of Physical Chemistry B</i> , 2022, 126, 5066-5080.	1.2	29
12171	Modeling of Multiresonant Thermally Activated Delayed Fluorescence Emitters—Properly Accounting for Electron Correlation Is Key!. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4903-4918.	2.3	32
12172	Spectroscopic Investigation, DFT Calculations, anti-Inflammatory Activity and Molecular Dynamic Simulation Study on Fagaramide Alkaloid. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-26.	1.4	1
12173	Simple and modestly scalable synthesis of. <i>Australian Journal of Chemistry</i> , 2022, 75, 331-344.	0.5	3
12174	Binary droplet interactions in shear water-in-oil emulsion: A molecular dynamics study. <i>Journal of Molecular Liquids</i> , 2022, 363, 119823.	2.3	7
12175	Synthesis, characterization and theoretical studies of the photovoltaic properties of novel bifunctional reactive disperse dyes based on aminothiazole derivatives. <i>Journal of Molecular Structure</i> , 2022, 1269, 133749.	1.8	2
12176	Intrinsically flexible all-carbon-nanotube electronics enabled by a hybrid organic-inorganic gate dielectric. <i>Npj Flexible Electronics</i> , 2022, 6, .	5.1	9
12177	Extraction of flavonoids from Glycyrrhiza residues using deep eutectic solvents and its molecular mechanism. <i>Journal of Molecular Liquids</i> , 2022, 363, 119848.	2.3	18
12178	Poly(3-aminophenylboronic acid) as a sensitive electrical and optical sensor material for detection of some air pollutants: A computational study. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113801.	1.1	5
12179	Study on the photopolymerization mechanism of allyl monomers: A photo-driven radical-mediated [3+2] cyclopolymerization mechanism to reduce degradation chain transfer. <i>Polymer</i> , 2022, 255, 125153.	1.8	4
12180	Multiple chlorinations to improve the performance of unfused electron-acceptor based organic photovoltaic cells. <i>Surfaces and Interfaces</i> , 2022, 32, 102185.	1.5	5
12181	Silicone elastomer with simultaneous enhanced healing and electrical resistance via fluorine substitution for actuator dielectrics. <i>Polymer</i> , 2022, 255, 125125.	1.8	6

#	ARTICLE	IF	CITATIONS
12182	Highly efficient Al-Ti gel as a coagulant for surface water treatment: Insights into the hydrolysate transformation and coagulation mechanism. <i>Water Research</i> , 2022, 221, 118826.	5.3	20
12183	Spectroscopic features and electronic properties on tetrazole-based energetic cocrystals under external electric field. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113802.	1.1	4
12184	Clarifying the effect of chemical structure on high-temperature resistance of polyimides based on DFT and ReaxFF based molecular dynamic simulation. <i>Polymer</i> , 2022, 255, 125119.	1.8	4
12185	Noncovalent π - π dimerization based on acridine and acid-responsive luminescence switching. <i>Dyes and Pigments</i> , 2022, 205, 110527.	2.0	4
12186	Superhalogen doping of aromatic heterocycles; effective approach for the enhancement of static and dynamic NLO response. <i>Vacuum</i> , 2022, 203, 111301.	1.6	4
12187	The role of Fe ₃ O ₄ @biochar as electron shuttle in enhancing the biodegradation of gaseous para-xylene by aerobic surfactant secreted strains. <i>Journal of Hazardous Materials</i> , 2022, 438, 129475.	6.5	13
12188	Schiff base-type Cu(I) complexes containing naphthylpyridyl-methanimine ligands featuring higher light-absorption capability: Synthesis, structures, and photophysical properties. <i>Polyhedron</i> , 2022, 224, 116002.	1.0	2
12189	Experimental spectroscopic investigations, solute-solvent interactions, topological analysis and biological evaluations of N-(9-Fluorenylmethoxycarbonyloxy)succinimide: An effective agent in anti-breast cancer activity. <i>Journal of Molecular Liquids</i> , 2022, 362, 119756.	2.3	10
12190	Supramolecular assemblies involving unconventional non-covalent contacts in pyrazole-based coordination compounds of Co(II) and Cu(II) pyridinedicarboxylates: Antiproliferative evaluation and theoretical studies. <i>Polyhedron</i> , 2022, 224, 116025.	1.0	2
12191	Surface modification of hydroxyapatite with enzyme-catalyzed reaction: Computation-supported experimental studies. <i>Materials Chemistry and Physics</i> , 2022, 289, 126448.	2.0	6
12192	Bifunctional mechanism and electrochemical performance of self-healing nitrile ether electrolyte additives in 4.5 V LiCoO ₂ /artificial graphite lithium-ion batteries. <i>Journal of Power Sources</i> , 2022, 542, 231799.	4.0	12
12193	Design and synthesis of various double donors for nonlinear optical chromophores with enhanced electro-optic activity. <i>Dyes and Pigments</i> , 2022, 205, 110546.	2.0	3
12194	Development of chromenoquinoline-fused coumarin dyes and their application in bioimaging. <i>Dyes and Pigments</i> , 2022, 205, 110530.	2.0	11
12195	Imidazobenzothiadiazole: A new multifunction dyes for mechanochromic luminescence, acid responding and mitochondrial staining. <i>Dyes and Pigments</i> , 2022, 205, 110531.	2.0	10
12196	Sensing properties of propylene oxide on Pt and Pd doped graphene sheets: A DFT Investigation. <i>Sensors and Actuators A: Physical</i> , 2022, 344, 113726.	2.0	6
12197	Regulating the competitive reaction pathway in glycerol conversion to lactic acid/glycolic acid selectively. <i>Journal of Catalysis</i> , 2022, 413, 407-416.	3.1	22
12198	Two-dimensional activated carbon nanosheets for rapid removal of tetracycline via strong π - π electron donor receptor interactions. <i>Bioresource Technology</i> , 2022, 360, 127544.	4.8	19
12199	First-principles study on the luminescence property of a single-molecule near metallic nanoclusters. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113813.	1.1	0

#	ARTICLE	IF	CITATIONS
12200	Tactfully improve the antioxidant activity of 2-hydroxychalcone with the strategy of substituent, solvent and intramolecular hydrogen bond effects. <i>Journal of Molecular Liquids</i> , 2022, 362, 119748.	2.3	9
12201	Hydrogen bonds in aqueous choline chloride solutions by DFT calculations and X-ray scattering. <i>Journal of Molecular Liquids</i> , 2022, 362, 119742.	2.3	5
12202	Sumanene as a delivery carrier for methimazole drug: DFT, AIM, SERS and solvent effects. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113811.	1.1	16
12203	Solvent effect on excited state intramolecular proton transfer and charge transfer in 3-((2E)-Tj ETQq1 1 0.784314 rgBT /Overlock 10 Luminescence, 2022, 250, 119118.	1.5	2
12204	Evaluation of the sequence-dependent relative activity of APE1 for optimal biosensing design. <i>Biosensors and Bioelectronics</i> , 2022, 214, 114539.	5.3	4
12205	The importance of intramolecular hydrogen bonds for structural stabilization. [Triphenyl-tetrazolium] [tetraphenyldichalcogenoimidodiphosphinates], [Ph ₃ CN ₄][Ph ₂ P(X)NP(Y)Ph ₂]. <i>Polyhedron</i> , 2022, 225, 116027.	1.0	2
12206	Liquid-liquid extraction and mechanism analysis of extracting fuel additive isopropanol from mixture with choline-based deep eutectic solvents as efficient extractants. <i>Fuel</i> , 2022, 326, 125048.	3.4	7
12207	A reactive molecular dynamics study of the effects of an electric field on n-dodecane combustion. <i>Combustion and Flame</i> , 2022, 244, 112238.	2.8	15
12208	Mitochondrial-targeted red-fluorescent chemodosimeter for hydrogen sulfide signaling and visualizing. <i>Sensors and Actuators B: Chemical</i> , 2022, 369, 132357.	4.0	7
12209	Quantifying the anion effect of gas solubility within ionic liquids using the solvation affinity index. <i>Chemical Engineering Science</i> , 2022, 260, 117851.	1.9	2
12210	Fluoride-selective chemosensor based on an anion imprinted fluorescent polymer. <i>Polyhedron</i> , 2022, 225, 116033.	1.0	3
12211	Secondary electron emission behavior of nanostructured fluorocarbon film. <i>Surfaces and Interfaces</i> , 2022, 33, 102195.	1.5	2
12212	Highly efficient toluene absorption with π -electron donor-based deep eutectic solvents. <i>Separation and Purification Technology</i> , 2022, 298, 121618.	3.9	16
12213	DFT and dynamic analysis of glucose alcoholysis conversion to 5-ethoxymethylfurfural and ethyl levulinate. <i>Fuel</i> , 2022, 326, 125075.	3.4	7
12214	New cadmium(II) porphyrin-based coordination dimer: Experimental and theoretic studies. <i>Journal of Solid State Chemistry</i> , 2022, 314, 123364.	1.4	2
12215	Exploration of the multiscale interaction mechanism between natural deep eutectic solvents and silybin by QC calculation and MD simulation. <i>Journal of Molecular Liquids</i> , 2022, 363, 119768.	2.3	4
12216	A comparison of the inhibition effect of Zn ²⁺ or Fe ²⁺ in the oxidation of α -thiophenol groups in coal. <i>Chemical Engineering Science</i> , 2022, 260, 117863.	1.9	2
12217	Advanced hydrogen adsorption on benzene: Cation- π interaction effects. <i>Chemical Physics</i> , 2022, 562, 111649.	0.9	0

#	ARTICLE	IF	CITATIONS
12218	Mixed matrix membranes containing Cu-based metal organic framework and functionalized ionic liquid for efficient NH ₃ separation. <i>Journal of Membrane Science</i> , 2022, 659, 120780.	4.1	8
12219	Toward green and efficient recycling of Au(III), Pd(II) and Pt(IV) from acidic medium using UCST-type ionic liquid. <i>Separation and Purification Technology</i> , 2022, 298, 121620.	3.9	8
12220	Iron oxide nanoparticles loaded smart hybrid hydrogel for anti-inflammatory drug delivery: Preparation and characterizations. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 650, 129631.	2.3	14
12221	The nonlinear optical properties and noncovalent interactions of supramolecular Donor-acceptor-donor assemblies between molecular tweezers and fullerenes. <i>Journal of Luminescence</i> , 2022, 250, 119094.	1.5	4
12222	Deep removal of chlorobenzene based volatile organic compounds from exhaust gas with ionic liquids. <i>Separation and Purification Technology</i> , 2022, 298, 121610.	3.9	17
12223	Co-extraction of Mn ²⁺ , Co ²⁺ , and a part of Ni ²⁺ from sulfuric acid solution containing Li ⁺ using the new ionic liquids. <i>Journal of Molecular Liquids</i> , 2022, 363, 119842.	2.3	2
12224	Removal intensification of basic and non-basic nitrides from liquid fuels by the optimization design of quaternary ammonium salt green solvents. <i>Fuel</i> , 2022, 326, 125093.	3.4	11
12225	Experimental and density functional theory investigation of the NO reduction mechanism by semichars preheated in Ar and CO ₂ /Ar atmospheres. <i>Fuel</i> , 2022, 326, 125080.	3.4	3
12226	Hydrogen bonding regulation enables indanthrone as a stable and high-rate cathode for lithium-ion batteries. <i>Energy Storage Materials</i> , 2022, 51, 172-180.	9.5	15
12227	The effect of conjugated groups for favourable molecular planarity and efficient suppression of charge recombination simultaneously of phenothiazine-based organic dyes for dye-sensitized solar cells. <i>Synthetic Metals</i> , 2022, 290, 117137.	2.1	7
12228	The new inspiration from the theoretical re-exploration of traditional autoxidation pathways leading to sulfate formation in the haze episode. <i>Atmospheric Environment</i> , 2022, 287, 119220.	1.9	0
12229	Experimental spectra, electronic properties (liquid and gaseous phases) and activity against SARS-CoV-2 main protease of Fluphenazine dihydrochloride: DFT and MD simulations. <i>Journal of Molecular Structure</i> , 2022, 1267, 133633.	1.8	1
12230	Interlayer intercalation of Li/Al-LDHs responsible for high-efficiency boron extraction. <i>Desalination</i> , 2022, 539, 115966.	4.0	12
12231	Structure-Property Relationship of Three 2-Chloro-4-fluoro Chalcone Derivatives: A Comprehensive Study on Linear and Non-linear Optical Properties, Structural Characterizations and Density Functional Theory. <i>Journal of Molecular Structure</i> , 2022, 1267, 133584.	1.8	10
12232	Citrate-regulated synthesis of hydrotalcite-like compounds as peroxymonosulfate activator - Investigation of oxygen vacancies and degradation pathways by combining DFT. <i>Applied Catalysis B: Environmental</i> , 2022, 317, 121704.	10.8	87
12233	Molecular structure, vibrational spectroscopy (FT-IR, Raman), solvent effects, molecular docking and DFT studies of 1-(4-chlorophenyl)-3-(4-ethoxyphenyl)-prop-2-en-1-one. <i>Journal of Molecular Structure</i> , 2022, 1267, 133660.	1.8	6
12234	Mechanism of the distinct toxicity level of imidacloprid and thiacloprid against honey bees: An in silico study based on cytochrome P450 9Q3. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108257.	1.3	2
12235	Ce(IV) activates peroxymonosulfate for the degradation of substituted PAHs. <i>Chemosphere</i> , 2022, 306, 135525.	4.2	16

#	ARTICLE	IF	CITATIONS
12236	Extraction of itaconic acid by endophytic <i>Aspergillus</i> sp., isolated from <i>Garcinia indica</i> : Spectroscopic, structural and quantum computational studies. <i>Journal of Molecular Structure</i> , 2022, 1268, 133635.	1.8	2
12237	Reaction site evolution during low-temperature oxidation of low-rank coal. <i>Fuel</i> , 2022, 327, 125195.	3.4	7
12238	The electronic structures and nonlinear optical properties of Alkali and Alkali earth metal atoms doped C ₆ H ₆ Cl ₆ : A density functional theoretical study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108263.	1.3	0
12239	Insights into the photophysical properties of 2-(2-hydroxyphenyl) benzazoles derivatives: Application of ESIPT mechanism on UV absorbers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 280, 121559.	2.0	5
12240	Study of detoxification of methyl parathion by dielectric barrier discharge (DBD) non-thermal plasma at gas-liquid interface: mechanism and bio-toxicity evaluation. <i>Chemosphere</i> , 2022, 307, 135620.	4.2	14
12241	Adsorption of toxic and non-toxic metals with new model of CX[4]: Experimental and computational investigation, Spectroscopic, QAIM, and Antibacterial activity analyses. <i>Journal of Molecular Structure</i> , 2022, 1268, 133618.	1.8	1
12242	An extension of electron acceptor sites around Thiazolothiazole unit for evaluation of large power conversion efficiency: A theoretical insight. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 281, 121610.	2.0	7
12243	From N atom to C-NO ₂ group: Achieving a high energy density material with a -NH ₂ -NO ₂ -NH ₂ -block. <i>Chemical Engineering Journal</i> , 2022, 450, 138094.	6.6	13
12244	Blue TiO ₂ nanotube electrocatalytic membrane electrode for efficient electrochemical degradation of organic pollutants. <i>Chemosphere</i> , 2022, 306, 135628.	4.2	16
12245	Tailoring co-assembly loading of doxorubicin in solvent-triggering gel. <i>Journal of Colloid and Interface Science</i> , 2022, 626, 619-628.	5.0	2
12246	Regulating excited state of sulfone-locked triphenylamine heteroaromatics for high-efficiency ultralong room-temperature phosphorescence. <i>Chemical Engineering Journal</i> , 2022, 449, 137834.	6.6	19
12247	Ratiometric detection and imaging of endogenous alkaline phosphatase activity by fluorescein-coumarin-based fluorescence probe. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 281, 121615.	2.0	5
12248	Covalent organic framework modified carbon nanotubes for removal of uranium (VI) from mining wastewater. <i>Chemical Engineering Journal</i> , 2022, 450, 138062.	6.6	10
12249	Structural benchmarking, density functional theory simulation, spectroscopic investigation and cancer chemotherapeutic agent. <i>Chemical Physics Impact</i> , 2022, 5, 100091.	1.7	79
12250	Comprehensive assessment of estrogenic activities of parabens by in silico approach and in vitro assays. <i>Science of the Total Environment</i> , 2022, 845, 157194.	3.9	7
12251	Theoretical investigation and antineoplastic potential of Zn (II) and Pd (II) complexes of 6-methylpyridine-2-carbaldehyde-N (4)-ethylthiosemicarbazone. <i>Chemical Physics Impact</i> , 2022, 5, 100094.	1.7	31
12252	A super stable Near-Infrared garnet phosphor resistant to thermal Quenching, thermal degradation and hydrolysis. <i>Chemical Engineering Journal</i> , 2022, 449, 137892.	6.6	22
12253	Bottom-up synthesis of cationic porphyrin-based porous organic polymers for highly efficient and selective recovery of gold. <i>Chemical Engineering Journal</i> , 2022, 449, 137758.	6.6	23

#	ARTICLE	IF	CITATIONS
12254	Effects of different dissolved organic matter on peroxymonosulfate activation over Co-Fe binary metal: Experiments and density functional theory. <i>Chemical Engineering Journal</i> , 2022, 450, 137770.	6.6	10
12255	N, N- TM -methylene-bridged nitroiodoazoles: Biocidal compounds with enhanced thermal stability. <i>Chemical Engineering Journal</i> , 2022, 450, 137841.	6.6	7
12256	Facile synthesis of hierarchical Ti ₃ C ₂ @FeOOH nanocomposites for antimony contaminated wastewater treatment: Performance, mechanisms, reutilization, and sustainability. <i>Chemical Engineering Journal</i> , 2022, 450, 138038.	6.6	14
12257	Peroxymonosulfate activation by iron self-doped sludge-derived biochar for degradation of perfluorooctanoic acid: A singlet oxygen-dominated nonradical pathway. <i>Chemical Engineering Journal</i> , 2022, 450, 137953.	6.6	40
12258	Comparison of UV and UV-LED activated sodium percarbonate for the degradation of O-desmethylvenlafaxine. <i>Journal of Environmental Sciences</i> , 2023, 126, 656-667.	3.2	4
12259	The Crystalline Behavior and Device Function of Nonfullerene Acceptors in Organic Solar Cells. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	26
12260	Structural modification on Dimethoxythienothiophene based non-fullerene acceptor molecule for construction of high-performance organic chromophores by employing DFT approach. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 170, 110906.	1.9	20
12261	Oxygen-coordinated low-nucleus cluster catalysts for enhanced electrocatalytic water oxidation. , 2023, 5, .		12
12262	Insight into pyrolysis mechanism of 1,2-propylene glycol: Based on density functional theory and wavefunction analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2022, , 108277.	1.3	0
12263	Crystal structures, optical analysis and theoretical calculations of two thiosemicarbazide and semicarbazide derivatives based on triphenylamine-thiophene. <i>Journal of Molecular Structure</i> , 2022, 1269, 133777.	1.8	0
12264	Enantio- and Regioselective Ni-Catalyzed <i>para</i> -C-H Alkylation of Pyridines with Styrenes via Intermolecular Hydroarylation. <i>Journal of the American Chemical Society</i> , 2022, 144, 13643-13651.	6.6	46
12265	Physicochemical and DFT studies of organic NLO single crystal 4-methoxy-N-(2-methyl-5-nitrophenyl) benzamide. <i>Molecular Crystals and Liquid Crystals</i> , 2023, 754, 43-67.	0.4	3
12266	Aromatic diglycosides from <i>Sophora tonkinensis</i> and a multi-step conformer filtering procedure for TDDFT calculation of flexible glycoside. <i>Journal of Asian Natural Products Research</i> , 2023, 25, 411-421.	0.7	2
12267	Impact of the Dicarboxylic Acid Chain Length on Intermolecular Interactions with Lidocaine. <i>Molecular Pharmaceutics</i> , 2022, 19, 2980-2991.	2.3	1
12268	Synthesis, Single-Crystal XRD, Spectral and Computational Analysis of 2-(3,4-Dimethoxyphenyl)-1H-Phenanthro[9,10-d] Imidazole as Electron-Transport and NLO Material. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 4924-4937.	1.4	2
12269	Photo-assisted reductive cleavage and catalytic hydrolysis-mediated persulfate activation by mixed redox-couple-involved CuFeS ₂ for efficient trichloroethylene oxidation in groundwater. <i>Water Research</i> , 2022, 222, 118885.	5.3	10
12270	Two-Dimensional Perovskites with Tunable Room-Temperature Phosphorescence. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	16
12271	Application of atomic electrostatic potential descriptors for predicting the eco-toxicity of ionic liquids towards leukemia rat cell line. <i>Chemical Engineering Science</i> , 2022, , 117941.	1.9	1

#	ARTICLE	IF	CITATIONS
12272	Theoretical insight into the reaction mechanism of ammonia dehydrogenation on iron-based clusters. <i>Materials Today Communications</i> , 2022, 32, 104088.	0.9	2
12273	Crystalline $\langle \text{scp} \rangle$ Germanium $\hat{\text{D}}$ ipyrrromethene $\langle / \text{scp} \rangle$ Radicals: from a Delocalized Neutral to a Localized Cation. <i>Chinese Journal of Chemistry</i> , 2022, 40, 2387-2392.	2.6	7
12274	Enhancing probe $\hat{\text{T}}$ Ms sensitivity for peroxyxynitrite through alkoxy modification of dicyanovinylchromene. <i>Analytical and Bioanalytical Chemistry</i> , 2022, 414, 6779-6789.	1.9	9
12275	Photochemical and Molecular Dynamics Studies of Halide Binding in Flavoenzyme Glucose Oxidase. <i>ChemBioChem</i> , 2022, 23, .	1.3	1
12276	Preparation of amidated pectins through enzymatic method: Structures, hydrogel properties and its application potential in fat substitutes. <i>Food Research International</i> , 2022, 160, 111719.	2.9	8
12277	Synthesis, vibrational analysis, molecular property investigation, and molecular docking of new benzenesulphonamide-based carboxamide derivatives against <i>Plasmodium falciparum</i> . <i>Journal of Molecular Structure</i> , 2022, 1269, 133796.	1.8	38
12278	Adsorption and breaking of hazardous methyl mercury on hybrid structures of ionic liquids and ZnO nanoclusters. <i>Journal of Molecular Liquids</i> , 2022, 364, 119957.	2.3	5
12279	Mechanism for the Intercalation of Aniline Cations into the Interlayers of Graphite. <i>Nanomaterials</i> , 2022, 12, 2486.	1.9	4
12280	A Ni(II) chetale of an unsymmetrical N2O3 donor ligand and its use as flexidentate metalloligand to synthesise heterometallic Ni(II)-Mn(II) complexes: recurrent CH $\hat{\text{A}}$ $\hat{\text{A}}$ $\hat{\text{I}}$ and $\hat{\text{I}}$ -stacking motifs in the structures. <i>Inorganica Chimica Acta</i> , 2022, , 121111.	1.2	1
12281	Bucket Effect to Improve $\langle \text{scp} \rangle$ Third $\hat{\text{O}}$ Order $\langle / \text{scp} \rangle$ Nonlinear Optical Response on $\langle \text{scp} \rangle$ Metal $\hat{\text{H}}$ eteroaromatic $\langle / \text{scp} \rangle$ Compounds. <i>Chinese Journal of Chemistry</i> , 2022, 40, 2611-2617.	2.6	6
12282	Ternary CE2Ba2 (E $\hat{\text{e}}$ $\hat{\text{o}}$ = $\hat{\text{a}}$ $\hat{\text{o}}$ As, Sb) Clusters: New Pentaatomic Planar Tetracoordinate Carbon Species with 18 Valence Electrons. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	2
12283	Modulating the strong metal-support interaction of single-atom catalysts via vicinal structure decoration. <i>Nature Communications</i> , 2022, 13, .	5.8	36
12284	Molecular design of silicon $\hat{\text{e}}$ containing diazenes: absorbance of E and Z isomers in near $\hat{\text{i}}$ nfrared region. <i>Chemistry - A European Journal</i> , 0, , .	1.7	1
12285	Unveiling the sensing mechanism and luminescence property of a new ESIPT-based fluorescent sensor for detecting Zn $\hat{\text{2}}$ +. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 282, 121650.	2.0	16
12286	Interfacial engineering boosting the piezocatalytic performance of Z-scheme heterojunction for carbamazepine degradation: Mechanism, degradation pathway and DFT calculation. <i>Applied Catalysis B: Environmental</i> , 2022, 317, 121793.	10.8	75
12287	Synergy of Mn-Fe-Al and reconstruction of chemisorption & physisorption in arsenic removal. <i>Separation and Purification Technology</i> , 2022, 299, 121748.	3.9	6
12288	Ionization energies and cationic bond dissociation energies of RuB, RhB, OsB, IrB, and PtB. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	5
12289	Spectral characterization, solvation effects on topological aspects, and biological attributes of Fmoc-L-glutamic acid 5 $\hat{\text{e}}$ tert $\hat{\text{e}}$ butyl ester: An effective reagent in anticancer evaluations. <i>Journal of Molecular Structure</i> , 2022, 1269, 133793.	1.8	11

#	ARTICLE	IF	CITATIONS
12290	Modification of g-C ₃ N ₄ with hydroxyethyl cellulose as solid proton donor via hydrogen bond to enhance H ₂ O ₂ production. <i>Applied Catalysis B: Environmental</i> , 2022, 318, 121749.	10.8	35
12291	Theoretical Study of the Structural, Optoelectronic, and Reactivity Properties of N-[5- ² -Methyl-3- ² -Isoxasolyl]-N-[(E)-1-(2-)]Methylidene] Amine and Some of Its Fe ²⁺ , Co ²⁺ , Ni ²⁺ , Cu ²⁺ , and Zn ²⁺ Complexes for OLED and OFET Applications. <i>Journal of Chemistry</i> , 2022, 2022, 1-18.	0.9	2
12292	Electronic structure analysis of copper photoredox catalysts using the quasi-restricted orbital approach. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	5
12293	Sulfonium and Selenonium Salts as Noncovalent Organocatalysts for the Multicomponent Groebke-Blackburn-Bienaym Reaction. <i>Journal of Organic Chemistry</i> , 2022, 87, 10199-10207.	1.7	20
12294	Performance evaluation and molecular dynamics simulation in the Liquid-liquid extraction process of low transition temperature mixture n-hexane-1,2-Dichloroethane. <i>Journal of Molecular Liquids</i> , 2022, 364, 119913.	2.3	2
12295	Physical mechanism on linear spectrum and nonlinear spectrum in double helical carbon nanomolecule-infinite. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 282, 121674.	2.0	11
12296	Wavelength-tunable fluorophores based on quinoline fused β -cyanovinyl derivatives: Synthesis, photophysics properties and imaging. <i>Tetrahedron Letters</i> , 2022, 104, 153996.	0.7	6
12297	DFT Investigation of Polyethylene-co-vinyl Acetate: Kinetics of Initiation and Propagation, Copolymer Composition, and Unit Sequence Distribution. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 10775-10789.	1.8	2
12298	A combined QTAIM/IRI topological analysis of the effect of axial/equatorial positions of NH ₂ and CN substituents in the [(PY5Me ₂)MoO] ⁺ complex. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108273.	1.3	3
12299	Experimental and theoretical investigation on degradation of dimethyl trisulfide by ultraviolet/peroxymonosulfate: Reaction mechanism and influencing factors. <i>Journal of Environmental Sciences</i> , 2023, 127, 824-832.	3.2	4
12301	Controllable design of high-efficiency triboelectric materials by functionalized metal-organic frameworks with a large electron-withdrawing functional group. <i>Nano Research</i> , 2022, 15, 9386-9391.	5.8	22
12302	Neutral Phosphine-Sulfonate Pd Complex-Catalyzed Copolymerization of 2-Methoxystyrene and Ethylene Polar Monomers: A DFT Mechanistic Study. <i>ACS Applied Polymer Materials</i> , 2022, 4, 5901-5908.	2.0	1
12303	Molecular Electrides: An In Silico Perspective. <i>ChemPhysChem</i> , 2022, 23, .	1.0	4
12304	A self-assembled aza-BODIPY linked dicyanostilbenzene with a large Stokes shift, AIE, mechanochromism and singlet oxygen yield. <i>Journal of Molecular Liquids</i> , 2022, 363, 119906.	2.3	5
12305	Study on spectral properties and active sites of glucose and fructose based on density functional theory. <i>Inorganic Chemistry Communication</i> , 2022, 143, 109775.	1.8	0
12306	Single bond activated AIE of platinum(II) complex achieving expeditious oxygen monitoring and high-efficiency felodipine identification. <i>Dyes and Pigments</i> , 2022, 205, 110582.	2.0	5
12307	Extractive separation of 1,8-cineole and β -terpinene with lactic acid-based deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2022, 363, 119828.	2.3	0
12308	Experimental and theoretical study of the sulfamic acid-urea deep eutectic solvent. <i>Journal of Molecular Liquids</i> , 2022, 363, 119859.	2.3	19

#	ARTICLE	IF	CITATIONS
12309	Effective absorption of dichloromethane using deep eutectic solvents. <i>Journal of Hazardous Materials</i> , 2022, 439, 129666.	6.5	19
12310	Construction and modulation of dual responsive AIE supramolecular aggregates combined with quantum chemistry simulation. <i>Journal of Molecular Liquids</i> , 2022, 363, 119881.	2.3	2
12311	Achieving the low interfacial tension by balancing crystallization and film-forming ability of the cathode interlayer for organic solar cells. <i>Journal of Colloid and Interface Science</i> , 2022, 627, 880-890.	5.0	6
12312	Research on interaction regularities and mechanisms between lactic acid and aroma compounds of Baijiu. <i>Food Chemistry</i> , 2022, 397, 133765.	4.2	13
12313	Uncovering the role of impurity sugars on the crystallization of d-tagatose crystal: Experiments and molecular dynamics simulations. <i>Food Chemistry</i> , 2022, 397, 133762.	4.2	6
12314	Experimental and computational investigation of a novel organic cation hexachlorostannate (IV) material (CHNO)(SnCl). <i>Journal of Molecular Structure</i> , 2022, 1269, 133757.	1.8	1
12315	Electrochemically driven FeO-activated sulfite oxidation for enhancing sludge dewaterability. <i>Chemical Engineering Journal</i> , 2022, 450, 138199.	6.6	10
12316	Shear Flow Induced Specific Ion Interfacial Effect on Enhanced Difference in Mass Transfer in the Boundary Layer. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12317	Theoretical studies on boron dimesityl-based thermally activated delayed fluorescence organic emitters: excited-state properties and mechanisms. <i>New Journal of Chemistry</i> , 2022, 46, 15678-15685.	1.4	1
12318	Benzothiazole-substituted 1,3-diaza-2-oxophenoxazine as a luminescent nucleobase surrogate for silver(II)-mediated base pairing. <i>Dalton Transactions</i> , 2022, 51, 13386-13395.	1.6	3
12319	Different Positions of Cyano Substitution Controlled Directionality of Esipt Processes with Two Asymmetric Proton Acceptors System: A Td-Dft Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12320	Theoretical analysis of sulfuric acid-dimethylamine-oxalic acid-water clusters and implications for atmospheric cluster formation. <i>RSC Advances</i> , 2022, 12, 22425-22434.	1.7	0
12321	Efficient Synthesis of PdIr Nanocatalysts with Controllable Surface Composition for Electrochemical Oxidation of Methanol. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12322	A bottom-up approach from medium-sized bilayer boron nanoclusters to bilayer borophene nanomaterials. <i>Nanoscale</i> , 2022, 14, 11443-11451.	2.8	12
12323	Quantitatively Regulating the Ketone Structure of Covalent Triazine-Based Frameworks for Efficient Visible-Light Photocatalytic Degradation of Organic Pollutants: Tunable Performance and Mechanisms. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12324	Aqueous microsolvation of 4-hydroxy-2-butanone: competition between intra- and inter-molecular hydrogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 19919-19926.	1.3	2
12325	A niobium pentafulvene ethylene complex: synthesis, properties and reaction pathways. <i>Dalton Transactions</i> , 2022, 51, 12502-12511.	1.6	3
12326	The Extraction of Aromatics Using Nmp: Liquid-Liquid Equilibrium Determination and Mechanistic Exploration. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
12327	Effects and mechanism of natural phenolic acids/fatty acids on copigmentation of purple sweet potato anthocyanins. <i>Current Research in Food Science</i> , 2022, 5, 1243-1250.	2.7	5
12328	Investigation on Molecular Dynamics Simulation for Predicting Kinematic Viscosity of Natural Ester Insulating Oil. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2022, 29, 1882-1888.	1.8	7
12329	A DFT study on the mechanism and regioselectivity of NHC-catalyzed double acylation of aromatic 1,2-diketones with α,β -unsaturated ketones. <i>New Journal of Chemistry</i> , 2022, 46, 17026-17031.	1.4	3
12330	Planar Inorganic Five-Membered Heterocycles with π - π Dual Aromaticity in Both S ₀ and T ₁ States. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	4
12331	Formation of the quasi-planar B ₅₆ boron cluster: topological path from B ₁₂ and disk aromaticity. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1
12332	Excited-state double proton transfer of 1,8-dihydroxy-2-naphthaldehyde: A MS-CASPT2//CASCF study. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 422-430.	0.6	2
12333	Collective total syntheses of cytochalasans and merocytochalasans. , 2022, 2, 100022.		1
12334	Pathway toward Optical Cycling and Laser Cooling of Functionalized Arenes. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 7029-7035.	2.1	15
12335	Basic-involved thermal interaction between arylamino[70]fullerenoarylaziridine and nitrocellulose. <i>Journal of Materials Science</i> , 2022, 57, 14265-14286.	1.7	1
12336	DFT investigates the mechanisms of cross-dehydrogenative coupling between heterocycles and acetonitrile. <i>Molecular Physics</i> , 0, , .	0.8	0
12337	The Distance between Minima of Electron Density and Electrostatic Potential as a Measure of Halogen Bond Strength. <i>Molecules</i> , 2022, 27, 4848.	1.7	7
12338	Synthesis, Formation Mechanism, and Structure of K[BH ₃ (CH ₃) ₃] and Its Application in Preparation of KB ₃ H ₈ . <i>Inorganic Chemistry</i> , 2022, 61, 12828-12834.	1.9	1
12339	Facile Access to Far-Red Fluorescent Probes with Through-Space Charge-Transfer Effects for In Vivo Two-Photon Microscopy of the Mouse Cerebrovascular System. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	15
12340	New QSPR model for prediction of corrosion inhibition using conceptual density functional theory. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	8
12341	Interaction of 5-fluorouracil anticancer drug with nucleobases: insight from DFT, TD-DFT, and AIM calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 5882-5893.	2.0	2
12342	Study of Pd-catalyzed Selective Mono- and Di-C(sp ³)-H Bond Activation: A Bi-ligand Model. <i>Journal of Organic Chemistry</i> , 2022, 87, 10958-10966.	1.7	1
12343	A DFT Comparative Study of Cyclo[18] Nanorings: Carbon, BN and BCN. <i>Journal of Cluster Science</i> , 2023, 34, 1465-1473.	1.7	4
12344	New Carboxamides and a New Polyketide from the Sponge-Derived Fungus <i>Arthrinium</i> sp. SCSIO 41421. <i>Marine Drugs</i> , 2022, 20, 475.	2.2	7

#	ARTICLE	IF	CITATIONS
12345	Solid-Grinded Cocrystals of Acridine and 3,5-Dinitrobenzoic Acid: A Cocrystal with Strong Cocrystallization Ability and Two-Photon Excited Fluorescence Property. <i>Journal of Physical Chemistry C</i> , 2022, 126, 13381-13387.	1.5	3
12346	Nucleotide Recognition by a Guanidinocalixarene Receptor in Aqueous Solution. <i>Chemical Research in Chinese Universities</i> , 2023, 39, 144-150.	1.3	4
12347	Influence of Silica-Supported Alkylaluminum on Heterogeneous Zwitterionic Anilinonaphthoquinone Nickel and Palladium-Catalyzed Ethylene Polymerization and Copolymerization with Polar Monomers. <i>ACS Catalysis</i> , 2022, 12, 9646-9654.	5.5	6
12348	Anion complexes of diborane derivatives inserted to benzene. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	1
12349	Glycol bearing perylene monoimide based non-fullerene acceptors with increased dielectric permittivity. <i>Monatshefte für Chemie</i> , 0, , .	0.9	2
12350	A Density Functional Theory and Information-Theoretic Approach Study of Interaction Energy and Polarizability for Base Pairs and Peptides. <i>Pharmaceuticals</i> , 2022, 15, 938.	1.7	9
12351	Advancing the Am Extractant Design through the Interplay among Planarity, Preorganization, and Substitution Effects. <i>Inorganic Chemistry</i> , 2022, 61, 11556-11570.	1.9	11
12352	Stability and interaction of biochar and iron Âmineral nanoparticles: effect of pH, ionic strength, and dissolved organic matter. <i>Biochar</i> , 2022, 4, .	6.2	5
12353	Two monoâ€•and dinuclear Bi(III) complexes combined with crystallographic, spectroscopic, and antibacterial activities, MEP/HSA, and TD/DFT calculations. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	1.7	11
12354	Probing the Molecular Assembly of a Metabolizer Drug with Î²-Cyclodextrin and Its Binding with CT-DNA in Augmenting Antibacterial Activity and Photostability by Physicochemical and Computational Methodologies. <i>ACS Omega</i> , 2022, 7, 26211-26225.	1.6	7
12355	Perfluoroarene Interaction-Controlled Chiral Phosphoric Acid-Catalyzed Enantioselective Michael Addition of Difluoroenoxy silanes to Azadienes: a Combination of Experimental and Theoretical Studies. <i>ACS Catalysis</i> , 2022, 12, 9655-9663.	5.5	12
12356	Activationâ€•Deactivation of Inter-Peptide Bond in Fluoro-N-(2-hydroxy-5-methyl phenyl)benzamide Isomers, Induced by the Position of the Halogen Atom in the Benzene Ring. <i>MolBank</i> , 2022, 2022, M1416.	0.2	0
12357	The Complexation between Siloxane Species and Methylsiloxane: Electronic Structure, Thermodynamic, and Interaction Characteristics. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0
12358	Facile Access to Farâ€•Red Fluorescent Probes with Throughâ€•Space Charge Transfer Effect for In Vivo Twoâ€•Photon Microscopy of Mouse Cerebrovascular System. <i>Angewandte Chemie</i> , 0, , .	1.6	1
12359	Highly efficient and persistent room temperature phosphorescence from cluster exciton enables ultrasensitive off-on VOC sensing. <i>Matter</i> , 2022, 5, 3499-3512.	5.0	62
12360	In Search of Preferential Macrocyclic Hosts for Sulfur Mustard Sensing and Recognition: A Computational Investigation through the New Composite Method r2SCAN-3c of the Key Factors Influencing the Host-Guest Interactions. <i>Nanomaterials</i> , 2022, 12, 2517.	1.9	5
12361	A Molecular Dynamics Approach to the Impacts of Oxidative Aging on the Engineering Characteristics of Asphalt. <i>Polymers</i> , 2022, 14, 2916.	2.0	7
12362	Insights into the Capture of CO2 by Nickel Hydride Complexes. <i>Catalysts</i> , 2022, 12, 790.	1.6	3

#	ARTICLE	IF	CITATIONS
12363	Noble Gas π -Silicon Cations: Theoretical Insights into the Nature of the Bond. <i>Molecules</i> , 2022, 27, 4592.	1.7	2
12364	Carbodefluorination of fluoroalkyl ketones via a carbene-initiated rearrangement strategy. <i>Nature Communications</i> , 2022, 13, .	5.8	22
12365	Bonding Nature of σ -Allylic Carbenes π in $[M_3(\mu_3)^3(CH_2)]$ -Containing Compounds: The Covalent Interaction. <i>Inorganic Chemistry</i> , 2022, 61, 12349-12355.	1.9	0
12366	Complexation of Astatine(III) with Ketones: Roles of NO_3^- Counterion and Exploration of Possible Binding Modes. <i>Inorganic Chemistry</i> , 2022, 61, 12087-12096.	1.9	8
12367	DFT study of common anions adsorption at graphene surface due to anion- π interaction. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	10
12368	Detection of cocoyl sarcosine utilizing an extended-gate-type organic field-effect transistor functionalized with a copper(II)-dipicolylamine complex. <i>MRS Communications</i> , 2022, 12, 592-596.	0.8	2
12369	Self-Assembling Behaviour of Perylene, Perylene Diimide, and Thionated Perylene Diimide Deciphered through Non-Covalent Interactions. <i>ChemPhysChem</i> , 2022, 23, .	1.0	6
12370	Lewis acids modulation in phosphine-sulfonate palladium catalyzed ethylene polymerization. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	1.7	3
12371	Ligand accommodation causes altered reactivity of silver clusters with iodomethane: superatomic stability of Ag_9^{12+} in mimicking XeF_2 . <i>Science China Chemistry</i> , 2022, 65, 1594-1600.	4.2	5
12372	Improving Insecticidal Activity of Chlorantraniliprole by Replacing the Chloropyridinyl Moiety with a Substituted Cyanophenyl Group. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 9645-9663.	2.4	12
12373	A Theoretical Design of Chiral Molecules through Conformational Lock towards Circularly Polarized Luminescence. <i>Photonics</i> , 2022, 9, 532.	0.9	0
12374	Computational chemistry of cluster: Understanding the mechanism of atmospheric new particle formation at the molecular level. <i>Chemosphere</i> , 2022, 308, 136109.	4.2	7
12375	π -Conjugated Hexaazatrinaphthylene-Based Azo Polymer Cathode Material Synthesized by a Reductive Homocoupling Reaction for Organic Lithium-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 36700-36710.	4.0	11
12376	Zn^{2+} -enhanced Ru (II) photoluminescence directed by double-clamp structural ligand for selective Zn^{2+} sensing and live-cell imaging. <i>Sensors and Actuators B: Chemical</i> , 2022, 371, 132513.	4.0	2
12377	Effects of Twisted Intramolecular Charge Transfer Behavior on Excited-State Intramolecular Proton Transfer Reactions of Methyl Benzoate Derivatives in Water Solution. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5126-5133.	1.1	11
12378	In silico study of tacrine and acetylcholine binding profile with human acetylcholinesterase: docking and electronic structure. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	6
12379	How Strain-Release Determines Chemoselectivity: A Mechanistic Study of Rhodium-Catalyzed Bicyclo[1.1.0]butane Activation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 7694-7701.	2.1	2
12380	Insights on π -Glucose Biosensors/Carriers Based on Boron-Nitride Nanomaterials from an Atomistic and Electronic Point of View. <i>ChemPhysChem</i> , 2022, 23, .	1.0	14

#	ARTICLE	IF	CITATIONS
12381	Structural Organization of Dibromodiazadienes in the Crystal and Identification of Br-Å-Å-O Halogen Bonding Involving the Nitro Group. <i>Molecules</i> , 2022, 27, 5110.	1.7	3
12382	Can We Merge the Weak and Strong Tetrel Bonds? Electronic Features of Tetrahedral Molecules Interacted with Halide Anions. <i>Molecules</i> , 2022, 27, 5411.	1.7	5
12383	Effects of First-Coordination Sphere and Buffers on the Nitrosyl-Nitrite Conversion Rate in Ru(II) Complexes. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	0
12384	Nascent Decomposition Pathways of CH ₄ Pyrolysis in Gas-Phase Metal Halides. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5900-5910.	1.1	2
12385	High-Sensitivity Green Photodetectors Using Subphthalocyanine Derivatives as Photoactive Donors. <i>Journal of Physical Chemistry C</i> , 2022, 126, 13496-13504.	1.5	7
12386	Molecular Structure, Spectroscopic, Quantum Computational, and Molecular Docking Investigations on Propyl Gallate. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 5747-5767.	1.4	1
12387	Geometric evolution, electronic structure, and vibrational properties of $\langle \text{ScGe} \rangle_n$ ($\langle \text{DFT} \rangle$ insight. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	3
12388	Impact of Protonation and Hydrogen Bonding Interactions on the Biological Properties of Antibacterial Compound 4-Dimethylaminopyridinium Salicylate Monohydrate: Correlation with Its Precursor Molecules. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 5892-5914.	1.4	1
12389	Energetic Gem-dinitro Salts with Improved Thermal Stability by Incorporating with A Fused Building Block. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 37975-37981.	4.0	12
12390	Intermolecular interactions induced desulfurization/denitrification of oil with deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2022, 366, 120159.	2.3	9
12391	Sensitive fluorescent detection and micromechanism of Mn-doped CuS probe for oxytetracycline hydrochloride. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 284, 121768.	2.0	8
12392	Methine initiated polypropylene-based disposable face masks aging validated by micromechanical properties loss of atomic force microscopy. <i>Journal of Hazardous Materials</i> , 2023, 441, 129831.	6.5	4
12393	Cu(II) carboxylate arene Ca ²⁺ functionalization: Tuning for nonradical pathways. <i>Science Advances</i> , 2022, 8, .	4.7	8
12394	Adsorption and Activation of O ₂ on Small Gold Oxide Clusters: the Reactivity Dominated by Site-Specific Factors. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5594-5603.	1.1	2
12395	Enhanced Aromaticity and Open-Shell Diradical Character in the Dianions of 9-Fluorenylidene-Substituted Expanded Radialenes. <i>Angewandte Chemie</i> , 0, , .	1.6	2
12396	Antituberculous Potential of Amino-(formylphenyl) Diazenyl-Hydroxyl and Nitro-Substituted Naphthalene-Sulfonic Acid Derivatives: Experimental and Theoretical Investigations. <i>Chemistry Africa</i> , 2022, 5, 1451-1467.	1.2	29
12397	DFT study on the disproportionation of methylchlorosilane catalyzed by AlCl ₃ /4Å-T-ZSM-5@MIL-53(Al) core-shell catalyst. <i>Structural Chemistry</i> , 0, , .	1.0	0
12398	Effect of structural modifications on the spectral and lasing characteristics of truxene-cored starbursts with/without diphenylamine end-cappers. <i>Science China Materials</i> , 2023, 66, 309-318.	3.5	4

#	ARTICLE	IF	CITATIONS
12399	Hybrid Quinoline Telluroether Ligand Derived Copper and Silver Complexes: Synthesis, Structural and Electronic Properties. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	3
12400	A small addition of reduced graphene oxide to protect fluorosilicone rubber from thermal oxidative degradation. <i>Polymers for Advanced Technologies</i> , 0, .	1.6	2
12401	Reduktive Bildung von Al ^{III} -B ^I -Bindungen in Alumaboranen: Einfache Spaltung polarer Mehrfachbindungen. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	2
12402	Reductive Al ^{III} -B ^I -Bond Formation in Alumaboranes: Facile Scission of Polar Multiple Bonds. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	7
12403	Water-Gas Shift Catalyzed by Iridium-Vanadium Oxide Clusters IrVO ₂ with Iridium in a Rare Oxidation State of ^{II} . <i>Journal of Physical Chemistry A</i> , 2022, 126, 5294-5301.	1.1	3
12404	Insight into Substrate Recognition by Urea-Based Helical Foldamer Catalysts Using a DFT Global Optimization Approach. <i>Journal of Organic Chemistry</i> , 2022, 87, 10726-10735.	1.7	2
12405	Controllable Reactivity Tuned by the Cooperativity in B/P and B/N Intermolecular Frustrated Lewis Pairs. <i>ChemCatChem</i> , 2022, 14, .	1.8	1
12406	Amphiphilic Nanointerface: Inducing the Interfacial Activation for Lipase. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 39622-39636.	4.0	6
12407	Experimental and Theoretical Analysis of Synthesized Poly(Pthalazinone Ether Sulfone Ketone) Copolymer-Modified Separators for Li ^S Batteries. <i>ChemElectroChem</i> , 2022, 9, .	1.7	1
12408	Quenching singlet oxygen via intersystem crossing for a stable Li-O ₂ battery. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	20
12409	Hydrogen storage capacity of Be ₂ (^{NLi}) ₂ cluster with ultra-short beryllium-beryllium distance. <i>Journal of Computational Chemistry</i> , 0, .	1.5	1
12410	Noncovalent interactions between benzoalchalcogenadiazoles and nitrogen bases. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	4
12411	An Organic Laser Based on Thermally Activated Delayed Fluorescence with Aggregation-Induced Emission and Local Excited State Characteristics. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	2
12412	Active Pharmaceutical Ingredient-Ionic Liquids (API-ILs): Nanostructure of the Glassy State Studied by Electron Paramagnetic Resonance Spectroscopy. <i>Molecules</i> , 2022, 27, 5117.	1.7	5
12413	Cycloaddition Reactivities Analyzed by Energy Decomposition Analyses and the Frontier Molecular Orbital Model. <i>Accounts of Chemical Research</i> , 2022, 55, 2467-2479.	7.6	28
12414	Modeling of Re(I) tricarbonyl complexes against SARS-CoV-2 receptor via DFT, in-silico molecular docking, and QSAR. <i>Chemical Physics Impact</i> , 2022, 5, 100105.	1.7	19
12415	[8]Cyclophenylmethine as a Super-Cyclooctatetraene: Dynamic Behavior, Global Aromaticity, and Open-Shell Diradical Character in the Neutral and Dicationic States. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	1
12416	Neutral Antiaromatic Bis(1,2-dithiolene)-Chelated Nickel Complexes Bearing Multiradical Characters. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5552-5558.	1.1	0

#	ARTICLE	IF	CITATIONS
12417	Experimental and theoretical studies of the influence of alkyl groups on the photovoltaic properties of (E)-6-((2, 3-dihydroxynaphthalene)diazenyl)-1H-benzoisoquinoline-1,3-dione-based organic solar cell. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	14
12418	On the reliability of atoms in molecules, noncovalent index, and natural bond orbital to identify and quantify noncovalent bonds. <i>Journal of Computational Chemistry</i> , 2022, 43, 1814-1824.	1.5	10
12419	Evaluating Znâ€Porphyrinâ€Based Nearâ€IRâ€Sensitive Nonâ€Fullerene Acceptors for Efficient Panchromatic Organic Solar Cells. <i>ChemistryOpen</i> , 2022, 11, .	0.9	5
12420	Natural ultralong hemicelluloses phosphorescence. <i>Cell Reports Physical Science</i> , 2022, 3, 101015.	2.8	17
12421	Bayâ€Monosubstitution with Electronâ€Donating Group as an Efficiently Strategy to Functionalize Perylene Imide Polymer for Enhancing Photocatalytic Oxygen Evolution Activity. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	12
12422	Synthesis of water-compatible noncovalent imprinted microspheres for acidic or basic biomolecules designed based on molecular dynamics. <i>Polymer</i> , 2022, 257, 125253.	1.8	6
12423	The role of hydrogen bonds on the stability of anticancer drug compounds TG/uracil, TG/5-fluorouracil and TG/gimeracil. <i>Structural Chemistry</i> , 0, , .	1.0	0
12424	Cyclized oligomer of tetracyanoquinodimethane-tetrathiafulvalene (TCNQ-TTF): a versatile macrocyclic molecule by DFT calculations. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2022, 102, 751-761.	0.9	2
12425	Versatile Dicyanomethylene-Based Fluorescent Probes for the Detection of Î²-Amyloid in Alzheimerâ€™s Disease: A Theoretical Perspective. <i>International Journal of Molecular Sciences</i> , 2022, 23, 8619.	1.8	3
12426	Crystal Structure and Noncovalent Interactions of Heterocyclic Energetic Molecules. <i>Molecules</i> , 2022, 27, 4969.	1.7	3
12427	Structural Evolution of Carbon-Doped Aluminum Clusters Al _n C _{sup>â€“</sup>} (^{â€“} = 6â€“15): Anion Photoelectron Spectroscopy and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5621-5631.	1.1	10
12428	Decoupling of thermoelectric parameters in two-dimensional hyperbranched platinum acetylides. <i>Chemical Engineering Journal</i> , 2023, 451, 138751.	6.6	3
12429	Experimental and Quantum Chemical Study on the Inhibition Characteristics of Glutathione to Coal Oxidation at Low Temperature. <i>ACS Omega</i> , 2022, 7, 31448-31465.	1.6	3
12430	[8]Cycloâ€phenylmethine as a Superâ€Cyclooctatetraene: Dynamic Behavior, Global Aromaticity, and Openâ€Shell Diradical Character in the Neutral and Dicationic States. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	9
12431	Photoâ€induced energy and charge transfer dynamics in Y6 dimers. <i>Journal of the Chinese Chemical Society</i> , 2023, 70, 625-636.	0.8	4
12432	The Pnictogen Bond, Together with Other Non-Covalent Interactions, in the Rational Design of One-, Two- and Three-Dimensional Organic-Inorganic Hybrid Metal Halide Perovskite Semiconducting Materials, and Beyond. <i>International Journal of Molecular Sciences</i> , 2022, 23, 8816.	1.8	11
12433	Stabilization of Zn group dimers: A theoretical study. <i>Journal of Computational Chemistry</i> , 2022, 43, 1719-1724.	1.5	1
12434	Molecular dynamics insight into phase separation and transport in anion-exchange membranes: Effect of hydrophobicity of backbones. <i>Journal of Membrane Science</i> , 2022, 661, 120922.	4.1	28

#	ARTICLE	IF	CITATIONS
12435	Site- and Enantioselective Manganese-Catalyzed Benzylic C-H Azidation of Indolines. <i>Journal of the American Chemical Society</i> , 2022, 144, 15383-15390.	6.6	22
12436	Modulating the Photocyclization Reactivity of Diarylethenes through Changes in the Excited-State Aromaticity of the π -Linker. <i>Journal of Organic Chemistry</i> , 2022, 87, 11565-11571.	1.7	3
12437	Solution-Phase Synthesis and Isolation of An Aza-Triangulene and Its Cation in Crystalline Form. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	7
12438	Effect Mechanisms of Sodium on NO Heterogeneous Reduction by Nitrogen-Containing Char: Experimental and DFT Investigation. <i>Combustion Science and Technology</i> , 0, , 1-26.	1.2	1
12439	External electric field-dependent photoinduced charge transfer in non-fullerene organic solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 284, 121763.	2.0	3
12440	Explaining the interaction of mangiferin with MMP-9 and NF- κ B: a computational study. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	5
12441	Charge Transport in Twisted Organic Semiconductor Crystals of Modulated Pitch. <i>Advanced Materials</i> , 2022, 34, .	11.1	19
12442	The Speciation of Americium Cations in Neat Water Implicated from DFT Studies. <i>Inorganic Chemistry</i> , 2022, 61, 13858-13867.	1.9	1
12443	A Stable Zn-MOF for Photocatalytic C ₃ -H Oxidation: Vinyl Double Bonds Boosting Electron Transfer and Enhanced Oxygen Activation. <i>ACS Catalysis</i> , 2022, 12, 10668-10679.	5.5	14
12444	Oxo-Carotenoids as Efficient Superoxide Radical Scavengers. <i>Antioxidants</i> , 2022, 11, 1525.	2.2	4
12445	Quantum Chemical and Experimental Insight into Structure, Physicochemical Properties and Dissolving Behavior of Deep Eutectic Solvents. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 883-907.	1.0	1
12446	One-Step Catalytic Activation Promoting Pore Development of Zhundong Coal-Based Activated Coke: A Compared Study with Conventional Carbonization-Activation Combined Process. <i>Energy & Fuels</i> , 2022, 36, 9171-9181.	2.5	6
12447	Synthesis and Coordination Chemistry of a Benzannulated Bipyridine: 6,6-Biphenanthridine. <i>Inorganic Chemistry</i> , 2022, 61, 13386-13398.	1.9	4
12448	Activation of molecular oxygen by tenorite and ascorbic acid: Generation of high-valent copper species for organic compound oxidation. <i>Journal of Hazardous Materials</i> , 2022, 440, 129839.	6.5	5
12449	Improving the solubility, hygroscopicity and permeability of enrofloxacin by forming 1:2 pharmaceutical salt cocrystal with neutral and anionic co-existing p-nitrobenzoic acid. <i>Journal of Drug Delivery Science and Technology</i> , 2022, 76, 103732.	1.4	6
12450	Theoretical Mechanistic Studies of the Polymerization of Functionalized Styrenes Catalyzed by Rare-Earth-Metal Complexes: Stereoselectivity Regulation. <i>Organometallics</i> , 2022, 41, 2466-2473.	1.1	3
12451	Density Functional Theory Study on NiN _x (x = 1, 2, 3, 4) Catalytic Hydrogenation of Acetylene. <i>Molecules</i> , 2022, 27, 5437.	1.7	1
12452	Physical Mechanisms of Intermolecular Interactions and Cross-Space Charge Transfer in Two-Photon BDBT-TCNB Co-Crystals. <i>Nanomaterials</i> , 2022, 12, 2757.	1.9	3

#	ARTICLE	IF	CITATIONS
12453	Bond Strength of a Diatomic Acceptor Ligand: A Reliable Measure of Its Antibond Occupation and Its Charge?. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	3
12454	Examining the Non-Covalent Interactions for Two Polymorphs of a 2,1,3-benzoxadiazole Derivative. <i>Crystals</i> , 2022, 12, 1143.	1.0	2
12455	<sc>Pentagonâ€Containing</sc> Doublet Graphene Fragments with <sc>Edgeâ€Dependent</sc> Spin/Charge Distribution. <i>Chinese Journal of Chemistry</i> , 2022, 40, 2525-2530.	2.6	5
12456	Designing Magnetic Superalkalis with Extremely Large Nonlinear Optical Responses. <i>Organometallics</i> , 2022, 41, 2406-2414.	1.1	1
12457	Atomically Precise Platinum Carbonyl Nanoclusters: Synthesis, Total Structure, and Electrochemical Investigation of [Pt₂₇(CO)₃₁]^{4â€} Displaying a Defective Structure. <i>Inorganic Chemistry</i> , 2022, 61, 12534-12544.	1.9	3
12458	Eco-Friendly Synthesis and Characterization of Double-Crossed Link 3D Graphene Oxide Functionalized With Chitosan for Adsorption of Sulfamethazine From Aqueous Solution: Experimental and DFT Calculations. <i>Frontiers in Environmental Science</i> , 0, 10, .	1.5	15
12459	Unveiling the effect of 2D silagraphene structural diversity on electronic properties: DFT, DOS, and ELF studies. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	0
12460	Influence of 5-Halogenation on the Base-Pairing Energies of Protonated Cytidine Nucleoside Analogue Base Pairs: Implications for the Stabilities of Synthetic <i>i</i>-Motif Structures for DNA Nanotechnology Applications. <i>Journal of the American Society for Mass Spectrometry</i> , 0, , .	1.2	1
12461	Enhanced Aromaticity and Openâ€Shell Diradical Character in the Dianions of 9â€Fluorenylideneâ€Substituted Expanded Radialenes. <i>Angewandte Chemie - International Edition</i> , 0, , .	7.2	4
12462	Tuning Intramolecular Stacking of Rigid Heteroaromatic Compounds for Highâ€Efficiency Deepâ€Blue Throughâ€Space Chargeâ€Transfer Emission. <i>Angewandte Chemie</i> , 0, , .	1.6	2
12463	Carrier Dynamics and Surface Reaction Boosted by Polymer-based Single-atom Photocatalysts. <i>Chemical Research in Chinese Universities</i> , 2022, 38, 1207-1218.	1.3	7
12464	Cyclopropenylidene: Clustering and Interaction with Water Molecules. <i>Journal of Physical Chemistry A</i> , 0, , .	1.1	1
12465	Toward a BT.2020 green emitter through a combined multiple resonance effect and multi-lock strategy. <i>Nature Communications</i> , 2022, 13, .	5.8	112
12466	Solutionâ€Phase Synthesis and Isolation of An Azaâ€Triangulene and Its Cation in Crystalline Form. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	29
12467	Synthesis of Î²-Arylseleno Sulfoximines: A Metal-Free Three-Component Reaction Mediated by Tetrabutylammonium Tribromide. <i>Journal of Organic Chemistry</i> , 2022, 87, 10684-10697.	1.7	12
12468	Microhydration of Phenyl Formate: Gasâ€Phase Laser Spectroscopy, Microwave Spectroscopy, and Quantum Chemistry Calculations. <i>ChemPhysChem</i> , 0, , .	1.0	2
12469	Photochemical environmental persistence of venlafaxine in an urban water reservoir: A combined experimental and computational investigation. <i>Chemical Engineering Research and Design</i> , 2022, 166, 478-490.	2.7	8
12470	Stability and catalytic properties of Ptâ€Ni clusters supported on pyridinic N-doped graphene nanoflakes: an auxiliary density functional theory study. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	6

#	ARTICLE	IF	CITATIONS
12471	Complexes of Ce(III) and Bis(pyrazolyl)borate Ligands: Synthesis, Structures, and Luminescence Properties. <i>Inorganic Chemistry</i> , 2022, 61, 14164-14172.	1.9	4
12472	TMGe8-17 ⁺ (TM=Ti, Zr, Hf, V, Nb, Ta) clusters: group determined properties. <i>European Physical Journal Plus</i> , 2022, 137, .	1.2	12
12473	Quantum chemistry study on the anthropomorphic molecules: characterization, photovoltaic properties, and application. <i>Journal of the Iranian Chemical Society</i> , 2023, 20, 47-55.	1.2	1
12474	Synthesis of Open-Cage Fullerenes Containing a H-Bond between the Encapsulated Water Molecule and the Amide Moiety on the Rim of the Orifice. <i>European Journal of Organic Chemistry</i> , 2022, 2022, .	1.2	3
12475	Ethanol Conversion to Butanol over Small Coinage Metal Clusters: An Experimental and Computational Study. <i>Journal of Cluster Science</i> , 2023, 34, 1735-1743.	1.7	2
12476	Molecular Structure, Spectroscopic Elucidation (FT-IR, FT-Raman, UV-Visible and NMR) with NBO, ELF, LOL, RDC, Fukui, Drug Likeness and Molecular Docking Analysis on Dimethomorph. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 3988-4031.	1.4	8
12477	Understanding structure-properties relationships of porphyrin linked to graphene oxide through π - π -stacking or covalent amide bonds. <i>Scientific Reports</i> , 2022, 12, .	1.6	6
12478	Distinguishing the Packing Modes of Planar Energetic Molecules with Two C_2H_2 Groups Based on π -Holes. <i>Crystal Growth and Design</i> , 2022, 22, 5390-5398.		5
12479	Thermally Activated Delayed Fluorescence of a Dinuclear Platinum(II) Compound: Mechanism and Roles of an Upper Triplet State. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	7
12480	Vibrational and structural properties of the Fe_2R_2 complexes.		

#	ARTICLE	IF	CITATIONS
12489	Electrochemical performance of various activated carbon-multi-walled carbon nanotubes symmetric supercapacitor electrodes in aqueous electrolytes. <i>Carbon Letters</i> , 2022, 32, 1481-1505.	3.3	17
12491	Synthesis and structure of polycyclic 1,2,3-triazolylmethyl-benzimidazole derivatives â€” Experimental and computational quantum chemical studies. <i>Journal of Molecular Structure</i> , 2022, 1270, 133978.	1.8	5
12492	DFT rationalization of metal-catalyst-controlled coupling of carbazole with diazo-naphthalen-2(1H)-one. <i>Molecular Catalysis</i> , 2022, 529, 112574.	1.0	1
12493	Bidentate Rh(I)â€”Phosphine Complexes for the Câˆ”H Activation of Alkanes: Computational Modelling and Mechanistic Insight. <i>ChemCatChem</i> , 2022, 14, .	1.8	1
12494	Cationic lithium polysulfides in lithiumâ€”sulfur batteries. <i>Chem</i> , 2022, 8, 3031-3050.	5.8	42
12495	Sensitive Detection of Aspartame and Vanillin by Combining Terahertz Fingerprinting With a Metamaterial. <i>IEEE Sensors Journal</i> , 2022, 22, 16513-16521.	2.4	8
12496	Enhanced indirect attack behavior of IO ₂ for photocatalytic H ₂ O ₂ production: Possible synergistic regulation of spin polarization and water bridge on photocatalytic reaction. <i>Journal of Catalysis</i> , 2022, 413, 1132-1145.	3.1	6
12497	Extractive desulfurization of model fuels with a nitrogen-containing heterocyclic ionic liquid. <i>Frontiers of Chemical Science and Engineering</i> , 2022, 16, 1735-1742.	2.3	4
12498	Unraveling the radical chain mechanism in the pyrolysis of Î²-O-4 linked lignin: The role of aliphatic substituents. <i>Proceedings of the Combustion Institute</i> , 2022, , .	2.4	3
12499	Developing new derivatives of 3â€”Xâ€”4â€”hydroxyâ€”2(1 <i>i>H</i>)-quinolone as quinolineâ€”based chemosensors for detecting fluoride: Theoretical study on nucleophilicity and hydrogenâ€”bonding via various analyses. <i>Journal of Physical Organic Chemistry</i>, 2022, 35, .</i>	0.9	2
12500	Mechanistic Study of Asymmetric Alkynylation of Isatin-Derived Ketimine Mediated by a Copper/Guanidine Catalyst. <i>Journal of Organic Chemistry</i> , 2022, 87, 11693-11707.	1.7	1
12501	An Efficient Synthesis and Study of Biological Activity of New Pyrimidoazepines Using Ag/Fe₃O₄/TiO₂/CuO@MWCNTs Magnetic Nanocomposites: A Combined Experimental and Theoretical Investigation. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-30.	1.4	1
12502	Construction of Laser-Sensitive High-Energy Metalâ€”Organic Frameworks Based on Hydroxyl-Functionalized Tetrazole. <i>Crystal Growth and Design</i> , 2022, 22, 5300-5306.	1.4	3
12503	The facile detection and micromechanism of ATMP and DTPMP by fluorescence sensor based on nitrogen-doped carbon nanomaterials. <i>Dyes and Pigments</i> , 2022, 207, 110659.	2.0	3
12504	Enhancement of Energetic Performance through the Construction of Trinitromethyl Substituted Î²-Bis(1,2,4-oxadiazole). <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 7824-7830.	2.1	9
12505	Hydrogen evolution reactions between small-sized Ga _n (M=Ga, Al; n=0, 1, 2, 3) clusters and water molecules. <i>Journal of Molecular Liquids</i> , 2022, 365, 120167.	2.3	2
12506	Mechanistic Insights about the Ligandâ€”Enabled Oxyâ€”arylation/vinylation of Alkenes via Au(I)/Au(III) Catalysis. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	11
12507	Janus dione derivatives: Novel high-mobility hole transport materials for perovskite solar cells. <i>Materials Today Communications</i> , 2022, 32, 104090.	0.9	0

#	ARTICLE	IF	CITATIONS
12508	Solubility Measurement, Thermodynamic Correlation, and Comprehensive Analysis of 3,5-Dinitrobenzoic Acid in 13 Pure Solvents. <i>Journal of Chemical & Engineering Data</i> , 2022, 67, 2833-2844.	1.0	3
12509	Stability, atomic charges, bond order analysis, and the directionality of lone electron pairs on nitriles and isocyanides. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, .	0.9	3
12510	Influence of Ionic Liquids on the Aggregation and Pre-aggregation Phenomena of Asphaltenes in Model Solvent Mixtures by Molecular Dynamics Simulations and Quantum Mechanical Calculations. <i>Energy & Fuels</i> , 2022, 36, 9048-9065.	2.5	3
12511	Photocatalytic activation of sulfite by N-doped porous biochar/MnFe ₂ O ₄ interface-driven catalyst for efficient degradation of tetracycline. <i>Green Energy and Environment</i> , 2024, 9, 481-494.	4.7	8
12512	Molecular Interaction Modulates Crystallization and Defects of Perovskite Films for High-Performance Solar Cells. <i>ACS Applied Energy Materials</i> , 2022, 5, 10572-10580.	2.5	2
12513	Insight into Isolation and Characterization of Phenolic Compounds from Hawthorn (<i>Crataegus</i>) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Foods for Human Nutrition, 2022, 77, 538-544.	1.4	5
12514	Paying Comprehensive Attention to the ESPT Mechanism and Luminescent Property of Salicylic Acid and Its Derivatives in Various Microenvironments. <i>Advanced Theory and Simulations</i> , 2022, 5, .	1.3	10
12515	Understanding the Kinetics and Topological Events Within the Thione to Thiol Rearrangement of Xanthates. <i>ChemistrySelect</i> , 2022, 7, .	0.7	1
12516	Crystal Structure Characterization, Interaction Energy Analysis and DFT Studies of 3-(4-Chlorophenyl)-N-phenylquinoxalin-2-amine. <i>Journal of Chemical Crystallography</i> , 0, , .	0.5	0
12517	Selective adsorption desulfurization by single Al atom anchoring on the surface of hexagonal boron nitride through S Al coordination. <i>Applied Surface Science</i> , 2022, 605, 154638.	3.1	9
12518	Dibenzo[b,f][1,4,5]chalcogenadiazepine Photoswitches: Conversion of Excitation Energy into Ring Strain. <i>Angewandte Chemie - International Edition</i> , 0, , .	7.2	1
12519	Environmentally compatible 3-dimensional star-shaped donor materials for efficient organic solar cells. <i>International Journal of Energy Research</i> , 2022, 46, 22145-22161.	2.2	19
12520	Ring Strain Energies of Three-Membered Homoatomic Inorganic Rings E ₃ and Diheterotetreliranes E ₂ Tt (Tt = C, Si, Ge): Accurate versus Additive Approaches. <i>Inorganic Chemistry</i> , 2022, 61, 13846-13857.	1.9	5
12521	Reconsideration of the Structures of Stemara-13(14)-en-18-ol and Related Diterpene Natural Products: Vinylic Hydrogen Chemical Shifts Are Key. <i>Journal of Natural Products</i> , 2022, 85, 1912-1917.	1.5	1
12522	Synthesis, crystal structure, Hirshfeld surface analysis, energy frameworks and computational studies of Schiff base derivative. <i>Heliyon</i> , 2022, 8, e10047.	1.4	4
12523	Simple and energetic: Novel combination of furoxan and 1,2,4-triazole rings in the synthesis of energetic materials. <i>Energetic Materials Frontiers</i> , 2022, 3, 146-153.	1.3	12
12524	Complete Inhibition of the Rotation in a Barrierless TICT Probe for Fluorescence-On Qualitative Analysis. <i>Analytical Chemistry</i> , 2022, 94, 11679-11687.	3.2	12
12525	Plasma-Assisted Coupling Reactions of Dinitrogen and Carbon Dioxide Mediated by Monometallic YB ₄ Anions: Carbon Nitrogen Bond Formation. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	2

#	ARTICLE	IF	CITATIONS
12526	Tuning Intramolecular Stacking of Rigid Heteroaromatic Compounds for High-Efficiency Deep-Blue Through-Space Charge-Transfer Emission. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	29
12527	An Organic Laser Based on Thermally Activated Delayed Fluorescence with Aggregation-Induced Emission and Local Excited State Characteristics. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	15
12528	Identification of Ge-O Double Bonds in Planar MnGe ₃ O and MnGe ₄ O Clusters: Anion Photoelectron Spectroscopy and <i>Ab Initio</i> Calculations. <i>Inorganic Chemistry</i> , 2022, 61, 12570-12576.	1.9	2
12529	Diterpene glycosides, acetophenone glycosides and tannins from polar extracts of the root of <i>Euphorbia fischeriana</i> with cytotoxicity and antibacterial activities. <i>Phytochemistry</i> , 2022, 203, 113382.	1.4	6
12530	Assessing the Experimental Hydrogen Bonding Energy of the Cyclic Water Dimer Transition State with a Cyclooctatetraene-Based Molecular Balance. <i>Journal of the American Chemical Society</i> , 2022, 144, 16965-16973.	6.6	3
12531	Novel Strategy to fabricate Antiwrinkle Cotton fabrics with 1,2,3,4-Butanetetracarboxylic Acid under a Low Temperature. <i>ACS Omega</i> , 2022, 7, 30093-30103.	1.6	4
12532	In silico Drug Repurposing of Anticancer Drug 5-FU and Analogues Against SARS-CoV-2 Main Protease: Molecular Docking, Molecular Dynamics Simulation, Pharmacokinetics and Chemical Reactivity Studies. <i>Advances and Applications in Bioinformatics and Chemistry</i> , 0, Volume 15, 59-77.	1.6	4
12533	Functional Pyromellitic Diimide as a Corrosion Inhibitor for Galvanized Steel: An Atomic-Scale Engineering. <i>ACS Omega</i> , 2022, 7, 27116-27125.	1.6	1
12534	UV-Visible Absorption Spectra of Solvated Molecules by Quantum Chemical Machine Learning. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4891-4902.	2.3	6
12535	Dual electronic effects achieving a high-performance Ni(II) pincer catalyst for CO ₂ photoreduction in a noble-metal-free system. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	9
12536	Bridging 1D Inorganic and Organic Synthesis to Fabricate Ultrathin Bismuth-Based Nanotubes with Controllable Size as Anode Materials for Secondary Li Batteries. <i>Small</i> , 2022, 18, .	5.2	1
12537	H ₃ PO ₄ activated biochars derived from different agricultural biomasses for the removal of ciprofloxacin from aqueous solution. <i>Particuology</i> , 2023, 75, 217-227.	2.0	14
12538	Structural evolution and relative stability of vanadium-doped boron clusters. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 445302.	0.7	7
12539	Mechanistic aspects of the Pd(OAc) ₂ (N ₃) catalyzed ethylene acetoxylation: A density functional theory study. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	1.7	1
12540	Nanoscale Polyelectrolyte Complex Vesicles from Bioinspired Peptidomimetic Homopolymers with Zwitterionic Property and Extreme Stability. <i>Macromolecules</i> , 2022, 55, 9257-9268.	2.2	1
12541	Supramolecular structure and tautomerism of trifluoromethanesulfonamidines. <i>Structural Chemistry</i> , 2023, 34, 139-152.	1.0	3
12542	Density functional theory model of <i>LiS</i> electrochemical system with explicit solvation of lithium polysulfides by sulfolane. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	2
12543	Single-atom nanozymes catalytically surpassing naturally occurring enzymes as sustained stitching for brain trauma. <i>Nature Communications</i> , 2022, 13, .	5.8	72

#	ARTICLE	IF	CITATIONS
12544	Cucurbit[n]urils (n = 7, 8) can strongly bind neutral hydrophilic molecules in water. <i>Science China Chemistry</i> , 2022, 65, 1733-1740.	4.2	9
12545	A strategy to design nonlinear optical materials: Self-assembly by π - π stacking. <i>Journal of the Chinese Chemical Society</i> , 0, , .	0.8	0
12546	Pyridine-2(1H)-thione as a bifunctional nucleophile in reaction with PdII and PtII aryl isocyanide complexes. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	2
12547	NQO-1 Enzyme-Activated NIR Theranostic Agent for Pancreatic Cancer. <i>Analytical Chemistry</i> , 2022, 94, 11159-11167.	3.2	12
12548	Prediction of Peptide-Induced Silica Formation under a Wide pH Range by Molecular Descriptors. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, , 130030.	2.3	0
12549	Dibenzo[b,f][1,4,5]chalcogenadiazepine Photoswitches: Conversion of Excitation Energy into Ring Strain. <i>Angewandte Chemie</i> , 0, , .	1.6	0
12550	Direct and Water-Mediated Adsorption of Stabilizers on SERS-Active Colloidal Bimetallic Plasmonic Nanomaterials: Insight into Citrate-AuAg Interactions from DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5236-5251.	1.1	3
12551	Insights into Solid-To-Solid Transformation of MOF Amorphous Phases. <i>Inorganic Chemistry</i> , 2022, 61, 13992-14003.	1.9	10
12552	The First-Principle Study on Tuning Optical Properties of MA2Z4 by Cr Replacement of Mo Atoms in MoSi2N4. <i>Nanomaterials</i> , 2022, 12, 2822.	1.9	4
12553	Spirothienoquinoline-based acceptor molecular systems for organic solar cell applications: DFT investigation. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	0
12554	Comparative study of the hydrogen bonding properties between allyl-functionalized/non-functionalized ionic liquids and DMSO. <i>Vibrational Spectroscopy</i> , 2022, 122, 103412.	1.2	4
12555	Highly efficient CO2 conversion on a robust metal-organic framework Cu(I)-MFU-4l: Prediction and mechanistic understanding from DFT calculations. <i>Journal of CO2 Utilization</i> , 2022, 63, 102148.	3.3	1
12556	NHC-catalyzed [3+4] annulation between 2-dromoenal and aryl 1,2-diamine: Insights into mechanisms, chemo and stereoselectivities. <i>Molecular Catalysis</i> , 2022, 530, 112604.	1.0	1
12557	A comparative study of the potential energy surfaces of (CO)2, CO-CS and (CS)2. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113849.	1.1	2
12558	(\pm)-Ferulasin, unusual sesquiterpene chromones from <i>Ferula sinkiangensis</i> . <i>Tetrahedron</i> , 2022, 122, 132953.	1.0	5
12559	Construction of internal electric field in imprinted poly (ionic liquid)-TiO2 composite nanoreactor for improving hole directional enrichment and selective photodegradation. <i>Composites Science and Technology</i> , 2022, 228, 109657.	3.8	16
12560	Stereospecific synthesis of monofluoroalkenes and their deuterated analogues via Ag-catalyzed decarboxylation. <i>Journal of Catalysis</i> , 2022, 413, 1089-1097.	3.1	3
12561	Mechanism of 9,10-Dihydro-9-oxa-10-phosphaphenanthrene-10-oxide degradation in UV light-emitting diodes lamp driven sodium sulfite activation process. <i>Chemical Engineering Research and Design</i> , 2022, 165, 704-715.	2.7	5

#	ARTICLE	IF	CITATIONS
12562	Carbon diffusion-engineered carbon nitride nanosheets for high-efficiency photocatalytic solar-to-fuels conversion. <i>Renewable Energy</i> , 2022, 197, 943-952.	4.3	4
12563	Investigations of cysteine isomers using Terahertz and Raman spectroscopies. <i>Infrared Physics and Technology</i> , 2022, 125, 104299.	1.3	4
12564	Trapping of CO, CO ₂ , H ₂ S, NH ₃ , NO, NO ₂ , and SO ₂ by polyoxometalate compound. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113826.	1.1	38
12565	Theoretical investigation on the sensing mechanism of a fluorescent probe 3TBN for cyanide anion detection. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113837.	1.1	2
12566	An investigation on chain transfer to monomers and initiators, termination of radicals in EVA copolymerization process based on DFT and microkinetic simulation. <i>Polymer</i> , 2022, 256, 125181.	1.8	2
12567	Adsorption of glyphosate on graphene and functionalized graphenes: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113840.	1.1	0
12568	Theoretical study on paramagnetic amino carbon nanotube as fluorouracil drug delivery system. <i>Journal of Drug Delivery Science and Technology</i> , 2022, 75, 103670.	1.4	3
12569	Influence of suppressing additive malachite green on superconformal cobalt electrodeposition. <i>Journal of Electroanalytical Chemistry</i> , 2022, 921, 116696.	1.9	8
12570	Quantum chemical design of near-infrared retinal-based pigments and evaluating their vibronic/electronic properties. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113835.	1.1	0
12571	The conformational control of small D-A-D organic solar cells for large power conversion efficiency: A deep quantum chemistry analysis. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113831.	1.1	5
12572	Acylation of blueberry anthocyanins with fatty acids: Improvement of their lipid solubility and antioxidant activities. <i>Food Chemistry: X</i> , 2022, 15, 100420.	1.8	11
12573	Highly efficient removal of organic contaminant with wide concentration range by a novel self-cleaning hydrogel: Mechanism, degradation pathway and DFT calculation. <i>Journal of Hazardous Materials</i> , 2022, 440, 129738.	6.5	14
12574	An efficient strategy for designing high-performance DSSCs: Using the terminal auxiliary acceptor to improve electronic transitions. <i>Dyes and Pigments</i> , 2022, 206, 110642.	2.0	2
12575	Over 1000Ånm photoresponse with cyclopentadithiophene-based non-fullerene acceptors for efficient organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2022, 1216, 113852.	1.1	15
12576	Bromochlorodifluoromethane interaction with pristine and doped BN nanosheets: A DFT study. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108367.	3.3	13
12577	Experimental and computational investigation on Polyaniline/ZnO nanocomposite for dye adsorption. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2022, 284, 115895.	1.7	11
12578	Adsorption process and mechanisms of AEO-3/dodecane mixed collector on low-rank coal surface driven by water flow: A non-equilibrium molecular dynamics simulation study. <i>Journal of Molecular Liquids</i> , 2022, 364, 119993.	2.3	4
12579	Extraction separation of lithium isotopes with Bromobenzene-15-crown-5/ionic liquids system: Experimental and theoretical study. <i>Journal of Molecular Liquids</i> , 2022, 364, 120020.	2.3	8

#	ARTICLE	IF	CITATIONS
12580	Aluminium carbide nano-sheet as a promising adsorbent for removal of carbendazim. <i>Inorganic Chemistry Communication</i> , 2022, 144, 109844.	1.8	0
12581	Luminescence color tuning of the four-coordinate N-heterocyclic carbene (NHC) copper(I) complexes with imidazolylidene ligand functionalized by thiazole/benzoxazole moiety. <i>Journal of Organometallic Chemistry</i> , 2022, 977, 122469.	0.8	1
12582	Charge transport properties of SARS-CoV-2 Delta variant (B.1.617.2). <i>Process Biochemistry</i> , 2022, 121, 656-660.	1.8	1
12583	Density Functional Study of the adsorption behavior of 6-mercaptopurine on Primary, Si, Al and Ti doped C60 fullerenes. <i>Chemical Physics Letters</i> , 2022, 804, 139910.	1.2	5
12584	Lipophilic phenanthroline diamide ligands in 1-octanol for separation of Am(III) from Eu(III). <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108401.	3.3	10
12585	A novel amorphous porous biochar for adsorption of antibiotics: Adsorption mechanism analysis via experiment coupled with theoretical calculations. <i>Chemical Engineering Research and Design</i> , 2022, 186, 362-373.	2.7	13
12586	One-pot fabrication of petroleum pitch derived hierarchical porous carbon via a recyclable MgO-templating strategy for p-nitrophenol removal. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108458.	3.3	4
12587	The effects of biologically important divalent and trivalent metal cations on the cyclization step of dopamine autoxidation reaction: A quantum chemical study. <i>Arabian Journal of Chemistry</i> , 2022, 15, 104153.	2.3	4
12588	Exploiting proton masking to protect amino achieve efficient capture CO ₂ by amino-acids deep eutectic solvents. <i>Separation and Purification Technology</i> , 2022, 299, 121787.	3.9	9
12589	Elucidating photolysis mechanisms of ketamine by quantum chemical calculations. <i>Computational and Theoretical Chemistry</i> , 2022, 1216, 113845.	1.1	1
12590	Interaction of CO ₂ with TiO ₂ /reduced graphene oxide as superior catalysts: Dispersion-corrected density functional theory simulation. <i>Diamond and Related Materials</i> , 2022, 128, 109279.	1.8	1
12591	Theoretical insight into the degradation of diclofenac by hydroxyl and sulfate radicals in aqueous-phase: Mechanisms, kinetics and eco-toxicity. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108311.	3.3	6
12592	Electronic structure calculations of the fundamental interactions in solvent extraction desalination. <i>Journal of Molecular Liquids</i> , 2022, 364, 119986.	2.3	6
12593	Terpolymers and additional π - π -bridges regulations for improving fill factors in efficient organic solar cells. <i>Dyes and Pigments</i> , 2022, 206, 110609.	2.0	2
12594	Improving electric field strength of interfacial electric double layer and cycle stability of Li-ion battery via LiCl additive. <i>Electrochimica Acta</i> , 2022, 429, 141060.	2.6	3
12595	Computational examination on monomeric, dimeric, trimeric structural and vibrational interactions, AIM, Hirshfeld, IGM and oxygenated solvent effect on optical properties for pyridine N-oxide. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100660.	1.3	1
12596	Computational design of a chitosan derivative for improving the color stability of anthocyanins: Theoretical calculation and experimental verification. <i>International Journal of Biological Macromolecules</i> , 2022, 219, 721-729.	3.6	5
12597	The effect of collectors on froth stability of frother: Atomic-scale study by experiments and molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , 2022, 364, 120035.	2.3	5

#	ARTICLE	IF	CITATIONS
12598	Differences in intermolecular interactions between 4-hydroxycoumarin and 7-hydroxycoumarin studied by terahertz spectroscopy and density functional theory. <i>Chemical Physics</i> , 2022, 562, 111676.	0.9	2
12599	Surface functionalization of Si ₆ Li ₆ cluster with superalkalis to achieve high nonlinear optical response: A DFT study. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 653, 129985.	2.3	7
12600	Benzothiazolyldiazine azomethine derivatives for efficient corrosion inhibition of mild steel in acidic environment: Integrated experimental and density functional theory cum molecular dynamics simulation approach. <i>Journal of Molecular Liquids</i> , 2022, 364, 120033.	2.3	37
12601	Insights into behavior and mechanism of tetracycline adsorption on virgin and soil-exposed microplastics. <i>Journal of Hazardous Materials</i> , 2022, 440, 129770.	6.5	27
12602	Synchronous regulation of bulk and interfacial defects by an ionic liquid for efficient and stable perovskite solar cells. <i>Applied Surface Science</i> , 2022, 603, 154410.	3.1	12
12603	Megastigmane sesquiterpenoids from whole plants of <i>Viola kunawurensis</i> . <i>Phytochemistry</i> , 2022, 203, 113361.	1.4	4
12604	3-Nitrophthalonitrile solubility and solvation thermodynamics in aqueous solutions. <i>Journal of Chemical Thermodynamics</i> , 2022, 174, 106873.	1.0	2
12605	DFT-based modeling of polypyrrole/B ₁₂ N ₁₂ nanocomposite for the photocatalytic applications. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 170, 110949.	1.9	4
12606	Six pairs of phenylpropanoid enantiomers from <i>Cinnamomum mollifolium</i> . <i>Phytochemistry</i> , 2022, 203, 113348.	1.4	4
12607	Selective flotation of chalcopyrite from galena using a novel collector benzoic diethylcarbamothioic thioanhydride: An experimental and theoretical investigation. <i>Journal of Molecular Liquids</i> , 2022, 365, 120027.	2.3	6
12608	A silane-based coupling strategy for enhancing the mechanical properties of proanthocyanidin nano-coatings on Ti dental implants. <i>Applied Surface Science</i> , 2022, 602, 154400.	3.1	3
12609	In-situ formed nanoscale FeO for fenton-like oxidation of thermosetting unsaturated polyester resin composites: Nondestructively recycle carbon fiber. <i>Chemosphere</i> , 2022, 307, 135780.	4.2	1
12610	Insight into the cation-regulated mechanism for the hydration of propargyl alcohols catalyzed by [Bu ₄ P ⁺][Im ⁻]. <i>Journal of Molecular Liquids</i> , 2022, 365, 120021.	2.3	1
12611	Synergistic co-reaction of Zn ²⁺ and H ⁺ with carbonyl groups towards stable aqueous zinc-organic batteries. <i>Energy Storage Materials</i> , 2022, 52, 386-394.	9.5	31
12612	Nonlinear optical (NLO) response of boron phosphide nanosheet by alkali metals doping: A DFT study. <i>Materials Science in Semiconductor Processing</i> , 2022, 151, 107007.	1.9	16
12613	Effect of temperature on Electron-Phonon coupling of carotenoids by Two-Dimensional correlation resonance Raman spectroscopy. <i>Journal of Molecular Liquids</i> , 2022, 365, 120148.	2.3	0
12614	Theoretical prediction for growth behavior and electronic properties of monoanionic Ru ₂ Gen ⁻ (n=3-20) clusters. <i>Inorganica Chimica Acta</i> , 2022, 542, 121141.	1.2	1
12615	Quaternary ammonium salts targeted regulate the surface charge distribution of activated carbon: A study of their binding modes and modification effects. <i>Environmental Research</i> , 2022, 214, 114103.	3.7	7

#	ARTICLE	IF	CITATIONS
12616	Au ₁₂ @Au ₃₀ core-shell molecule: A stable l symmetry nanoparticle. <i>Physica B: Condensed Matter</i> , 2022, 645, 414246.	1.3	0
12617	Enhanced photocatalytic degradation of bisphenol A by a novel donor-acceptor g-C ₃ N ₄ : π - π interactions boosting the adsorption and electron transfer behaviors. <i>Separation and Purification Technology</i> , 2022, 300, 121947.	3.9	23
12618	Reevaluation of radical-induced differentiation in UV-based advanced oxidation processes (UV/hydrogen peroxide, UV/peroxydisulfate, and UV/chlorine) for metronidazole removal: Kinetics, mechanism, toxicity variation, and DFT studies. <i>Separation and Purification Technology</i> , 2022, 301, 121905.	3.9	14
12619	DFT insight into Cd ²⁺ , Hg ²⁺ , Pb ²⁺ , Sn ²⁺ , As ³⁺ , Sb ³⁺ , and Cr ³⁺ heavy metal ions adsorption onto surface of bowl-like B30 nanosheet. <i>Journal of Molecular Liquids</i> , 2022, 365, 120131.	2.3	19
12620	Excellent foaming properties of anionic-zwitterionic-Gemini cationic compound surfactants for gas well deliquification: Experimental and computational investigations. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 653, 129944.	2.3	6
12621	DFT study of super-halogen (Al ₇) doped carbon nitride (C ₂ N) and its nonlinear optical properties. <i>Journal of Molecular Structure</i> , 2022, 1270, 133910.	1.8	4
12622	Computational study of Pd-Cd bimetallic crystals: Spectroscopic properties, hirshfeld surface analysis, non-covalent interaction, and sensor activity. <i>Journal of Molecular Liquids</i> , 2022, 365, 120111.	2.3	23
12623	Colorimetric probing and fluorescent chemosensor features of functionalized sulphamide-azomethine derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 433, 114188.	2.0	6
12624	Revealing the non-covalent interactions between oxygen-containing demulsifiers and interfacially active asphaltenes: A multi-level computational simulation. <i>Fuel</i> , 2022, 329, 125375.	3.4	13
12625	Effect of molecular structure and ionization state on aggregation of carboxymethyl chitosan: A molecular dynamics study. <i>Carbohydrate Polymers</i> , 2022, 297, 119993.	5.1	7
12626	Experimental and computational analyses of the cocrystal of tetrahydrofuran-2,3,4,5-tetracarboxylic acid and urea. <i>Journal of Molecular Structure</i> , 2022, 1269, 133820.	1.8	2
12627	Direct Z-scheme Bi ₂ MoO ₆ /UiO-66-NH ₂ heterojunctions for enhanced photocatalytic degradation of ofloxacin and ciprofloxacin under visible light. <i>Applied Catalysis B: Environmental</i> , 2022, 318, 121820.	10.8	87
12628	Thermodynamic and density functional theory study the removal of different forms of gas arsenic by using aluminum nitride nanotube. <i>Fuel</i> , 2022, 329, 125395.	3.4	2
12629	Anomalous pressure-responsive emission enhancement of FCO-CzS due to molecular configuration and electronic structure changes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 283, 121723.	2.0	2
12630	A conjugated polymer with Electron-withdrawing cyano group enables for flexible asymmetric electrochromic supercapacitors. <i>Chemical Engineering Journal</i> , 2022, 450, 138386.	6.6	20
12631	Intensification of van der Waals interaction for efficient peroxymonosulfate activation and accuracy re-evaluation of quenching experiments for reactive oxidation species identification. <i>Chemical Engineering Journal</i> , 2022, 450, 138353.	6.6	13
12632	N-doped carbon intercalated Fe-doped MoS ₂ nanosheets with widened interlayer spacing: An efficient peroxymonosulfate activator for high-salinity organic wastewater treatment. <i>Journal of Colloid and Interface Science</i> , 2022, 628, 318-330.	5.0	17
12633	Synthesis, photophysical, electrochemical and computational investigation of dimethine and trimethine cyanine-based dyes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 433, 114189.	2.0	6

#	ARTICLE	IF	CITATIONS
12634	Theoretical study on photophysical properties of twisted D-A interaction TPA-BSM derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 433, 114191.	2.0	0
12635	Synthesis, characterization and theoretical calculations of four chiral schiff base materials for second harmonic generation applications. <i>Journal of Molecular Structure</i> , 2022, 1269, 133868.	1.8	2
12636	Boron induced strong metal-support interaction for high sintering resistance of Pt-based catalysts toward oxygen reduction reaction. <i>Applied Surface Science</i> , 2022, 604, 154466.	3.1	14
12637	A computational investigation about the effect of metal substitutions on the electronic spectra of porphyrin donors in the visible and near infrared regions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 282, 121676.	2.0	1
12638	Highly efficient electro-cocatalytic Fenton-like reactions for the degradation of recalcitrant naphthenic acids: Exploring reaction mechanisms and environmental implications. <i>Chemical Engineering Journal</i> , 2022, 450, 138331.	6.6	11
12639	Study the effect of zeolite pore size and acidity on the catalytic pyrolysis of Kraft lignin. <i>Fuel Processing Technology</i> , 2022, 237, 107467.	3.7	14
12640	Experimental and computational study on the inhibitory effect of phytic acid on U(VI) biomineralization by <i>Shewanella putrefaciens</i> . <i>Chemical Engineering Journal</i> , 2022, 450, 138364.	6.6	8
12641	Influence of the S-containing ligand on adsorption of platinum single atom on a carbon nanotube: A DFT study. <i>Journal of Molecular Structure</i> , 2022, 1270, 133850.	1.8	1
12642	Synthesis, structure elucidation, Hirshfeld surface analysis, energy frameworks and DFT studies of novel ethyl 2-(5-methyl-2-oxopyridin-N-yl)acetate (OPA). <i>Journal of Molecular Structure</i> , 2022, 1270, 133928.	1.8	5
12643	Rotational spectrum of anisole-CO ₂ : Cooperative C-H...O tetrel bond and C-H...O hydrogen bond. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 282, 121677.	2.0	4
12644	Fluorescent adenine analogues with ESPT characteristic utilized for real-time detecting DNA adduct. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 282, 121675.	2.0	3
12645	Synthesized thiazole-based hydrazides and their spectral characterization along with biological studies: Promising quantum chemical insights. <i>Journal of Molecular Structure</i> , 2022, 1270, 133923.	1.8	11
12646	A novel oxazole-based fluorescence sensor towards Ga ³⁺ and PPI for sequential determination and application. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 433, 114202.	2.0	4
12647	Terahertz spectral vibrational properties and weak interactions analysis of caffeic acid and ferulic acid. <i>Journal of Molecular Structure</i> , 2022, 1270, 133960.	1.8	2
12648	Experimental and theoretical study on the evolution of functional groups in cellulose char during oxidative pyrolysis. <i>Fuel</i> , 2022, 329, 125400.	3.4	4
12649	Photodegradation of dye using Polythiophene/ZnO nanocomposite: A computational approach. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 117, 108285.	1.3	14
12650	Synthesis, vibrational spectra, Hirshfeld surface analysis, DFT calculations, and in silico ADMET study of 3-(2-chloroethyl)-2,6-bis(4-fluorophenyl)piperidin-4-one: A potent anti-Alzheimer agent. <i>Journal of Molecular Structure</i> , 2022, 1269, 133845.	1.8	11
12651	Viscosity reduction mechanism of functionalized silica nanoparticles in heavy oil-water system. <i>Fuel Processing Technology</i> , 2022, 237, 107454.	3.7	12

#	ARTICLE	IF	CITATIONS
12652	An iron chlorophyll derivative for enhanced degradation of bisphenol A: New insight into the generation mechanism of high-valent iron oxo species. <i>Chemical Engineering Journal</i> , 2023, 451, 138688.	6.6	5
12653	Promoting charge migration of Co(OH) ₂ /g-C ₃ N ₄ by hydroxylation for improved PMS activation: Catalyst design, DFT calculation and mechanism analysis. <i>Chemical Engineering Journal</i> , 2023, 451, 138503.	6.6	29
12654	Insights into CQDs-doped perylene diimide photocatalysts for the degradation of naproxen. <i>Chemical Engineering Journal</i> , 2023, 451, 138571.	6.6	15
12655	Application of experiments and density function theory on the formation mechanism of NH ₃ during O ₂ /Ar and O ₂ /H ₂ O combustion process of demineralized coals. <i>Fuel</i> , 2023, 331, 125730.	3.4	9
12656	Separation of anthracene and carbazole from crude anthracene via imidazolium-based ionic liquids. <i>Fuel</i> , 2023, 331, 125704.	3.4	7
12657	Degradation of three typical hydroxamic acids collectors via UVA-B activated H ₂ O ₂ and persulfate: Kinetics, transformation pathway, DFT calculation and toxicity evaluation. <i>Chemical Engineering Journal</i> , 2023, 451, 138639.	6.6	17
12658	Structural characterization of ((9-fluorenylidene) (ferrocenyl)methyl)palladium iodide as the catalytic intermediate in the synthesis of 9-(ferrocenyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 497 Td ((ferrocenylethyl)methylene)-9<i>i>	6.6	17
12659	Highly Durable and Ultrafast Cycling of Dual- Li^+ Ion Batteries via In Situ Construction of Cathode-Electrolyte Interphase. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	18
12660	Pd-Catalyzed MIA-Directed Acetoxylation of Benzylamines and Computational Study. <i>European Journal of Organic Chemistry</i> , 2022, 2022, .	1.2	2
12662	Topological Analysis of Functions on Arbitrary Grids: Applications to Quantum Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 6077-6091.	2.3	2
12663	Unexpected Pyridinyl Group-Mediated Metal-Free Wacker-Type Oxidation en Route to Pyrido[2,1-a]isoindol-5-ium Salts. <i>Synthesis</i> , 0, , .	1.2	0
12664	Structure and bonding of proximity-enforced main-group dimers stabilized by a rigid naphthyridine diimine ligand. <i>Journal of Computational Chemistry</i> , 2023, 44, 456-467.	1.5	1
12665	Density Functional Theory Study of the Regioselectivity in Copolymerization of bis-Styrenic Molecules with Propylene Using Zirconocene Catalyst. <i>Catalysts</i> , 2022, 12, 1039.	1.6	3
12666	Aggregation-Dependent Circularly Polarized Luminescence and Thermally Activated Delayed Fluorescence from Chiral Carbene-Cu ^I -Amide Enantiomers. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	15
12667	A comparison of hydrogen abstraction reaction between allyl-type monomers with thioxanthone-based photoinitiators without amine synergists. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	0
12668	Insights into the Kinetics, Theoretical Model and Mechanism of Free Radical Synergistic Degradation of Micropollutants in UV/Peroxydisulfate Process. <i>Water (Switzerland)</i> , 2022, 14, 2811.	1.2	1
12669	Encapsulated layer induces boundary effect and twist angle adjust absorption in h-BN/graphene/h-BN heterostructure. <i>Materials Research Express</i> , 2022, 9, 095004.	0.8	0
12670	Theoretical study of the Meisenheimer and charge-transfer complexes formed upon colorimetric determination of nitroaromatic explosives. <i>FirePhysChem</i> , 2022, , .	1.5	1

#	ARTICLE	IF	CITATIONS
12671	A Cephalosporin-Tripodalamine Conjugate Inhibits Metallo- β -Lactamase with High Efficacy and Low Toxicity. <i>Antimicrobial Agents and Chemotherapy</i> , 2022, 66, .	1.4	2
12672	Thermodynamics and Spectroscopy of Halogen- and Hydrogen-Bonded Complexes of Haloforms with Aromatic and Aliphatic Amines. <i>Molecules</i> , 2022, 27, 6124.	1.7	2
12673	Six-component synthesis and biological activity of novel spiropyridoindolepyrrolidine derivatives: A combined experimental and theoretical investigation. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	1
12674	Hydrogen Bond Effects: A Strategy for Improving Controllability in Organocatalytic Photoinduced Controlled Radical Polymerization Targeting High Molecular Weight. <i>ACS Catalysis</i> , 2022, 12, 11606-11614.	5.5	5
12675	Benzothiadiazole-Based Green Hybridized Local and Charge-Transfer (HLCT) Fluorophores as Solution-Processed Non-Doped Emitters for Simple Structured Electroluminescent Devices. <i>ChemPhotoChem</i> , 2022, 6, .	1.5	1
12676	New insight of Fe valence state change using leaves-A combined experimental and theoretical study. <i>Chinese Physics Letters</i> , 0, , .	1.3	0
12677	Effects of intermolecular interactions and solvent properties on the solid-liquid phase equilibrium of isosorbide 5-mononitrate. <i>Journal of Molecular Liquids</i> , 2022, 364, 119974.	2.3	3
12678	Theoretical study the mechanism of ESIPT process for pyridine-hydrazone-substituted naphthalimide receptor 4a-E. <i>Chemical Physics Letters</i> , 2022, 805, 139933.	1.2	0
12679	Synthesis, single crystal (XRD), spectral characterization, computational (DFT), quantum chemical modelling and anticancer activity of di(p-bromobenzyl) (dibromo) (1, 10-phenanthroline) tin (IV) complex. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100714.	1.3	9
12680	Effect of caffeic acid esters on antioxidant activity and oxidative stability of sunflower oil: Molecular simulation and experiments. <i>Food Research International</i> , 2022, 160, 111760.	2.9	7
12681	Acid-triggered polyether sulfone - Polyvinyl pyrrolidone blend anion exchange membranes for the recovery of titania waste acid via diffusion dialysis. <i>Journal of Membrane Science</i> , 2022, 662, 120980.	4.1	6
12682	Favipiravir attachment to a conical nanocarbon: DFT assessments of the drug delivery approach. <i>Computational and Theoretical Chemistry</i> , 2022, 1216, 113866.	1.1	9
12683	Spectroscopic, Computational(DFT), Quantum mechanical studies and protein-ligand interaction of Schiff base 6,6-((1,2-phenylenebis(azaneylylidene))bis(methaneylylidene))bis(2-methoxyphenol) from o-phenylenediamine and 3- methoxysalicylaldehyde. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100713.	1.3	27
12684	FexN produced in pharmaceutical sludge biochar by endogenous Fe and exogenous N doping to enhance peroxymonosulfate activation for levofloxacin degradation. <i>Water Research</i> , 2022, 224, 119022.	5.3	51
12685	Novel adamantane substituted polythiophenes as competitors to Poly(3-Hexylthiophene). <i>Polymer</i> , 2022, 258, 125274.	1.8	0
12686	Synthesis, spectral, computational, wavefunction and molecular docking studies of 4-((thiophene-2-ylmethylene)amino)benzenesulfonamide from sulfanilamide and thiophene-2-carbaldehyde. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100718.	1.3	16
12687	Simultaneous removal of tetracycline and arsenic(III) using copper-manganese composite oxide: Competition behaviors and removal mechanisms. <i>Journal of Water Process Engineering</i> , 2022, 49, 103117.	2.6	3
12688	Discharge Mechanism Difference Analysis Between Natural Ester and Mineral Oil Under Impulse Electric Field: A DFT Investigation. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2022, 29, 1803-1810.	1.8	7

#	ARTICLE	IF	CITATIONS
12689	Structures of Streptococcus pyogenes class A sortase in complex with substrate and product mimics provide key details of target recognition. <i>Journal of Biological Chemistry</i> , 2022, 298, 102446.	1.6	8
12690	Application of QSAR for investigation on coagulation mechanisms of textile wastewater. <i>Ecotoxicology and Environmental Safety</i> , 2022, 244, 114035.	2.9	5
12691	Nitrogen and oxygen-codoped microporous carbon derived from acid-base interaction of carboxylic acid polymers and urea for enhanced CO ₂ capture. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108526.	3.3	4
12692	Experimental and DFT investigation on the role of aromaticity on the stability of hydrogen bonded complexes of cyclohexanone with amines and hydroxyl compounds. <i>Journal of Molecular Liquids</i> , 2022, 366, 120221.	2.3	1
12693	Catalytic effects on decomposition of formic acid in the atmosphere – A kinetic and thermochemical investigation. <i>Chemical Physics Letters</i> , 2022, 806, 140038.	1.2	0
12694	Evaluating the photoelectric performance of D- π -A dyes with different π -conjugated bridges for DSSCs. <i>Chemical Physics Letters</i> , 2022, 806, 140035.	1.2	6
12695	Hierarchically structural layered double oxides with stretchable nanopores for highly effective removal of protein-bound uremic toxins. <i>Separation and Purification Technology</i> , 2022, 301, 122033.	3.9	9
12696	Molecular insights into the CO ₂ separation mechanism of GO supported deep eutectic solvent membrane. <i>Journal of Molecular Liquids</i> , 2022, 366, 120248.	2.3	6
12697	Hydrothermal and photocatalytic synergistic pretreatment to improve the full utilization of corn stalk. <i>Bioresource Technology</i> , 2022, 363, 127989.	4.8	7
12698	Investigation of atropisomeric transformation of a novel PDE4 inhibitor with tetrahydroisoquinoline-based amide group and its primary study of binding to HSA. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2022, 221, 115056.	1.4	0
12699	Theoretical study and molecular design of thermally activated delayed fluorescence molecules based on intramolecular-locked strategy. <i>Journal of Luminescence</i> , 2022, 251, 119263.	1.5	6
12700	A theoretical study of CO ₂ capture by highly hydrophobic type III deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2022, 366, 120285.	2.3	7
12701	On the influence of pnictogen bonding on acidity. <i>Polyhedron</i> , 2022, 227, 116145.	1.0	2
12702	Modulating the ESIPT dynamics of 3HF derivatives via substitution and solvent effect: A theoretical study. <i>Journal of Molecular Liquids</i> , 2022, 366, 120295.	2.3	6
12703	Analysis of solid-liquid equilibrium behavior of highly water-soluble beet herbicide metamitron in thirteen pure solvents using experiments and molecular simulations. <i>Journal of Molecular Liquids</i> , 2022, 366, 120121.	2.3	7
12704	A combined QTAIM, DFT and molecular dynamics study on the nanoscale dynamical and structural organization of imidazolium-based dicationic ionic liquids. <i>Journal of Molecular Liquids</i> , 2022, 365, 120186.	2.3	4
12705	Functionalization of poly(glycidylmethacrylate) with iminodiacetate and imino phosphonate groups for enhanced sorption of neodymium - sorption performance and molecular modeling. <i>Reactive and Functional Polymers</i> , 2022, 180, 105389.	2.0	5
12706	Thermally activated delayed fluorescence materials based on acridin-9(10H)-one acceptor for organic light-emitting diodes. <i>Dyes and Pigments</i> , 2022, 207, 110701.	2.0	4

#	ARTICLE	IF	CITATIONS
12707	Carbazole and triazine-based bipolar hosts with extremely low efficiency roll-offs for green PhOLEDs. <i>Dyes and Pigments</i> , 2022, 207, 110727.	2.0	2
12708	DFT molecular modeling of A2-D-A1-D-A2 type DF-PCIC based small molecules acceptors for organic photovoltaic cells. <i>Chemical Physics Letters</i> , 2022, 806, 140026.	1.2	17
12709	Experimental and DFT studies of 2-methyl-quinoxaline and its silver (I) complex: Non-covalent interaction analysis, antimicrobial activity and molecular docking study. <i>Inorganic Chemistry Communication</i> , 2022, 145, 109935.	1.8	6
12710	Mechanism study of ternary deep eutectic solvents with protonic acid for lignin fractionation. <i>Bioresource Technology</i> , 2022, 363, 127887.	4.8	15
12711	The chemistry of Fe-N,S -chelated Ru(II) complexes with 1,4-diethynylbenzene. <i>Polyhedron</i> , 2022, 227, 116120.	1.0	2
12712	Theoretical insight and molecular recognition of oxatub[4]arene-based organic macrocycle as a supramolecular host for antipsychotic drug risperidone. <i>Journal of Molecular Liquids</i> , 2022, 366, 120195.	2.3	2
12713	The Alkaline-earthides based parallel-stacked dimer and trimer of Janus face $\text{C}_6\text{H}_6\text{F}_6$ showing extremely large nonlinear optical responses. <i>Polyhedron</i> , 2022, 227, 116119.	1.0	6
12714	Molecular dynamics simulation of CO_2 hydrate growth in salt water. <i>Journal of Molecular Liquids</i> , 2022, 366, 120237.	2.3	10
12715	The molecular structure, spectroscopic properties and partition functions of $\text{C}_3\text{H}_2\text{S}$ isomers: An ab initio study. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113877.	1.1	1
12716	Nitrate promoted defluorination of perfluorooctanoic acid in UV/sulfite system: Coupling hydrated electron/reactive nitrogen species-mediated reduction and oxidation. <i>Environmental Pollution</i> , 2022, 313, 120172.	3.7	8
12717	A Gd^{3+} -doped blue TiO_2 nanotube array anode for efficient electrocatalytic degradation of iohexol. <i>Separation and Purification Technology</i> , 2022, 301, 122007.	3.9	4
12718	Specific recognition and solid phase extraction of three primary aromatic amines based on molecularly imprinted polymer monolith for the migration detection in food contact materials. <i>Microchemical Journal</i> , 2022, 182, 107895.	2.3	3
12719	Design of novel dual functional ionic liquids and DFT study on their CO_2 absorption mechanism. <i>Journal of Molecular Liquids</i> , 2022, 366, 120340.	2.3	4
12720	Study on the activation mechanism of protactinium and NH_3 by density functional theory. <i>Chemical Physics Letters</i> , 2022, 806, 140072.	1.2	0
12721	Enhanced active corrosion protection coatings for aluminum alloys with two corrosion inhibitors co-incorporated in nanocontainers. <i>Corrosion Science</i> , 2022, 208, 110663.	3.0	24
12722	Cooperation of multiple active species generated in hydrogen peroxide activation by iron porphyrin for phenolic pollutants degradation. <i>Environmental Pollution</i> , 2022, 313, 120097.	3.7	11
12723	Computational study of toxic gas removal. <i>Journal of Molecular Liquids</i> , 2022, 365, 120213.	2.3	22
12724	Relationship between cellulolytic enzyme lignin structural and lignin nanoparticle-polyvinyl alcohol membrane property: Insights from monolignols and molecular dynamics simulations. <i>Industrial Crops and Products</i> , 2022, 188, 115673.	2.5	3

#	ARTICLE	IF	CITATIONS
12725	Insight into the anti-corrosion behavior of Reineckia Carnea leaves extract as an eco-friendly and high-efficiency corrosion inhibitor. <i>Industrial Crops and Products</i> , 2022, 188, 115640.	2.5	23
12726	Acetate improves catalytic performance for rapid removal of Cr(VI) by sodium borohydride in aqueous environments. <i>Separation and Purification Technology</i> , 2022, 301, 122051.	3.9	5
12727	Molecular modeling of the photovoltaic properties of amino naphthalene and N-alkylated-isoquinoline dye. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100739.	1.3	12
12728	Transesterification reactive extractive distillation process using ionic liquids as entrainers: From molecular insights to process integration. <i>Separation and Purification Technology</i> , 2022, 301, 122002.	3.9	11
12729	A separation strategy of Au(III), Pd(II) and Pt(IV) based on hydrophobic deep eutectic solvent from hydrochloric acid media. <i>Journal of Molecular Liquids</i> , 2022, 365, 120200.	2.3	11
12730	Theoretical investigation on the structure and physicochemical properties of choline chloride-based deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2022, 366, 120243.	2.3	7
12731	Experimental and theoretical insight into the transformation behaviors and risk assessment of Flutamide in UV/O ₃ /PMS system. <i>Journal of Cleaner Production</i> , 2022, 375, 134167.	4.6	7
12732	Spectroscopic studies of 5-fluoro-1H-pyrimidine-2,4-dione adsorption on nanorings, solvent effects and SERS analysis. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113873.	1.1	2
12733	Photo- and electro-luminescent properties of difluoroboron complexes based on the carbazole-functionalized 2-(benzo[d]thiazol-2-yl)phenol ligands. <i>Dyes and Pigments</i> , 2022, 207, 110738.	2.0	1
12734	Spectral (FT-IR, FT-Raman, NMR, UV-vis), electronic structure (DFT, TD-DFT), and molecular docking investigations on 1-((1H-benzo[d]imidazol-1-yl)methyl)urea – A bioactive Mannich base system. <i>Chemical Physics Letters</i> , 2022, 806, 140047.	1.2	5
12735	Nonlinear optical properties of benzanthrone derivatives with N'-methylpiperazin-1-yl and N'-phenylpiperazin-1-yl substituents: Experimental and quantum chemical study. <i>Optics and Laser Technology</i> , 2022, 156, 108616.	2.2	4
12736	A green and facile strategy to enhance thermal stability and flame retardancy of unidirectional flax fabric based on fully bio-based system. <i>Industrial Crops and Products</i> , 2022, 188, 115610.	2.5	5
12737	Investigation of solid-liquid equilibrium and thermodynamic models of D-Tagatose in mono-solvents and binary solvents. <i>Chemical Thermodynamics and Thermal Analysis</i> , 2022, 8, 100084.	0.7	0
12738	Regenerable neodymium-doped zirconium-based MOF adsorbents for the effective removal of phosphate from water. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108610.	3.3	19
12739	Effects of substituent and excess electron attachment on proton transfer between the radiosensitizer base pairs in aqueous solution. <i>Journal of Molecular Liquids</i> , 2022, 366, 120216.	2.3	3
12740	Research on dissolution behavior of N-hydroxyphthalimide in three binary solvents: Measurement, modeling, molecular simulation and thermodynamics. <i>Journal of Molecular Liquids</i> , 2022, 365, 120190.	2.3	3
12741	Effects of environmental factors on the fleroxacin photodegradation with the identification of reaction pathways. <i>Chemosphere</i> , 2022, 308, 136373.	4.2	2
12742	Theoretical insight and experimental exploration of designing biocompatible functionalized ionic liquids for efficient separation of typical organic Lewis acid compound indole from coal-based fuel pyrolysis product. <i>Journal of Molecular Liquids</i> , 2022, 367, 120439.	2.3	7

#	ARTICLE	IF	CITATIONS
12743	Investigation of the adsorption of a DNA based purine derivative on N/B-doped coronene and coronene by means of DFT and NCI interaction analysis. <i>Journal of Molecular Liquids</i> , 2022, 367, 120373.	2.3	12
12744	Effect of oligothiophene spacer length on photogenerated charge transfer from perylene diimide to boron-doped diamond electrodes. <i>Solar Energy Materials and Solar Cells</i> , 2022, 248, 111984.	3.0	2
12745	Achieving simultaneous hydrogen evolution and organic pollutants degradation through the modification of Ag ₃ PO ₄ using Cs ₂ AgBiBr ₆ quantum dots and graphene hydrogel. <i>Separation and Purification Technology</i> , 2022, 302, 122079.	3.9	3
12746	Designing and theoretical characterization of D- π -A ₁ - π -A ₂ typed organic small molecule donor materials. <i>Materials Science in Semiconductor Processing</i> , 2022, 152, 107097.	1.9	3
12747	Human hair rich in pyridinic nitrogen-base DNA biosensor for direct electrochemical monitoring of palbociclib-DNA interaction. <i>Bioelectrochemistry</i> , 2022, 148, 108264.	2.4	8
12748	Size-controllable crown ether-embedded 2D nanosheets for the host-guest ion segregation and recovery: Insights from DFT simulations. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 171, 110983.	1.9	6
12749	A rare class of multiply bonded trigonal-planar pnictogen complexes: Rational syntheses, versatile reactivities, and unique semiconducting properties. <i>Inorganica Chimica Acta</i> , 2022, 543, 121202.	1.2	1
12750	Reaction of the thallium(I) cation with [2.2]paracyclophane: Experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2022, 543, 121205.	1.2	1
12751	Comparative study on the deep eutectic solvents formed by choline chloride and cresol isomers from theoretical and experimental perspectives. <i>Journal of Molecular Liquids</i> , 2022, 367, 120420.	2.3	9
12752	Selective hydroconversion of 5-hydroxymethylfurfural to 2,5-bis(hydroxymethyl)furan using carbon nanotubes-supported nickel catalysts. <i>Carbon Resources Conversion</i> , 2022, 5, 289-298.	3.2	7
12753	Physicochemical characteristics of three-phase products of low-rank coal by hydrothermal carbonization: experimental research and quantum chemical calculation. <i>Energy</i> , 2022, 261, 125347.	4.5	9
12754	Fluorescent probe disclosing hydroxyl radical generation in mitochondria and nucleoli of cells during ferroptosis. <i>Sensors and Actuators B: Chemical</i> , 2022, 373, 132707.	4.0	10
12755	Photochemical reactions of dinuclear organometallic complexes with diphenyl dichalcogenides. <i>Journal of Organometallic Chemistry</i> , 2022, 982, 122517.	0.8	0
12756	Improved properties of 3d transition metal nanoclusters deposited on defective hexagonal boron nitride quantum dots. <i>Materials Today Communications</i> , 2022, 33, 104466.	0.9	0
12757	Radical-induced pyrolysis mechanism in C=O and C=Cal bond cleavage. <i>Fuel Processing Technology</i> , 2022, 238, 107494.	3.7	4
12758	Antibacterial Z-scheme ZnIn ₂ S ₄ /Ag ₂ MoO ₄ composite photocatalytic nanofibers with enhanced photocatalytic performance under visible light. <i>Chemosphere</i> , 2022, 308, 136386.	4.2	14
12759	Transdermal release behaviors of bioactive deep eutectic solvents as natural skin care and mechanism. <i>Journal of Molecular Liquids</i> , 2022, 367, 120412.	2.3	1
12760	Solvent extraction for lithium isotope separation by 4-NO ₂ -B15C5/[BMIm][NTf ₂] system. <i>Journal of Molecular Liquids</i> , 2022, 367, 120357.	2.3	12

#	ARTICLE	IF	CITATIONS
12761	Assessing p-tolyloxy-1,3,4-oxadiazole acetamides as lipoxygenase inhibitors assisted by in vitro and in silico studies. <i>Bioorganic Chemistry</i> , 2022, 129, 106144.	2.0	6
12762	5,6-Biheterocyclic pentazole salts as promising energetic materials: a new design strategy. <i>Materials Today Communications</i> , 2022, 33, 104379.	0.9	1
12763	Unveiling the molecular mechanism of spiropyran-based receptors toward cyanide sensing: A theoretical study. <i>Materials Today Communications</i> , 2022, 33, 104346.	0.9	0
12764	Electrostatic potential of the incorporated asymmetry molecules induced high charge separation efficiency of the modified carbon nitride copolymers. <i>Applied Catalysis B: Environmental</i> , 2022, 319, 121922.	10.8	15
12765	Enhancement of ultrafast nonlinear absorption by different substituted positions in pyrene-containing twistacenes isomers. <i>Optics and Laser Technology</i> , 2022, 156, 108563.	2.2	0
12766	Broad-specificity antibody profiled by hapten prediction and its application in immunoassay for fipronil and major metabolites. <i>Journal of Hazardous Materials</i> , 2023, 441, 129931.	6.5	12
12767	Rational design of near-infrared ratiometric fluorescent probes for real-time tracking of β -galactosidase in vivo. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 285, 121879.	2.0	3
12768	Enhancement of perovskites performance for coal tar decomposition by pore structure and acid-base modification. <i>Fuel</i> , 2023, 331, 125654.	3.4	6
12769	Regulation of defects and nitrogen species on carbon nanotube by plasma-etching for peroxydisulfate activation: Inducing non-radical/radical oxidation of organic contaminants. <i>Journal of Hazardous Materials</i> , 2023, 441, 129905.	6.5	23
12770	Enhanced photodegradation of tylosin in the presence of natural montmorillonite: Synergistic effects of adsorption and surface hydroxyl radicals. <i>Science of the Total Environment</i> , 2023, 855, 158750.	3.9	4
12771	Revealing the activity origin of oxygen-doped amorphous carbon material for SO ₂ catalytic oxidation: A descriptor considering dynamic electron transfer during O ₂ activation. <i>Carbon</i> , 2023, 201, 37-48.	5.4	11
12772	Study on oxidation characteristics and conversion of sulfur-containing model compounds in coal. <i>Fuel</i> , 2023, 331, 125756.	3.4	6
12773	Ammonium benzenesulfonate as an electrolyte additive to relieve the irreversible accumulation of lithium sulfide for high-energy density lithium-sulfur battery. <i>Journal of Colloid and Interface Science</i> , 2023, 629, 368-376.	5.0	9
12774	X-ray diffraction, IR spectrum, optical properties, AIM, NBO, RDC, HS, Fukui function, biological and molecular docking analysis of a novel hybrid compound (C ₉ H ₁₅ N ₃)[CuCl ₄ (H ₂ O)]. <i>Journal of Molecular Structure</i> , 2023, 1271, 134094.	1.8	6
12775	Theoretical insight on the saturated stimulated emission intensity of a squaraine dye for STED nanoscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 284, 121793.	2.0	2
12776	Exergy, economic, and exergoenvironmental analyses of new combined heat and power process based on mechanism analysis of working fluid screening. <i>Energy</i> , 2023, 262, 125308.	4.5	2
12777	Synthesis, structural characterization, DNA interaction, dye adsorption properties and theoretical studies of copper (II) carboxylates. <i>Journal of Molecular Structure</i> , 2023, 1272, 134104.	1.8	4
12778	Morphology constraint of β -HMX in polymeric carbon nitrides towards hybrid energetic materials. <i>Chemical Engineering Journal</i> , 2023, 452, 138981.	6.6	7

#	ARTICLE	IF	CITATIONS
12779	Solvent controlled excited state intramolecular proton transfer (ESIPT) behavior and luminescent property of a novel phthalimide-based fluorophore: A TD-DFT Study. <i>Journal of Molecular Structure</i> , 2023, 1272, 134123.	1.8	5
12780	Persistent free radicals on carbon nanotubes and their catalytic effect on benzoyl peroxide decomposition. <i>Carbon</i> , 2023, 201, 473-482.	5.4	3
12781	Self-crystallization behavior of paraffin and the mechanism study of SiO ₂ nanoparticles affecting paraffin crystallization. <i>Chemical Engineering Journal</i> , 2023, 452, 139287.	6.6	5
12782	Sensing cyclosarin (a chemical warfare agent) by Cucurbit[n]urils: A DFT/TD-DFT study. <i>Journal of Molecular Structure</i> , 2023, 1272, 134163.	1.8	0
12783	Theoretical perspective for substitution effect on luminescent properties of through space charge transfer-based thermally activated delayed fluorescence molecules. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 285, 121899.	2.0	7
12784	Comprehending of florfenicol (form A) dissolution behavior in aqueous low alcohol blends: Solubility, solvation thermodynamics as well as inter-molecular interactions. <i>Journal of Chemical Thermodynamics</i> , 2023, 176, 106925.	1.0	4
12785	Structural insights, spectral, fluorescence, Z-scan, C-H⋯O/N-H⋯O hydrogen bonding and AIM, RDG, ELF, LOL, FUKUI analysis, NLO activity of N-2(Methoxy phenyl) acetamide. <i>Journal of Molecular Structure</i> , 2023, 1272, 134140.	1.8	27
12786	Multi-function hollow nanorod as an efficient sulfur host accelerates sulfur redox reactions for high-performance Li-S batteries. <i>Journal of Colloid and Interface Science</i> , 2023, 629, 65-75.	5.0	8
12787	Stereospecific redox-mediated clusterization reconstruction for constructing long-lived, color-tunable, and processable phosphorescence cellulose. <i>Chemical Engineering Journal</i> , 2023, 451, 138923.	6.6	16
12788	Study on ionic association behavior in sodium nitrate solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 285, 121888.	2.0	1
12789	Comparative study of the cocrystals with layered/cavity structure in regulating in vitro pharmaceutical properties of diuretic acetazolamide. <i>Journal of Molecular Structure</i> , 2023, 1271, 134035.	1.8	0
12790	Cyclo[18]carbonâ€A new class of electron acceptor for organic solar cells applications. <i>Journal of Molecular Structure</i> , 2023, 1271, 134025.	1.8	4
12791	Establishing a high-speed electron transfer channel via CuS/MIL-Fe heterojunction catalyst for photo-Fenton degradation of acetaminophen. <i>Applied Catalysis B: Environmental</i> , 2023, 320, 121979.	10.8	41
12792	From small molecules to solid-state materials: A brief discourse on an example of carbon compounds. , 2023, , 93-115.		1
12793	Experimental and theoretical study of the physicochemical properties of the novel imidazole-based eutectic solvent. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 118, 108319.	1.3	3
12794	Study on the mechanism of free radical scavenger TEMPO blocking in coal oxidation chain reaction. <i>Fuel</i> , 2023, 331, 125853.	3.4	12
12795	The Molecular Nature of the Eliminating Azeotrope in Extractive Distillation by Ionic Liquid Entrainer. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12796	Mechanistic study of the bismuth mediated fluorination of arylboronic esters and further rational design. <i>RSC Advances</i> , 2022, 12, 24208-24216.	1.7	2

#	ARTICLE	IF	CITATIONS
12797	Spin engineering of triangulenes and application for nano nonlinear optical materials design. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18529-18542.	1.3	6
12798	The role of halogen bonds in the catalytic mechanism of the iso-Nazarov cyclization reaction: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18877-18887.	1.3	4
12799	Heterovalent chalcogen bonding: supramolecular assembly driven by the occurrence of a tellurium(Te^{II}) $\cdots\text{Ch}^{\text{I}}$ (Ch = S, Se, Te) linkage. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 5635-5644.	3.0	5
12800	Adsorption Sites and Electron Transfer Characteristics of Methyl Orange on Three-Dimensional Hierarchical Flower-Like Nanostructures of Co-Al-Layered Double Hydroxides: Experimental and Dft Investigation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12801	The role of phosphoric acid in the crystallization of lenalidomide form DMSO-water system. <i>CrystEngComm</i> , 2022, 24, 6357-6366.	1.3	0
12802	Strong Be \cdots Be bonds in double-aromatic bridged Be ₂ (η^4 -SO) molecules. <i>Dalton Transactions</i> , 2022, 51, 12596-12603.	1.6	5
12803	Molecular recognition and spectral tuning of organic dyes in water by amide naphthotubes. <i>Chemical Communications</i> , 2022, 58, 9413-9416.	2.2	6
12804	Deciphering the Cooperative Effect of Base and N-Substituents on the Origin of Regioselectivity Switching for Mannich Reactions of Glycinate by Carbonyl Catalysts. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12805	Insights of Adsorption and Dissociation of Hydrogen on Ni Doped Mg ₄ Clusters: A Dft Study. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12806	Unveiling the Effect of Solvent Polarity on the Excited State Intramolecular Proton Transfer and Hydrogen Bond Mechanisms of Dhp. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12807	Lanthanide/actinide boride nanoclusters and nanomaterials based on boron frameworks consisting of conjoined B _n rings ($n = 7-9$). <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 21078-21084.	1.3	1
12808	Study on the Mechanism of Free Radical Trapping Agent Tempo Blocking in Coal Oxidation Chain Reaction. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12809	DFT studies of electronic and nonlinear optical properties of a novel class of excess electron compounds based on multi-alkali metal atoms-doped Janus face C ₁₃ H ₁₀ F ₁₂ . <i>New Journal of Chemistry</i> , 2022, 46, 15334-15343.	1.4	3
12810	DFT studies on rhodium(Rh^{III})-catalyzed synthesis of indanones from <i>N</i> -methoxybenzamides via C-H activation reaction. <i>New Journal of Chemistry</i> , 2022, 46, 16576-16583.	1.4	0
12811	Recognition and mechanistic investigation of anion sensing by ruthenium(Ru^{II}) arene complexes and bio-imaging application. <i>Dalton Transactions</i> , 2022, 51, 13071-13084.	1.6	5
12812	The role of conformational dynamics in the activity of polymer-conjugated CalB in organic solvents. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 22028-22037.	1.3	1
12813	Tuning ESIPT-coupled luminescence by expanding π -conjugation of a proton acceptor moiety in ESIPT-capable zinc(Zn^{II}) complexes with 1-hydroxy-1 <i>H</i> -imidazole-based ligands. <i>Dalton Transactions</i> , 2022, 51, 15166-15188.	1.6	11
12814	Hydroboration of carbon dioxide with pinacolborane catalyzed by various aluminum hydrides: a comparative mechanistic study. <i>Catalysis Science and Technology</i> , 2022, 12, 6129-6141.	2.1	2

#	ARTICLE	IF	CITATIONS
12815	Synthesis and reactivity of dinuclear copper(<i>scp</i>) pyridine diimine complexes. Dalton Transactions, 2022, 51, 13396-13404.	1.6	2
12816	Fumarato and phthalato bridged dinuclear metal-organic Cu(<i>scp</i>) and Mn(<i>scp</i>) compounds involving infinite fumarate-water assemblies and unusual structure-guiding H-bonded synthons: antiproliferative evaluation and theoretical studies. New Journal of Chemistry, 2022, 46, 17817-17833.	1.4	0
12817	Theoretical studies on the effects of π -bridge engineering on the photoelectric performance of Y6. New Journal of Chemistry, 2022, 46, 19963-19974.	1.4	1
12818	The mechanism of intramolecular halogen bonding enhanced the quantum efficiency of ultralong organic phosphorescence in the aggregated state. Physical Chemistry Chemical Physics, 2022, 24, 22905-22917.	1.3	8
12819	Pushing the limits of the hydrogen bond enhanced halogen bond—the case of the C-H hydrogen bond. Chemical Science, 2022, 13, 11156-11162.	3.7	9
12820	A natural deep eutectic solvent-based aqueous biphasic system coupled with MoS ₂ photocatalytic reduction for green recovery of gold from thiosulfate solution. Green Chemistry, 2022, 24, 8330-8344.	4.6	6
12821	Realization of switching between TADF and HLCT emissions through modulation of the intramolecular charge transfer character. Journal of Materials Chemistry C, 2022, 10, 13124-13136.	2.7	8
12822	Direct (hetero)arylation (DHAP) polymerization of conjugated polymers – new A – B – A monomer design for P(NDI2OD-T2) & the challenges of adopting DHAP for continuous flow processes. Journal of Materials Chemistry C, 2022, 10, 13025-13039.	2.7	8
12823	Asymmetric assembly of pyrazole and 1,2,3-triazole with a methylene bridge: regioisomerism and energetic properties. Chemical Communications, 2022, 58, 10647-10650.	2.2	18
12824	Side Chain effect on the electrochemical and optical properties of thieno[3,4-c]pyrrole-4,6-dione based donor acceptor donor type monomers and polymers. Molecular Systems Design and Engineering, 0, .	1.7	3
12825	Correlating the orbital overlap area and vibrational frequency shift of an isocyanide moiety adsorbed on Pt and Pd covered Au(111) surfaces. Physical Chemistry Chemical Physics, 2022, 24, 23301-23308.	1.3	3
12826	Trimetallic clusters in the sumanene bowl for dinitrogen activation. Physical Chemistry Chemical Physics, 2022, 24, 23265-23278.	1.3	8
12827	Halonium, chalconium, and pnictonium salts as noncovalent organocatalysts: a computational study on relative catalytic activity. Organic and Biomolecular Chemistry, 2022, 20, 7632-7639.	1.5	8
12828	Template-assisted alloying of atom-precise silver nanoclusters: a new approach to generate cluster functionality. Chemical Science, 2022, 13, 11394-11404.	3.7	14
12829	Hopping transport in perylene diimide based organic solar cells: a DFT approach. New Journal of Chemistry, 2022, 46, 19357-19372.	1.4	6
12830	On the importance of π -stacking interactions in the complexes of copper and zinc bearing pyridine-2,6-dicarboxylic acid <i>N</i> -oxide and <i>N</i> -donor auxiliary ligands. CrystEngComm, 2022, 24, 6677-6687.	1.3	2
12831	Revisiting indeno[1,2- <i>bc</i>]fluorene by steric promoted synthesis while isolating the second stable 4 <i>n</i> -indeno[2,1- <i>ac</i>]fluorene. Organic and Biomolecular Chemistry, 2022, 20, 8071-8077.	1.5	8
12832	Characteristic guaiane sesquiterpenes from <i>Daphne penicillata</i> and ECD/NMR-based assignment of C-1 configuration. Organic Chemistry Frontiers, 2022, 9, 6213-6222.	2.3	7

#	ARTICLE	IF	CITATIONS
12833	Structural evolution, photoelectron spectra and vibrational properties of anionic GdGe ₂ (Z = 54) nanoalloy clusters: a DFT insight. RSC Advances, 2022, 12, 22020-22030.	1.7	5
12834	Synergistic Pretreatment of Hydrothermal and Photocatalytic for Improving the Full Component Utilization of Corn Stalk Based on Lignin First Biorefining. SSRN Electronic Journal, 0, , .	0.4	0
12835	A temperature-dependent tricoloured mechanochromic fluorescent material with polymorphic structures. Journal of Materials Chemistry C, 0, , .	2.7	5
12836	A comparative study on the reactivity of ditantalum deuteride cluster anions Ta ₂ D ₂ and Ta ₂ D ₄ toward N ₂ . Physical Chemistry Chemical Physics, 2022, 24, 24950-24958.	1.3	1
12837	Unveiling the origin of the chemoselectivity of bismacrocyclic-mediated C-H arylation of phenols: from mechanism concept to new coupling design. Organic Chemistry Frontiers, 2022, 9, 4890-4901.	2.3	0
12838	Dual antioxidant activity and the related mechanisms of a novel pentapeptide GLP4 from the fermented mycelia of <i>Ganoderma lingzhi</i> . Food and Function, 2022, 13, 9032-9048.	2.1	5
12839	A theoretical study on the donor ability adjustment of tris(2,4,6-trichlorophenyl)methyl-triarylamine (TTM-TPA) radicals aiming to develop better organic luminescent materials. New Journal of Chemistry, 2022, 46, 16325-16332.	1.4	5
12840	Effects of a long-short axis skeleton on the excited-state properties of ultraviolet hot exciton molecules: luminescence mechanism and molecular design. Physical Chemistry Chemical Physics, 2022, 24, 22309-22318.	1.3	0
12841	Flexibility is the key to tuning the transport properties of fluorinated imide-based ionic liquids. Chemical Science, 2022, 13, 9176-9190.	3.7	14
12842	Comprehending radicals, diradicals and their bondings in aggregates of imide-fused polycyclic aromatic hydrocarbons. Chemical Science, 2022, 13, 9985-9992.	3.7	2
12843	Nitrogen defect-containing polymeric carbon nitride for efficient photocatalytic H ₂ evolution and RhB degradation under visible light irradiation. RSC Advances, 2022, 12, 24713-24723.	1.7	2
12844	A theoretical insight into excited-state decay and proton transfer of <i>p</i> -nitrophenol in the gas phase and methanol solution. Physical Chemistry Chemical Physics, 2022, 24, 20517-20529.	1.3	2
12845	Insights of Adsorption and Dissociation of Hydrogen on Ni Doped Mg ₄ Clusters: A Dft Study. SSRN Electronic Journal, 0, , .	0.4	0
12846	Fischer-Helferich glycosidation mechanism of glucose to methyl glycosides over Al-based catalysts in alcoholic media. RSC Advances, 2022, 12, 23416-23426.	1.7	1
12847	A theoretical study based on DFT calculations on the different influence of functional groups on the C-H activation process via Pd-catalysed I ² -X elimination. RSC Advances, 2022, 12, 26116-26122.	1.7	1
12848	Semimetal Bi/CoF-Based Adsorptive Catalyst for Plasmon-Enhanced Photodegradation of Phenolic Pollutants. SSRN Electronic Journal, 0, , .	0.4	0
12849	Establishing Ta-Pb/Cu and Sa-Pb/Cu Interface Catalyst Shells on Hmx Surfaces Via in Situ Coprecipitation to Ameliorate the Performances of Hmx. SSRN Electronic Journal, 0, , .	0.4	0
12850	Molecular Insights into the Dispersibility of Asphaltene and Crude Oil Rheological Properties Under the Effect of Multi-Alkylated Aromatic Amides. SSRN Electronic Journal, 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
12851	Photochemistry of phosphenic chloride (ClPO ₂): isomerization with chlorine metaphosphite (ClOPO) and reduction by carbon monoxide. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20828-20836.	1.3	2
12852	The role of the intermediate triplet state in iron-catalyzed multi-state C-H activation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20721-20727.	1.3	1
12853	Functionalized nona-silicide [Si ₉ R ₃] Zintl clusters: a new class of superhalogens. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 21105-21111.	1.3	6
12854	Over 17% efficiency all-small-molecule organic solar cells based on an organic molecular donor employing a 2D side chain symmetry breaking strategy. <i>Energy and Environmental Science</i> , 2022, 15, 4338-4348.	15.6	63
12855	CB ₆ Al ⁰⁺ : Planar hexacoordinate boron (phB) in the global minimum structure. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 22634-22644.	1.3	11
12856	Sensitive structural motifs separately distributed in azide-based 3D EMOFs: a primary explosive with an excellent initiation ability and enhanced stability. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 5884-5892.	3.0	19
12857	Hydroxamate based transition metal-organic coordination polymers with semiconductive properties. <i>Dalton Transactions</i> , 2022, 51, 12709-12716.	1.6	5
12858	Establishing design strategies for emissive materials with an inverted singlet-triplet energy gap (INVEST): a computational perspective on how symmetry rules the interplay between triplet harvesting and light emission. <i>Journal of Materials Chemistry C</i> , 2022, 10, 12680-12698.	2.7	24
12859	Single-factor analysis of Ni-BAC-catalyzed β -pinene hydrogenation based on hierarchical analysis. <i>RSC Advances</i> , 2022, 12, 28560-28571.	1.7	0
12860	In-Situ Growth of 2d Magnesium Hydroxide on Zirconium-Based Metal Organic Frameworks for Phosphate Removal: An Experimental and Theoretical Exploration of Adsorption Behavior. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12861	Mechanistic insight into borrowing-hydrogen N-alkylation catalyzed by an MLC catalyst with dual proton-responsive sites. <i>Dalton Transactions</i> , 2022, 51, 16215-16223.	1.6	1
12862	Polyethyleneimine-capped copper nanoclusters for detection and discrimination of 2,4,6-trinitrotoluene and 2,4,6-trinitrophenol. <i>Analytical Methods</i> , 2022, 14, 4485-4494.	1.3	7
12863	A functional electrolyte additive enabling robust interphases in high-voltage Li-LiNi _{0.8} Co _{0.1} Mn _{0.1} O ₂ batteries at elevated temperatures. <i>Journal of Materials Chemistry A</i> , 2022, 10, 21912-21922.	5.2	10
12864	A double-spiro ring-structured mechanophore with dual-signal mechanochromism and multistate mechanochemical behavior: non-sequential ring-opening and multimodal analysis. <i>Polymer Chemistry</i> , 2022, 13, 5507-5514.	1.9	3
12865	Thiazoloisindigo-based ambipolar polymers for excellent balanced hole and electron mobility. <i>Materials Chemistry Frontiers</i> , 2022, 6, 3369-3381.	3.2	4
12866	Interaction-determined extraction capacity between rare earth ions and extractants: taking lanthanum and lutetium as models through theoretical calculations. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 5360-5370.	3.0	4
12867	Synthesis, Single Crystal Characterization and Anti-AD Activities of a Novel Complex of Cu(II) with β -sitin Formed Protonated Chrysin Derivative Ligand. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12868	The photoisomerization mechanism of methacrolein oxide (MACR-OO): the cyclic dioxole formation pathway revealed. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 22531-22537.	1.3	1

#	ARTICLE	IF	CITATIONS
12869	Molecular reaction and dynamic mechanism of iodate reduction to molecular iodine by nitrogen(N_2) in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 22889-22897.	1.3	0
12870	Efficient fluorescent recognition of ATP/GTP by a water-soluble bisquinolinium pyridine-2,6-dicarboxamide compound. Crystal structures, spectroscopic studies and interaction mode with DNA. <i>RSC Advances</i> , 2022, 12, 27826-27838.	1.7	3
12871	Engineering of W-shaped benzodithiophenedione-based small molecular acceptors with improved optoelectronic properties for high efficiency organic solar cells. <i>RSC Advances</i> , 2022, 12, 21801-21820.	1.7	12
12872	The smallest 4f-metalla-aromatic molecule of cyclo-PrB ₂ with Pr ^{III} multiple bonds. <i>Chemical Science</i> , 2022, 13, 10082-10094.	3.7	4
12873	Recyclable rhodium-catalyzed C-H activation/[4 + 2] annulation with unconventional regioselectivity at ambient temperature: experimental development and mechanistic insight. <i>Green Chemistry</i> , 2022, 24, 7012-7021.	4.6	9
12874	Tailored ternary hydrophobic deep eutectic solvents for synergistic separation of yttrium from heavy rare earth elements. <i>Green Chemistry</i> , 2022, 24, 7148-7161.	4.6	10
12875	An intramolecular-locked strategy for designing nonlinear optical materials with remarkable first hyperpolarizability. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 21800-21805.	1.3	2
12876	Tetraphenylnaphthosilole (TPNS): a potential building block for deep-blue emitter featured aggregation-induced blue-shifted emission. <i>Journal of Materials Chemistry C</i> , 2022, 10, 14517-14524.	2.7	1
12877	Achieving tricolor luminescence switching from a stimuli-responsive luminophore based on a bisarylic methanone derivative. <i>New Journal of Chemistry</i> , 2022, 46, 15657-15665.	1.4	2
12878	Enhanced Bone Regeneration Via Zif-8 Decorated Hierarchical Polyvinylidene Fluoride Piezoelectric Foam Nanogenerator: Coupling of Bioelectricity, Angiogenesis, and Osteogenesis. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12879	Design New Organic Material Based on Indandione as an Electron Acceptor for High Performance Solar Cells. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12880	Visible-emitting Cu(I) complexes with <i>N</i> -functionalized benzotriazole-based ligands. <i>New Journal of Chemistry</i> , 2022, 46, 18938-18951.	1.4	3
12881	Sulfuric acid-dimethylamine particle formation enhanced by functional organic acids: an integrated experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 23540-23550.	1.3	2
12882	Comparison of the hydrogen extraction reactions of isopentane molecules and ions. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
12883	Design and computational insight into two novel CL-20 analogues, BNMTNIW and BNIMTNIW: high performance energetic materials. <i>New Journal of Chemistry</i> , 2022, 46, 16693-16701.	1.4	5
12884	Synthesis and Characterization of a Hierarchical Nanoadsorbent Fe ₃ O ₄ @SiO ₂ @PAA-So ₃ h For Pb(II) and Cu(II) Removal from Water. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12885	Cyclometalated iridium complexes based on monodentate aminophosphanes. <i>Dalton Transactions</i> , 2022, 51, 12334-12351.	1.6	1
12886	Efficient degradation of organic dyes using peroxymonosulfate activated by magnetic graphene oxide. <i>RSC Advances</i> , 2022, 12, 21026-21040.	1.7	3

#	ARTICLE	IF	CITATIONS
12887	Theoretical study on the reaction mechanism of Si ₂ Cl ₆ and HCl catalyzed by amine catalysts. <i>New Journal of Chemistry</i> , 2022, 46, 17977-17984.	1.4	2
12888	A structurally simple linear conjugated polymer toward practical application of organic solar cells. <i>Energy and Environmental Science</i> , 2022, 15, 4789-4797.	15.6	27
12889	Heterogeneous ethylene hydroformylation on polymer supported Rh-based catalysts: a DFT analysis of the mechanism and Rh ⁺ P effect. <i>Catalysis Science and Technology</i> , 2022, 12, 6740-6750.	2.1	1
12890	Theoretical insights into the mechanism and origin of chemoselectivity in the catalyst- and directing group-dependent oxidative cyclization of diynes with pyridine <i>N</i> -oxides. <i>Organic Chemistry Frontiers</i> , 2022, 9, 5168-5177.	2.3	2
12891	Achieving circularly polarized luminescence and large piezoelectric response in hybrid rare-earth double perovskite by a chirality induction strategy. <i>Materials Horizons</i> , 2022, 9, 2450-2459.	6.4	20
12892	Impact of various heterocyclic π -linkers and their substitution position on the opto-electronic attributes of the A ⁺ π -D ⁺ π -A type IECIO-4F molecule: a comparative analysis. <i>RSC Advances</i> , 2022, 12, 20792-20806.	1.7	22
12893	Identification of chlorinated products from tyrosine and tyrosyl dipeptides during chlorination: a computational study. <i>Environmental Sciences: Processes and Impacts</i> , 2022, 24, 2345-2356.	1.7	1
12894	Direct synthesis of a stable radical doped electrically conductive coordination polymer. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 5016-5023.	3.0	3
12895	Rational designs of structurally similar TADF and HLCT emitters with benzo- or naphtho-carbazole units as electron donors. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1
12896	Two-photon absorption and triplet excited state quenching of near-IR region aza-BODIPY photosensitizers <i>via</i> a triphenylamine moiety despite heavy bromine atoms. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 25495-25505.	1.3	3
12897	Molecular tuning of non-fullerene electron acceptors in organic photovoltaics: a theoretical study. <i>New Journal of Chemistry</i> , 2022, 46, 20204-20216.	1.4	3
12898	Simultaneous Strengthening and Toughening Lignin/Cellulose Nanofibril Composite Films: Effects from Flexible Hydrogen Bonds. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12899	Carbazolylgold(III) complexes with thermally activated delayed fluorescence switched on by ligand manipulation as high efficiency organic light-emitting devices with small efficiency roll-offs. <i>Chemical Science</i> , 2022, 13, 10129-10140.	3.7	8
12900	Existence of noble gas-inserted phosphorus fluorides: FN _g PF ₂ and FN _g PF ₄ with Ng ⁺ P covalent bond (Ng = Ar, Kr, Xe and Rn). <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20466-20479.	1.3	2
12901	Chemical Bonding and Aromaticity Analyses of Petroporphyrins with Vanadium or Nickel. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12902	Studying noncovalent or covalent bond problem between smoothened and cholesterol by molecular dynamics simulation and Markov state model. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 19564-19575.	1.3	0
12903	Isomerization of two-dimensional non-fullerene electron acceptor materials for developing high-performance organic solar cells. <i>Journal of Materials Chemistry C</i> , 2022, 10, 11286-11295.	2.7	2
12904	Efficient separation of electrode active materials and current collector metal foils from spent lithium-ion batteries by a green deep eutectic solvent. <i>Green Chemistry</i> , 2022, 24, 8131-8141.	4.6	12

#	ARTICLE	IF	CITATIONS
12905	Single and double deprotonation/dearomatization of the N,S-donor pyridinophane ligand in ruthenium complexes. Dalton Transactions, 2022, 51, 14734-14746.	1.6	2
12906	Robust and promising hydrogen and oxygen evolution reactions by a nanostructured bifunctional FeCoPd alloy electrocatalyst. Journal of Materials Chemistry A, 2022, 10, 23731-23743.	5.2	12
12907	A three dimensional graphdiyne-like porous triptycene network for gas adsorption and separation. RSC Advances, 2022, 12, 28299-28305.	1.7	4
12908	Nitrogen, phosphorus co-doped hollow porous carbon microspheres as an oxidase-like electrochemical sensor for baicalin. New Journal of Chemistry, 2022, 46, 16341-16351.	1.4	6
12909	Phenanthrene-based deep-blue fluorophores with balanced carrier transport ability for high-performance OLEDs with a CIE _y < 0.04. Journal of Materials Chemistry C, 2022, 10, 14711-14721.	2.7	9
12910	The destructive mechanism of A β 1-42 protofibrils by norepinephrine revealed via molecular dynamics simulations. Physical Chemistry Chemical Physics, 2022, 24, 19827-19836.	1.3	6
12911	Identification of 4-acrylamido-N-(pyridazin-3-yl)benzamide as anti-COVID-19 compound: a DFTB, molecular docking, and molecular dynamics study. RSC Advances, 2022, 12, 24178-24186.	1.7	3
12912	The Intramolecular Assembly of Polynitrobiazoles and Ether-Bridge: A Facile Strategy to Access High-Energy and Thermostable Polynitro-Functionalized Diazole-1,3,6-Oxadiazepines. SSRN Electronic Journal, 0, , .	0.4	0
12913	Disarming the alkoxide trap to access a practical FeCl ₃ system for borrowing-hydrogen N-alkylation. Organic Chemistry Frontiers, 2022, 9, 4803-4817.	2.3	6
12914	Activation of Persulfate by Vanadium Oxide Modified Carbon Nanotube for 17 β -Estradiol Degradation in Soil : Mechanism, Application and Ecotoxicity Assessment. SSRN Electronic Journal, 0, , .	0.4	0
12915	Intratumoral synthesis of transformable metal-phenolic nanoaggregates with enhanced tumor penetration and retention for photothermal immunotherapy. Theranostics, 2022, 12, 6258-6272.	4.6	12
12916	Theoretical Studies on Sensing of Transition Metals Using C _{2n} Surface. SSRN Electronic Journal, 0, , .	0.4	0
12917	A two-dimensional Be ₂ Au monolayer with planar hexacoordinate s-block metal atoms: a superconducting global minimum Dirac material with two perfect Dirac node-loops. Chemical Science, 2022, 13, 11099-11109.	3.7	5
12918	Achieving the highest density and energy within diazo-oxide compounds. Materials Chemistry Frontiers, 2022, 6, 2670-2677.	3.2	7
12919	Energetics of carboxylic acid-pyridine heterosynthon revisited: A computational study of intermolecular hydrogen bond domination on phenylacetic acid-nicotinamide cocrystals. Open Chemistry, 2022, 20, 949-957.	1.0	0
12920	Experimental study and quantum chemical calculation of free radical reactions in ciprofloxacin degradation during the UV/chlorine oxidation process. Environmental Science: Water Research and Technology, 2022, 8, 2744-2760.	1.2	2
12921	Computational Underpinnings for the Photocatalytic Transformation of Para-Aminothiophenol to Dimercaptoazobenzene on Copper Surface. SSRN Electronic Journal, 0, , .	0.4	0
12922	Theoretical investigation of triplet potential energy surfaces for (C [*]) cyclometalated platinum(ⁱⁱ) complexes and the corresponding control strategies. New Journal of Chemistry, 2022, 46, 18306-18315.	1.4	0

#	ARTICLE	IF	CITATIONS
12923	Coronene-based quantum dots for the delivery of the doxorubicin anticancer drug: a computational study. <i>New Journal of Chemistry</i> , 2022, 46, 18518-18534.	1.4	2
12924	Studies of a bola-type bis(dithiafulvene) molecular system: synthesis, crystal structure, and electrochemical properties. <i>New Journal of Chemistry</i> , 2022, 46, 18133-18145.	1.4	1
12925	Molecular Encapsulation of Bioactive Ingredients from Xuefu Zhuyu Decoction by Cyclodextrin-Assisted Extraction. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12926	Data-Mining Based Assembly of Promising Metal-Organic Frameworks on Xe/Kr Separation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12927	Unravelling the robustness of magnetic anisotropy of a nickelocene molecule in different environments: a first-principles-based study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 21122-21130.	1.3	0
12928	Bicarbonate insertion triggered self-assembly of chiral octa-gold nanoclusters into helical superstructures in the crystalline state. <i>Chemical Science</i> , 2022, 13, 10523-10531.	3.7	15
12929	Unveiling the Effect of Solvent Polarity on the Excited State Intramolecular Proton Transfer and Hydrogen Bond Mechanisms of Dhp. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12930	Two-dimensional covalent organic frameworks with p- and bipolar-type redox-active centers for organic high-performance Li-ion battery cathodes. <i>Journal of Materials Chemistry A</i> , 2022, 10, 16595-16601.	5.2	20
12931	A novel acid-controlled second-order nonlinear optical switch based on dimethyldihydropyrene/cyclophanediene photoswitch. <i>Journal of Materials Chemistry C</i> , 2022, 10, 12338-12349.	2.7	4
12932	Modulation of Halogen-Bonded 2d Self-Assemblies of Benzothiadiazole Derivative: Concentration and Solvent Effects. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12933	Turning conventional non-TADF units into high-lying reverse intersystem crossing TADF emitters: different symmetric D ⁺ -A ⁻ -D-type modified donor units. <i>New Journal of Chemistry</i> , 2022, 46, 15168-15174.	1.4	1
12934	Renaissance of dinitroazetidene: novel hybrid energetic boosters and oxidizers. <i>Dalton Transactions</i> , 2022, 51, 14088-14096.	1.6	9
12935	Exploring the evolution patterns of melem from thermal synthesis of melamine to graphitic carbon nitride. <i>RSC Advances</i> , 2022, 12, 24311-24318.	1.7	3
12936	Molecular electrostatic potential as a general and versatile indicator for electronic substituent effects: statistical analysis and applications. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 25740-25752.	1.3	11
12937	Molecular dynamics simulation study of adsorption of anionic/nonionic surfactants at oil/water interfaces. <i>RSC Advances</i> , 2022, 12, 27330-27343.	1.7	6
12938	Dual metal Co-anchored nanosheets to catalyze advanced oxidation processes for highly efficient oxytetracycline degradation. <i>Environmental Science: Nano</i> , 2022, 9, 4214-4232.	2.2	4
12939	Physical Insight into the Mechanism of Photoinduced Charge-Transfer and its Effects on Gas Mixture Adsorption in the Metal-Organic Framework: A Study Combining Quantum Mechanics Calculations and Molecular Mechanics Simulations. <i>SSRN Electronic Journal</i> , 0, , .	0.4	1
12940	Environmental-Friendly Hydrochar-Montmorillonite Composite for Efficient Catalytic Degradation of Dicamba and Alleviating its Damage to Crops. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
12941	Development of Highly-Efficient Od/1d/Od Dual Z-Scheme Cds/ZnWO ₄ /Zns Heterojunction Photocatalysts in Pollutant Removal and Involved Mechanism. SSRN Electronic Journal, 0, , .	0.4	0
12942	Crystal engineering of molecules with through-space $\hat{I}\pm$ -effect hydrogen bonds: 3a,6a-diepoxybenzo[<i>c</i>]isoquinolines possessing a free amino group. CrystEngComm, 2022, 24, 6093-6100.		0
12943	Discovering Crystal Forms of the Bio-based Nylon 50 Monomer 1,5-pentanediamine-O-phthalate: Insight into the Crystal Structures, Transformations and Stability. CrystEngComm, 0, , .	1.3	0
12944	A comprehensive study on the photophysical and non-linear optical properties of thienyl-chalcone derivatives. Physical Chemistry Chemical Physics, 2022, 24, 21927-21953.	1.3	4
12945	The mechanism of direct reductive amination of aldehyde and amine with formic acid catalyzed by boron trifluoride complexes: insights from a DFT study. Catalysis Science and Technology, 2022, 12, 5679-5686.	2.1	1
12946	Insights into the spontaneous multi-scale supramolecular assembly in an ionic liquid-based extraction system. Physical Chemistry Chemical Physics, 2022, 24, 25950-25961.	1.3	2
12947	Atmospheric-pressure synthesis of glycerol carbonate from CO ₂ and glycerol catalyzed by protic ionic liquids. Green Chemistry, 2022, 24, 8292-8301.	4.6	17
12948	Effect of conformational disorder on exciton states of an azobenzene aggregate. Physical Chemistry Chemical Physics, 2022, 24, 24002-24006.	1.3	3
12949	Micro-physical parameter dynamic evolution behaviour of a natural ester molecular chain under a changing electric field and its correlation mechanism with lightning impulse discharge: theoretical analysis. Physical Chemistry Chemical Physics, 2022, 24, 23427-23436.	1.3	4
12950	Charge transfer regulated by domain differences between host and guest donors in ternary organic solar cells. Journal of Materials Chemistry A, 2022, 10, 22477-22487.	5.2	4
12951	Mechanistic insight into the disruption of Tau R3 \hat{E} R4 protofibrils by curcumin and epinephrine: an all-atom molecular dynamics study. Physical Chemistry Chemical Physics, 2022, 24, 20454-20465.	1.3	13
12952	Theoretical investigations on the antioxidant potential of 2,4,5-trihydroxybutyrophenone in different solvents: A DFT approach. Results in Chemistry, 2022, 4, 100515.	0.9	4
12953	Theoretical insights into the central \hat{E} acceptor \hat{E} bridge function on the whole visible light and near-infrared emission in tetraphenylpyrazine-based luminogens. New Journal of Chemistry, 2022, 46, 16932-16940.	1.4	3
12954	A Molecular Dynamics Simulation Study of Amine-Carboxyl Ionic Interactions and Their Distribution in a Polysiloxanes Network. Journal of Macromolecular Science - Physics, 2022, 61, 844-859.	0.4	1
12955	A DENSITY FUNCTIONAL THEORY (DFT) STUDY ON SILICON DOPED CARBON NANOTUBE Si-CNT AS A CARRIER FOR BMSF-BENZ DRUG USED FOR OSTEOPOROSIS DISEASE. Momento, 2022, , 1-24.	0.3	1
12956	Structural investigations and theoretical insights of a polymethoxy chalcone derivative: Synthesis, crystal structure, 3D energy frameworks and SARS CoV-2 docking studies. Journal of Molecular Structure, 2023, 1272, 134226.	1.8	7
12957	Environmental-friendly hydrochar-montmorillonite composite for efficient catalytic degradation of dicamba and alleviating its damage to crops. Science of the Total Environment, 2023, 856, 158917.	3.9	8
12958	Synthesis of durable hydrophobic fluorinated polyurethanes with exceptional cavitation erosion resistance. Tribology International, 2023, 177, 107973.	3.0	7

#	ARTICLE	IF	CITATIONS
12959	Investigation of the adsorption performance and mechanism of 2-mercaptoethane sulfonic acid intercalated modified layered double hydroxide on heavy metal ions. <i>Journal of Colloid and Interface Science</i> , 2023, 629, 948-959.	5.0	13
12960	Design of highly stable thermally activated delayed fluorescence emitters via the overlap degree of HOMO-LUMO distributions. <i>Journal of Molecular Structure</i> , 2023, 1272, 134213.	1.8	9
12961	Co-operation between multidentate ligand and inorganic salts: preparation of solvent-free primary explosives based on 4-amino-1,2,5-oxadiazole-3-carbohydrazide. <i>Chemical Engineering Journal</i> , 2023, 452, 139472.	6.6	17
12962	Efficient synthesis of PdIr nanocatalysts with controllable surface composition for electrochemical oxidation of methanol. <i>Fuel</i> , 2023, 332, 126105.	3.4	10
12963	A flexible, sensitive and stable humidity sensor based on an all-polymer nanofiber film. <i>Materials Letters</i> , 2023, 330, 133268.	1.3	9
12964	Nitazoxanide in aqueous co-solvent solutions of isopropanol/DMF/NMP: Solubility, solvation thermodynamics and intermolecular interactions. <i>Journal of Chemical Thermodynamics</i> , 2023, 176, 106928.	1.0	3
12965	Simple and high-precision DFT-QSPR prediction of enthalpy of combustion for sesquiterpenoid high-energy density fuels. <i>Fuel</i> , 2023, 332, 126157.	3.4	3
12966	Proton-insertion dominated polymer cathode for high-performance aqueous zinc-ion battery. <i>Chemical Engineering Journal</i> , 2023, 452, 139324.	6.6	32
12967	Synthesis, crystal structure and computational studies of new steroidal hemisuccinyl ester derivatives. <i>Journal of Molecular Structure</i> , 2023, 1272, 134191.	1.8	1
12968	Violet phosphorus-Fe ₃ O ₄ as a novel photocatalysis-self-Fenton system coupled with underwater bubble plasma to efficiently remove norfloxacin in water. <i>Chemical Engineering Journal</i> , 2023, 452, 139481.	6.6	7
12969	Probing the effect of microenvironment on the enzyme-like behavior of catalytic peptide assemblies. <i>Journal of Colloid and Interface Science</i> , 2023, 629, 683-693.	5.0	3
12970	Supramolecular association of (1,4-phenylenedimethanaminium) bis(perchlorate) monohydrate: A combined experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2023, 1272, 134212.	1.8	4
12971	Theoretical study of 36Adz based alkaline earthides M+(36Adz)M ⁺ (M+ = Li & Na; M ⁺ = Be, Mg & Ca) Tj ETQq0 0 0 rgBT /Overlo 153, 107119.	1.9	6
12972	Interface engineering for achieving efficient and stable perovskite solar cells by Bphen-fullerene dimer. <i>Chemical Engineering Journal</i> , 2023, 452, 139412.	6.6	6
12973	Perovskite/metal-organic framework photocatalyst: A novel nominee for eco-friendly uptake of pharmaceuticals from wastewater. <i>Journal of Alloys and Compounds</i> , 2023, 930, 167322.	2.8	7
12974	Piezo-photo coupling effect and extended optical absorption of piezoelectric-based hybrids for efficient bisphenol A degradation. <i>Chemical Engineering Journal</i> , 2023, 452, 139456.	6.6	8
12975	Experimental and Quantum Chemical Approaches for Hydrazide-based Crystalline Organic Chromophores: Synthesis, SC-XRD, Spectroscopic and Nonlinear Optical Properties. <i>Journal of Molecular Structure</i> , 2023, 1272, 134208.	1.8	5
12976	Bi modified oxidized tubular carbon nitride with high-yield singlet oxygen for propylparaben degradation: Implication for a novel oxygen activation mechanism. <i>Applied Catalysis B: Environmental</i> , 2023, 321, 122025.	10.8	10

#	ARTICLE	IF	CITATIONS
12977	Ultra-sensitive fluorescent and colorimetric probes for femtomolar detection of picric acid: Mechanochromic, latent fingerprinting, and pH responsive character with AIE properties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 435, 114318.	2.0	13
12978	Efficient removal of polybrominated diphenyl ethers from soil washing effluent by dummy molecular imprinted adsorbents: Selectivity and mechanisms. <i>Journal of Environmental Sciences</i> , 2023, 129, 45-57.	3.2	7
12979	DFT Study on the Effect of Na on NO Reduction with Nitrogen-Containing Char from Zhundong Coal. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6148-6159.	1.1	1
12980	EXPERIMENTAL AND THEORETICAL STUDY OF A SANDWICH-LIKE PHENOXY-BRIDGED HETEROBIMETALLIC ZINC(II)â€“MANGANESE(III) 3-MeOSALPHEN COMPLEX. <i>Journal of Structural Chemistry</i> , 2022, 63, 1242-1255.	0.3	46
12981	Growth, Structure, and Dielectric and Optics Properties of a Novel Optical Crystal with High Optical Nonlinearity. <i>Crystal Growth and Design</i> , 2022, 22, 5895-5903.	1.4	13
12982	Developing a QSPR Model of Organic Carbon Normalized Sorption Coefficients of Perfluorinated and Polyfluoroalkyl Substances. <i>Molecules</i> , 2022, 27, 5610.	1.7	1
12983	Hybridized Ag-CuCrO ₂ Nanostructured Composites for Enhanced Gas Sensing. <i>ACS Applied Nano Materials</i> , 2022, 5, 12690-12698.	2.4	4
12984	Silver-Catalyzed Synthesis of 2-Cyano-5-pyrazolyl-2 <i>H</i> -tetrazole: A Promising Precursor to Insensitive Energetic Compounds. <i>Crystal Growth and Design</i> , 2022, 22, 6140-6147.	1.4	2
12985	Isoyanide and Cyanide Entities Form Isostructural Halogen Bond-Based Supramolecular Networks Featuring Five-Center Tetrafurcated Halogenâ€“C/N Bonding. <i>Crystal Growth and Design</i> , 2022, 22, 6079-6087.	1.4	8
12986	Synergistic Extraction of 1,3-Propanediol from Fermentation Broths Using Multialcohol Extractants. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 11891-11901.	3.2	3
12987	Significance of Antisolvents on Solvation Structures Enhancing Interfacial Chemistry in Localized High-Concentration Electrolytes. <i>ACS Central Science</i> , 2022, 8, 1290-1298.	5.3	24
12988	A Competitive Solvation of Ternary Eutectic Electrolytes Tailoring the Electrode/Electrolyte Interphase for Lithium Metal Batteries. <i>ACS Nano</i> , 2022, 16, 14558-14568.	7.3	19
12989	Anion Photoelectron Spectroscopy and Quantum Chemical Calculations of Bimetallic Oxide Clusters YCu ₂ O _x (<i>n</i> = 2â€“5). <i>Journal of Physical Chemistry A</i> , 2022, 126, 6067-6079.	1.1	1
12990	Photocatalytic Carbon Dioxide Reduction and Density Functional Theory Investigation of 2,6-(Pyridin-2-yl)-1,3,5-triazine-2,4-diamine and Its Cobalt and Nickel Complexes. <i>ACS Applied Energy Materials</i> , 2022, 5, 11077-11090.	2.5	4
12991	QSTR Modeling to Find Relevant DFT Descriptors Related to the Toxicity of Carbamates. <i>Molecules</i> , 2022, 27, 5530.	1.7	4
12992	A graphyne spoked wheel. <i>CheM</i> , 2022, 8, 2831-2842.	5.8	20
12993	Iridium(III) Complexes Based on Indolo[3,2- <i>h</i>]carbazole Derivatives for Narrowband Organic Light-Emitting Diodes with External Quantum Efficiency of 32.3% and Low Efficiency Roll-Off. <i>Advanced Energy and Sustainability Research</i> , 2022, 3, .	2.8	4
12994	Exploring the Mechanism of Ionic Liquids to Improve the Extraction Efficiency of Essential Oils Based on Density Functional Theory and Molecular Dynamics Simulation. <i>Molecules</i> , 2022, 27, 5515.	1.7	3

#	ARTICLE	IF	CITATIONS
12995	Extraction of Uranium in Nitric Media with Novel Asymmetric Tetra-Alkylcarbamide. <i>Molecules</i> , 2022, 27, 5527.	1.7	1
12996	From Nâ€H Nitration to Controllable Aromatic Mononitration and Dinitrationâ€The Discovery of a Versatile and Powerful <i>N</i> -Nitropyrazole Nitrating Reagent. <i>Jacs Au</i> , 2022, 2, 2152-2161.	3.6	11
12997	A family of oligo(<i>p</i> -phenylenevinylene) derivative aggregationâ€induced emission probes: Ultrasensitive, rapid, and antiâ€interfering fluorescent sensing of perchlorate via precise alkyl chain length modulation. <i>Aggregate</i> , 2023, 4, .	5.2	13
12998	<i>Si</i> ₆ C ₁₈ : A bispentalene derivative with two planar tetracoordinate carbons. <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	2
12999	Simultaneously Enhanced Dewaterability and Biopolymer Release of Sludge by Natural Deep Eutectic Solvents: Performance, Mechanisms, and Insights of Theoretical Calculations. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 11926-11938.	3.2	9
13000	Targeting Protein Pockets with Halogen Bonds: The Role of the Halogen Environment. <i>Journal of Chemical Information and Modeling</i> , 0, , .	2.5	7
13001	Uncovering the Morphological Regulation Mechanism of Low Sensitivity and Highly Energetic Materials in Solvents: Changing Crystal Morphology Induced by Hydrogen Bonding. <i>Crystal Growth and Design</i> , 2022, 22, 5935-5946.	1.4	8
13002	Effect of Static Jahnâ€Teller Distortion on the <i>Li</i> ⁺ Transport in a Copper Hexacyanoferrate Framework. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6814-6825.	1.1	1
13003	Hydride Relay Exchange Mechanism for the Heterocyclic Câ€H Arylation of Benzofuran and Benzothiophene Catalyzed by Pd Complexes. <i>Journal of Organic Chemistry</i> , 2022, 87, 12997-13010.	1.7	2
13004	Asymmetric synthesis of bedaquiline based on bimetallic activation and non-covalent interaction promotion strategies. <i>Science China Chemistry</i> , 2022, 65, 1968-1977.	4.2	12
13005	Mechanistic Basis for the High Enantioselectivity and Activity in the Multichiral Bimetallic Complex-Mediated Enantioselective Copolymerization of <i>meso</i> -Epoxides. <i>ACS Catalysis</i> , 2022, 12, 12268-12280.	5.5	8
13006	Selective adsorption of liquid long-chain α -olefin/paraffin on Mg-MOF-74: Adsorption behavior and interaction mechanism. <i>Nano Research</i> , 2023, 16, 1595-1605.	5.8	4
13008	A Waterâ€Stable and Redâ€Emissive Radical Cation for Mutp53 Cancer Therapy. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	9
13009	Affinities to Oxaliplatin: Vitamins from B Group vs. Nucleobases. <i>International Journal of Molecular Sciences</i> , 2022, 23, 10567.	1.8	2
13010	Unraveling origin of chemoselectivity and regioselectivity of iridiumâ€catalyzed B(4)â€H functionalization of <i>o</i> -carborane by alkyne. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	0
13011	Enhanced blue thermally activated delayed fluorescence with rigid adamantane as non-conjugated linker for space-confined donor-acceptor charge transfer: a theoretical study. <i>Journal of Physics: Conference Series</i> , 2022, 2338, 012022.	0.3	0
13012	Oxidation mechanism of ammonia-N/coal-N during ammonia-coal co-combustion. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 35498-35514.	3.8	18
13013	A Systemic Insight into Exohedral Actinides and Endohedral Borospherenes: An&Bm and An@Bn (An=U, Np, Pu; m = 28, 32, 34, 36, 38, 40; n = 36, 38, 40). <i>Molecules</i> , 2022, 27, 6047.	1.7	3

#	ARTICLE	IF	CITATIONS
13014	Chloride Binding Modulated by Anion Receptors Bearing Tetrazine and Urea. <i>ChemPhysChem</i> , 0, , .	1.0	2
13016	Aggregation-Dependent Circularly Polarized Luminescence and Thermally Activated Delayed Fluorescence from Chiral Carbene-Cu(I)-Amide Enantiomers. <i>Angewandte Chemie</i> , 0, , .	1.6	0
13017	Exploring of catalytic oxygen reduction reaction activity of lattice carbons of vanadium and niobium doped nitrogen codoped carbon nanotubes by density functional theory. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	2
13018	Mechanistic elucidation of Diels-Alder cycloaddition reactions between quinoflavonoid and substituted butadiene using LOL, ELF, QTAIM, and DFT studies. <i>Structural Chemistry</i> , 2023, 34, 959-969.	1.0	2
13019	Stimuli responsive silylene: Electromerism induced reversible switching between mono- and bis-silylene. <i>Angewandte Chemie</i> , 0, , .	1.6	0
13020	Synthesis, Anticancer Activity and Molecular Docking Studies of Novel N-Mannich Bases of 1,3,4-Oxadiazole Based on 4,6-Dimethylpyridine Scaffold. <i>International Journal of Molecular Sciences</i> , 2022, 23, 11173.	1.8	7
13021	RhB-Embedded Zirconium-Biquinoline-Based MOF Composite for Highly Sensitive Probing Cr(VI) and Photochemical Removal of CrO ₄ ²⁻ , Cr ₂ O ₇ ²⁻ , and MO. <i>Inorganic Chemistry</i> , 2022, 61, 15213-15224.	1.9	18
13022	Exploring Differences between Bis(aldimino)- and amino-aldimino- <i>N</i> , <i>C</i> , <i>N</i> -Pincer-Stabilized Pnictinidenes: Limits of Synthesis, Structure, and Reversible Tautomerization-Controlled Oxidation. <i>Organometallics</i> , 2022, 41, 2535-2550.	1.1	7
13023	Bright short-wavelength infrared organic light-emitting devices. <i>Nature Photonics</i> , 2022, 16, 752-761.	15.6	18
13024	Intermolecular Interactions between Nitrosourea and Polyoxometalate compounds. <i>ChemistrySelect</i> , 2022, 7, .	0.7	32
13025	Tri-explosophoric groups driven fused energetic heterocycles featuring superior energetic and safety performances outperforms HMX. <i>Nature Communications</i> , 2022, 13, .	5.8	46
13026	Enhancement of SO ₂ sensing performance of micro-ribbon graphene sensors using nitrogen doping and light exposure. <i>Applied Surface Science</i> , 2023, 608, 155059.	3.1	6
13027	Pnictogen-Bridged Diphenyl Sulfones as Photoinduced Pnictogen Bond Forming Emission Motifs. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	2
13028	An Experimental and Theoretical Study on Essential Oil of <i>Aethionema sancakense</i> : Characterization, Molecular Properties and RDG Analysis. <i>Molecules</i> , 2022, 27, 6129.	1.7	21
13029	Probing intra- and inter-molecular interactions through rotational spectroscopy: The case of the odorant 2- ² -aminoacetophenone and its 1:1 water and neon complexes. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	4
13030	Metal-Free Phosphination and Continued Functionalization of Pyridine: A Theoretical Study. <i>Molecules</i> , 2022, 27, 5694.	1.7	2
13031	Theoretical calculation of nitro-(2,4,6-trinitrophenyl)-azoles energetic compounds. <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	0
13032	Boosting the Energetic Performance of Trinitromethyl-1,2,4-oxadiazole Moiety by Increasing Nitrogen-Oxygen in the Bridge. <i>International Journal of Molecular Sciences</i> , 2022, 23, 10002.	1.8	6

#	ARTICLE	IF	CITATIONS
13033	A pocket-based 3D molecule generative model fueled by experimental electron density. <i>Scientific Reports</i> , 2022, 12, .	1.6	8
13034	Density Functional Theory Study of Low-Dimensional (2D, 1D, 0D) Boron Nitride Nanomaterials Catalyzing Acetylene Acetate Reaction. <i>International Journal of Molecular Sciences</i> , 2022, 23, 9997.	1.8	1
13035	Investigations of 6-Fluoro-4-Oxo-3,4-Dihydro-2H-Chromene-2-Carboxylic Acid by Quantum Computational, Spectroscopic, TD-DFT with Various Solvents and Molecular Docking Studies. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-18.	1.4	1
13036	Theoretical study on the interaction between 3,4-dinitroimidazole and cyclotetramethylene tetranitramine. <i>Monatshefte für Chemie</i> , 0, , .	0.9	0
13037	Chemical bonding between thorium and novel BN nanomaterials. <i>Journal of Applied Physics</i> , 2022, 132, 124302.	1.1	0
13038	Theoretical study of the interaction of fullerenes with the emerging contaminant carbamazepine for detection in aqueous environments. <i>Scientific Reports</i> , 2022, 12, .	1.6	6
13039	Extremely Stable Thorium-MOF Assembly of Tetraphenylethylene Derivative With Tunable AIE Property and Highly Selective Detection of Nitro Aromatic Compounds. <i>Advanced Materials Interfaces</i> , 2022, 9, .	1.9	8
13040	Trace Immunosensing of Multiple Neonicotinoid Insecticides by a Novel Broad-Specific Antibody Obtained from a Rational Screening Strategy. <i>Biosensors</i> , 2022, 12, 716.	2.3	3
13041	Al-Decorated C ₂ N Monolayer as a Potential Catalyst for NO Reduction with CO Molecules: A DFT Investigation. <i>Molecules</i> , 2022, 27, 5790.	1.7	3
13042	Triel Bond Formed by Malondialdehyde and Its Influence on the Intramolecular H-Bond and Proton Transfer. <i>Molecules</i> , 2022, 27, 6091.	1.7	2
13043	Process Simulation and Multiobjective Optimization for High-Purity Hexane Recovery Using Deep Eutectic Solvent. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 13929-13943.	1.8	2
13044	The ionic salts with super oxidizing ions O ₂ ⁺ and N ₅ ⁺ : Potential candidates for high-energy oxidants. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	0
13045	Aryldiazonium salts can serve as nitrogen-based Lewis acid catalysts and their applications in the formation of photoactive charge transfer complexes. <i>Chinese Chemical Letters</i> , 2023, 34, 107821.	4.8	4
13046	2-D Molecular Alloy Ru-M (M = Cu, Ag, and Au) Carbonyl Clusters: Synthesis, Molecular Structure, Catalysis, and Computational Studies. <i>Inorganic Chemistry</i> , 2022, 61, 14726-14741.	1.9	4
13047	Tris(2-Pyridyl)arsine as a New Platform for Design of Luminescent Cu(I) and Ag(I) Complexes. <i>Molecules</i> , 2022, 27, 6059.	1.7	10
13048	Aromaticity study of singlet- and triplet-state corannulene dianion and dication. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	2
13049	Hydroamination of Unactivated Alkenes with Aliphatic Azides. <i>Journal of the American Chemical Society</i> , 2022, 144, 16316-16324.	6.6	10
13050	Electronic structures and photophysical properties of carbazole and thiophene based organic compounds used as hole-injecting layer for organic light-emitting diodes (OLEDs). <i>Canadian Journal of Chemical Engineering</i> , 0, , .	0.9	1

#	ARTICLE	IF	CITATIONS
13051	Improving the performance of DSSCs by modulating the electron donor and electron acceptor of dye molecules with the DTPBT group as π -bridge. <i>Molecular Physics</i> , 0, , .	0.8	0
13052	Sonophotocatalytic degradation of ciprofloxacin by Bi ₂ MoO ₆ /FeVO ₄ heterojunction: Insights into performance, mechanism and pathway. <i>Separation and Purification Technology</i> , 2022, 303, 122251.	3.9	25
13053	Multicolor ultralong phosphorescence from perovskite-like octahedral $\text{I}^{\pm}\text{-AlF}_3$. <i>Nature Communications</i> , 2022, 13, .	5.8	9
13054	Theoretical study on a series of naphthalimide-contained two-photon fluorescent hypochlorite probe targeting endoplasmic reticulum: response mechanism and receptor effect. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	0
13055	Linear Axially Chiral Conjugated Polymers Exhibiting Ultralong Low-Temperature Phosphorescence and Intense Circularly Polarized Luminescence. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	22
13056	Design and Synthesis of a π -Conjugated N-Heteroaromatic Material for Aqueous Zinc-Organic Batteries with Ultrahigh Rate and Extremely Long Life. <i>Advanced Materials</i> , 2023, 35, .	11.1	33
13057	Luminescent fac-[ReX(CO) ₃ (phenyl-pyta)] (X = Cl, Br, I) complexes: influence of the halide ligand on the electronic properties in solution and in the solid state. <i>Photochemical and Photobiological Sciences</i> , 2023, 22, 169-184.	1.6	2
13058	Enantioseparation of planar chiral ferrocenes on cellulose-based chiral stationary phases: Benzoate versus carbamate pendant groups. <i>Electrophoresis</i> , 2023, 44, 203-216.	1.3	1
13059	Effects of boron/nitrogen/phosphorus doping on the scavenging action of armchair single-walled carbon nanotubes (armchair-SWCNT) for OH radicals: a DFT study. <i>Carbon Letters</i> , 2023, 33, 99-113.	3.3	2
13060	Temperature-Resistant Intrinsic High Dielectric Constant Polyimides: More Flexibility of the Dipoles, Larger Permittivity of the Materials. <i>Molecules</i> , 2022, 27, 6337.	1.7	8
13061	Conformational Heterogeneity and Interchain Percolation Revealed in an Amorphous Conjugated Polymer. <i>ACS Nano</i> , 2022, 16, 14432-14442.	7.3	4
13063	Modelling of Aminothiophene-Carbonitrile Derivatives as Potential Drug Candidates for Hepatitis B and C. <i>Iranian Journal of Science and Technology, Transaction A: Science</i> , 2022, 46, 1399-1412.	0.7	37
13064	Thermodynamic and Computational (DFT) Study of Non-Covalent Interaction Mechanisms of Charge Transfer Complex of Linagliptin with 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) and Chloranilic acid (CHA). <i>Molecules</i> , 2022, 27, 6320.	1.7	10
13065	Exploring of spacer fluorination effect on the characteristics and physicochemical properties of the newly designed task specific dicationic imidazolium-based ionic liquids: A quantum chemical approach. <i>Journal of Fluorine Chemistry</i> , 2022, 261-262, 110026.	0.9	3
13066	Critical Role of Iodous Acid in Neutral Iodine Oxoacid Nucleation. <i>Environmental Science & Technology</i> , 2022, 56, 14166-14177.	4.6	12
13067	Rational Synthesis of an Unsymmetric Pt Complex Unit Having Two Kinds of Pyrazolate Ligands: Elucidating Steric and Electronic Effects of Pyrazolate Ligands in Pt-Ag Sandwich Complexes. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	5
13068	Simulation Study on the Screening of Hydrophobic Surface Materials for Pipeline Drag Reduction Based on Adsorption Properties. <i>Langmuir</i> , 2022, 38, 11236-11249.	1.6	5
13069	Designing a Four-Ring Tubular Boron Motif through Metal Doping. <i>Inorganic Chemistry</i> , 2022, 61, 14553-14559.	1.9	4

#	ARTICLE	IF	CITATIONS
13070	Bivalent metal complexes of a novel Schiff base of vitamin B6: green synthesis, characterization, DFT studies, AIM analysis and antibacterial studies. <i>Research on Chemical Intermediates</i> , 0, .	1.3	0
13071	Computational study of the effects of static electric field on the interaction of 5-Fluorouracil anti-cancer drug with pristine and Sc- and Ti-doped B12P12 nanocage as drug delivery. <i>Chemical Papers</i> , 2023, 77, 277-294.	1.0	4
13074	Understanding the reaction mechanism of the CO ₂ and cyclohexene oxide copolymerization catalyzed by zinc(II) and magnesium(II) catalysts: a DFT approach. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	0
13075	Efficient Synthesis of Itaconate Polyesters with Amine-Triggered Rapid Degradation and Outstanding Mechanical Properties: An Experimental and Theoretical Study on Degradation Mechanisms. <i>Macromolecules</i> , 2022, 55, 8002-8013.	2.2	2
13076	Solubility measurement, correlation, thermodynamic analysis and molecular simulation of 1-nitronaphthalene in twelve pure solvents. <i>Journal of Molecular Liquids</i> , 2022, 367, 120475.	2.3	5
13077	Pyramid-Like Au ₂ -CNC under an External Electric Field: Charge Transfer, UV-Vis Absorption Spectra, and Nonlinear Optical Property. <i>Journal of Physical Chemistry C</i> , 2022, 126, 16236-16242.	1.5	4
13078	Understanding the Chemical Shifts of Aqueous Electrolyte Species Adsorbed in Carbon Nanopores. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 8953-8962.	2.1	1
13079	Rationalizing the Substituent Effects in Diels-Alder Reactions of Triazolinediones with Anthracene. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6657-6667.	1.1	2
13080	Microscopic reaction mechanism for CO ₂ gasification of cellulose based on reactive force field molecular dynamics simulations. <i>Renewable Energy</i> , 2022, 200, 334-343.	4.3	7
13081	Molecular oxidation-reduction junctions for artificial photosynthetic overall reaction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	18
13082	Nucleophilicity Prediction Using Graph Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 4319-4328.	2.5	6
13083	Coupling of pseudoradical centers in the synthesis of oxazine fused-spiroindoline: a two-stage one-step double cyclization. <i>Journal of Chemical Sciences</i> , 2022, 134, .	0.7	2
13084	Deciphering the role of (anti)aromaticity in cofacial excimers of linear acenes. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	4
13085	Adsorption of Chloromethine Anti-Cancer Drug on Pure and Aluminum-Doped Boron Nitride Nanocarriers: A Comparative DFT Study. <i>Pharmaceuticals</i> , 2022, 15, 1181.	1.7	7
13086	A DFT, TDDFT and QTAIM study of the acridine pincer ligand-based Ru(II) and Rh(III) complexes: detailed analysis of the metal-F bonding. <i>Chemical Papers</i> , 2023, 77, 47-61.	1.0	1
13087	Stimuli Responsive Silylene: Electromerism Induced Reversible Switching Between Mono- and Bis-Silylene. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	4
13088	Elongation of a Trigonal-Prismatic Copper Cluster by Diphosphine Ligands with Longer Spacers. <i>Inorganic Chemistry</i> , 2022, 61, 15144-15151.	1.9	5
13089	Theoretical studies on donor-acceptor based macrocycles for organic solar cell applications. <i>Scientific Reports</i> , 2022, 12, .	1.6	5

#	ARTICLE	IF	CITATIONS
13090	Theoretical perspective for the relationship between molecular structures and circularly polarised thermally activated delayed fluorescence properties. <i>Molecular Physics</i> , 0, , .	0.8	0
13091	Improved Stability of Blue Colour of Anthocyanins from <i>Lycium ruthenicum</i> Murr. Based on Copigmentation. <i>Molecules</i> , 2022, 27, 6089.	1.7	3
13092	Câ€H Insertion in Dirhodium Tetracarboxylate-Catalyzed Reactions despite Dynamical Tendencies toward Fragmentation: Implications for Reaction Efficiency and Catalyst Design. <i>Journal of the American Chemical Society</i> , 2022, 144, 17219-17231.	6.6	10
13093	Ionization of Decamethylmanganocene: Insights from the DFT-Assisted Laser Spectroscopy. <i>Molecules</i> , 2022, 27, 6226.	1.7	2
13094	Synthesis and dissolution behaviour of nateglinideâ€nicotinamide cocrystals by simple slurry crystallization. <i>Canadian Journal of Chemical Engineering</i> , 2023, 101, 2611-2620.	0.9	0
13095	Fluoride Additive as a Simple Tool to Qualitatively Improve Performance of Nickel-Catalyzed Asymmetric Michael Addition of Malonates to Nitroolefins. <i>Journal of Organic Chemistry</i> , 2022, 87, 12182-12195.	1.7	2
13096	Exploring the Photophysics of a Zn²⁺ Fluorescence Sensor and Its Sensing Mechanism. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6124-6134.	1.1	0
13097	Exploring the pyrolysis chemistry of 1,3,5-trimethylcyclohexane with insight into fuel isomeric and multiple substitution effects. <i>Proceedings of the Combustion Institute</i> , 2022, , .	2.4	0
13098	Weak interactions between epinephrine and thymine. <i>Letters in Organic Chemistry</i> , 2022, 19, .	0.2	0
13099	Singlet Fission from Upper Excited States of Bodipy Crystalline Film and Single Crystal. <i>Journal of Physical Chemistry C</i> , 2022, 126, 17212-17222.	1.5	3
13100	Mechanism of Ultrafast Triplet Exciton Formation in Single Cocrystals of Î€-Stacked Electron Donors and Acceptors. <i>Journal of the American Chemical Society</i> , 2022, 144, 18607-18618.	6.6	16
13101	Spiropyran/Merocyanine Amphiphile in Various Solvents: A Joint Experimentalâ€Theoretical Approach to Photophysical Properties and Self-Assembly. <i>International Journal of Molecular Sciences</i> , 2022, 23, 11535.	1.8	1
13102	Size-dependent adsorption performance of ZnO nanoclusters for drug delivery applications. <i>Structural Chemistry</i> , 2023, 34, 1061-1071.	1.0	9
13103	Theoretical Insights into Phenanthroline-Based Ligands toward the Separation of Am(III)/Eu(III). <i>Inorganic Chemistry</i> , 2022, 61, 15423-15431.	1.9	8
13104	Halogen Bonding Involving Gold Nucleophiles in Different Oxidation States. <i>Inorganic Chemistry</i> , 2022, 61, 15398-15407.	1.9	13
13105	Solid-liquid convertible fluorinated terthiophene as additives in mediating morphology and performance of organic solar cells. <i>Chemical Engineering Journal</i> , 2023, 453, 139489.	6.6	9
13106	Systematic research on gallium atom-doped neutral small- and medium-sized gas-phase magnesium clusters: A DFT study of GaMg_n (n=2â€12) clusters. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	8
13107	Methane Activation by Vanadium Oxide Cluster Anions (V₂O₅)<i> _N</i>O^{âˆ™} (<i>N</i> = 1âˆ™18). <i>Journal of Chemical Physics</i> , 0, , .	1.2	4

#	ARTICLE	IF	CITATIONS
13108	From Density Functional Theory to Conceptual Density Functional Theory and Biosystems. <i>Pharmaceuticals</i> , 2022, 15, 1112.	1.7	11
13109	Long-term corona behaviour and performance enhancing mechanism of SiC/epoxy nanocomposite in SF ₆ gas environment. <i>Plasma Science and Technology</i> , 2023, 25, 035501.	0.7	1
13110	Facile Access to 2-Selenoxo-1,2,3,4-tetrahydro-4-quinazolinone Scaffolds and Corresponding Diselenides via Cyclization between Methyl Anthranilate and Isoselenocyanates: Synthesis and Structural Features. <i>Molecules</i> , 2022, 27, 5799.	1.7	4
13111	CO ₂ Adsorption over 3d Transition-Metal Nanoclusters Supported on Pyridinic N ₃ -Doped Graphene: A DFT Investigation. <i>Materials</i> , 2022, 15, 6136.	1.3	3
13112	Insight into the Formation of Cocrystal and Salt of Tenoxicam from the Isomer and Conformation. <i>Pharmaceutics</i> , 2022, 14, 1968.	2.0	9
13113	Probing the Hyperconjugative Aromaticity of Cyclopentadiene and Pyrroliums Containing Group 7 Transition Metal Substituents. <i>Organometallics</i> , 2022, 41, 2742-2752.	1.1	5
13114	2-(Pyridin-2-ylmethylene)indan-1-ones: The first study of E/Z isomerization of cyclic chalcones with electron-deficient hetaryl moiety. <i>Tetrahedron</i> , 2022, 123, 133005.	1.0	1
13115	Pentacoordinate Carbon Atoms in a Ferrocene Dication Derivative [Fe(Si ₂ - $\dot{\text{I}}$ -5-C ₅ H ₂) ₂] ²⁺ . <i>Chemistry</i> , 2022, 4, 1092-1100.	0.9	4
13116	Cluster formation between an oxadiazole derivative with metal nanoclusters (Ag/Au/Cu), graphene quantum dot sheets, SERS studies, and solvent effects. <i>Structural Chemistry</i> , 2023, 34, 867-877.	1.0	6
13117	Organocatalytic synthesis of chiral allene catalyzed by chiral phosphoric acid via asymmetric 1,8-addition of indole imine methide: Mechanism and origin of enantioselectivity. <i>Molecular Catalysis</i> , 2022, 530, 112648.	1.0	1
13118	A theoretical investigation on the interaction mechanism between 1-methyl-3,4,5-trinitropyrazole and 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane. <i>Chemical Papers</i> , 2023, 77, 451-461.	1.0	2
13119	Super-Excimer: Anomalous Bonding in a Metastable Excited-State Dimer of Superatomic Dimers. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 8455-8461.	2.1	2
13120	Manifesting Direction-Specific Complexation in [HFIP ₂ ⋯H ₂ O ₂] ⁺ : Exclusive Formation of a High-Lying Conformation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 8607-8612.	2.1	3
13121	Effects of the pH Value on the Electrodeposition of Fe-P Alloy as a Magnetic Film Material. <i>Journal of Physical Chemistry C</i> , 2022, 126, 15472-15484.	1.5	6
13122	Structural prediction of anion thiolate protected gold clusters of [Au _{28+7n} (SR) _{17+3n}] ⁺ (n = 0-4). <i>Journal of Chemical Physics</i> , 2022, 157, 124303.	1.2	2
13123	Explaining the High Catalytic Activity in Bis(indenyl) Methyl Zirconium Cation Using Combined EDA-NOCV/QTAIM Approach. <i>ChemPhysChem</i> , 0, , .	1.0	1
13124	Experimental Spectroscopic, Quantum Chemical, Molecular Docking, and Molecular Dynamic Simulation Studies on Hydantoin (Monomer and Dimer). <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 6627-6653.	1.4	0
13125	Gelation behavior and mechanism of <i>Nicandra physalodes</i> (Linn.) Gaertn. seeds pectin induced by Glucono- δ -lactone. <i>Carbohydrate Polymers</i> , 2023, 299, 120151.	5.1	8

#	ARTICLE	IF	CITATIONS
13126	Regulating the Acidity of SO ₃ H ⁺ -Functionalized Ionic Liquids: Hydrogen Bonding or Electrostatic Potential?. <i>ChemPlusChem</i> , 0, , .	1.3	0
13127	Redox induced electron transfer in lithium polysulfide â€“ A DFT study. <i>Journal of Sulfur Chemistry</i> , 2023, 44, 1-11.	1.0	2
13128	Annihilating Actinic Photochemistry of the Pyruvate Anion by One and Two Water Molecules. <i>Journal of the American Chemical Society</i> , 2022, 144, 19317-19325.	6.6	5
13129	Theoretical Investigation of the Mechanism of Rh(III)-catalyzed Annulation of 2-Biphenylboronic Acid with Activated Alkene. <i>Chemical Research in Chinese Universities</i> , 0, , .	1.3	0
13130	Curcumin and Diclofenac Therapeutic Efficacy Enhancement Applying Transdermal Hydrogel Polymer Films, Based on Carrageenan, Alginate and Poloxamer. <i>Polymers</i> , 2022, 14, 4091.	2.0	6
13131	Unusual Enantiodivergence in Chiral Br ⁺ -catalyzed Asymmetric Allylation with ² Alkenyl Allylic Boronates. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	9
13132	Unique Dispersion-Induced Tetrel Bond with Co-operative π -hole-Induced Pnicogen Bond in the POCl ₃ -Acetone Heterodimer: Experimental Confirmation at Low Temperatures. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6637-6647.	1.1	1
13133	Stacking Interactions: A Supramolecular Approach to Upgrade Weak Halogen Bond Donors. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	9
13134	Deep Trap Origins, Characteristics, and Related Mechanisms in Chemically Grafted Polypropylene with Enhanced Direct Current Volume Resistivity. <i>Journal of Physical Chemistry C</i> , 2022, 126, 16280-16288.	1.5	9
13135	â€“Holes in Iodonium Ylides: Halogenâ€“Bond Activation of Carboxylic Acids, Phenols and Thiophenols May Enable Their Xâ€“H Insertion Reactions. <i>Chemistry - A European Journal</i> , 0, , .	1.7	2
13136	An insight into interaction of the uracil, thymine and cytosine biomolecules with methimazole anti-thyroid drug: DFT and GD3â€“DFT approaches. <i>Structural Chemistry</i> , 0, , .	1.0	2
13137	Computational study of the relative stability of some glass-ionomer cement-forming molecules. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	1
13138	High-Voltage and Intrinsically Safe Sodium Metal Batteries Enabled by Nonflammable Fluorinated Phosphate Electrolytes. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 43387-43396.	4.0	7
13139	Abietane diterpenoids from <i>Phlegmariusus carinatus</i> and their biological activities. <i>Phytochemistry</i> , 2022, 204, 113457.	1.4	2
13140	On the Periodicity of the Information Theory and Conceptual DFT-Based Reactivity Descriptors. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6801-6813.	1.1	1
13141	Rapid 3D roll-up of gas-phase planar gold clusters and affinity and alienation for Mg and Ge: A theoretical study of MgGeAu _n (n=1â€“12) clusters. <i>IScience</i> , 2022, 25, 105215.	1.9	5
13142	Detection of Carbon, Sulfur, and Nitrogen Dioxide Pollutants with a 2D Ca ₁₂ O ₁₂ Nanostructured Material. <i>ACS Omega</i> , 2022, 7, 34929-34943.	1.6	17
13143	Theoretical investigation of the mechanism of ethanol to propene catalyzed by phosphorus-modified FAU zeolite. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	2

#	ARTICLE	IF	CITATIONS
13145	Clustering Analysis, Structure Fingerprint Analysis, and Quantum Chemical Calculations of Compounds from Essential Oils of Sunflower (<i>Helianthus annuus</i> L.) Receptacles. <i>International Journal of Molecular Sciences</i> , 2022, 23, 10169.	1.8	2
13146	Quantum chemistry calculation and experimental research on the component proportion of black disperse dye. <i>Textile Research Journal</i> , 2023, 93, 750-761.	1.1	1
13147	DFT calculations, structural analysis, solvent effects, and non-covalent interaction study on the para-aminosalicylic acid complex as a tuberculosis drug: AIM, NBO, and NMR analyses. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	2
13148	Properties and Stabilities of Cyclic and Open Chains of Halogen Bonds. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6443-6455.	1.1	6
13149	Substituent Effect on Vibrationally Resolved Absorption Spectra and Exciton Dynamics of Dipyrrolonaphthyridinedione Aggregates. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6395-6406.	1.1	3
13150	In silico exploration of noble gas dimer enforced by noncovalent interaction. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	3
13151	Synthesis, Crystal Structure, and Properties of Phenylsilicon(IV) Bis-catecholate Complexes. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2022, 48, 647-658.	0.3	1
13152	Annealing, solvation, and mirror-plating effects in phosphonium chloroaluminate ionic liquids. <i>Nano Research</i> , 0, , .	5.8	0
13153	Fabrication of the polyethersulfone/functionalized mesoporous carbon nanocomposite nanofiltration membrane for dyes and heavy metal ions removal: Experimental and quantum mechanical simulation method. <i>Polymers for Advanced Technologies</i> , 0, , .	1.6	1
13154	The key role of molecular aggregation in rechargeable organic cathodes. <i>Matter</i> , 2022, 5, 4467-4479.	5.0	7
13155	Theoretical investigation of the effect of O M $\{TiZr\}$	1.3	4
13156	Costunolide covalently targets NACHT domain of NLRP3 to inhibit inflammasome activation and alleviate NLRP3-driven inflammatory diseases. <i>Acta Pharmaceutica Sinica B</i> , 2023, 13, 678-693.	5.7	16
13157	Intrinsic Analysis of Thermally Activated Delayed Fluorescence (TADF) for Ag(I) Complex Based on the Path Integral Approach: Origin of the Effective Spin-Flipping Channel and Vibrational Spin-Orbit Coupling Effect. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6695-6709.	1.1	2
13158	Xanthine oxidase inhibitory study of eight structurally diverse phenolic compounds. <i>Frontiers in Nutrition</i> , 0, 9, .	1.6	9
13159	Application of DFT Calculations in Designing Polymer-Based Drug Delivery Systems: An Overview. <i>Pharmaceutics</i> , 2022, 14, 1972.	2.0	15
13161	Unique Fluorescence Turn-On and Turn-Off Responses to Acids by a Carbazole-Based Metal-Organic Framework and Theoretical Studies. <i>Journal of the American Chemical Society</i> , 2022, 144, 17054-17063.	6.6	36
13162	Semi-Empirical Calculation of Bodipy Aggregate Spectroscopic Properties through Direct Sampling of Configurational Ensembles. <i>International Journal of Molecular Sciences</i> , 2022, 23, 10955.	1.8	1
13163	Novel family of nitrogen-rich energetic (1,2,4-triazoly) furoxan salts with balanced performance. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	8

#	ARTICLE	IF	CITATIONS
13165	Degradation mechanism of BPA under VUV irradiation: efficiency contribution and DFT calculations. <i>Environmental Science and Pollution Research</i> , 2023, 30, 12813-12824.	2.7	4
13166	Sb-Fe bimetallic non-aqueous phase desulfurizer for efficient absorption of hydrogen sulfide: A combined experimental and DFT study. <i>Korean Journal of Chemical Engineering</i> , 2022, 39, 3305-3314.	1.2	4
13167	High efficient room temperature phosphorescent materials constructed with methylene molecular configuration. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	1
13168	Computational Design of Crescent Shaped Promising Nonfullerene Acceptors with 1,4-Dihydro-2,3-quinoxalinedione Core and Different Electron-withdrawing Terminal Units for Photovoltaic Applications. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7110-7126.	1.1	2
13169	Structural evolution and electronic properties of pure and semiconductor atom doped in clusters: $\text{In}^{\text{+}}$, $\text{In}^{\text{-}}$, $\text{Si}^{\text{+}}$, and $\text{Ge}^{\text{+}}$ ($\text{In}^{\text{+}}$ = 16). <i>Journal of Computational Chemistry</i> , 2022, 43, 1978-1984.	1.5	9
13170	Polyamide composite membranes for enhanced organic solvent nanofiltration performance by metal ions assisted interfacial polymerization method. <i>AIChE Journal</i> , 2023, 69, .	1.8	7
13171	Understanding the influence of alkyl-chains and hetero-atom (C, S, O) doped electron-acceptor fullerene-free benzothiazole for application in organic solar cell: first principle perception. <i>Optical and Quantum Electronics</i> , 2022, 54, .	1.5	14
13172	Polarity-triggered anti-Kasha system for high-contrast cell imaging and classification. <i>Aggregate</i> , 2023, 4, .	5.2	1
13173	Aziridination Reactivity of a Manganese(II) Complex with a Bulky Chelating Bis(Alkoxide) Ligand. <i>Molecules</i> , 2022, 27, 5751.	1.7	0
13175	Density functional theory studies on N4 and N8 species: Focusing on various structures and excellent energetic properties. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	5
13177	Synthesis and X-ray Characterization of 4,5-Dihydropyrazolyl-Thiazoles Bearing a Coumarin Moiety: On the Importance of Antiparallel π -Stacking. <i>ChemistrySelect</i> , 2022, 7, .	0.7	8
13178	Halogenated Zn^{2+} Solvation Structure for Reversible Zn Metal Batteries. <i>Journal of the American Chemical Society</i> , 2022, 144, 18435-18443.	6.6	95
13179	Competitor hydrogen-bond acceptors in the $\text{SP}(\text{NH})_3$ -based structures: Comparison of structural features - computational/database and experimental. <i>Polyhedron</i> , 2022, , 116157.	1.0	0
13180	Mixed-Isocyanide Complexes of Technetium under Steric and Electronic Control. <i>Inorganic Chemistry</i> , 2022, 61, 16163-16176.	1.9	10
13181	Synthetic Doping of Acenaphthylene through BN/CC Isosterism and a Direct Comparison with BN-Acenaphthene. <i>Journal of Organic Chemistry</i> , 2022, 87, 12986-12996.	1.7	4
13182	A comprehensive theoretical investigation on the thiophene hydrodesulphurisation mechanism over sulphided Co-Mo catalysts supported by ZSM-5, FAU, Beta and MCM-22 zeolites. <i>Molecular Simulation</i> , 0, , 1-24.	0.9	0
13183	Nitrogen-rich polycyclic pentazolates as promising energetic materials: theoretical investigating. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	1
13184	Van der Waals Interaction-Driven Self-Assembly of V_2O_5 Nanoplates and MXene for High-Performing Zinc-Ion Batteries by Suppressing Vanadium Dissolution. <i>ACS Nano</i> , 2022, 16, 14539-14548.	7.3	100

#	ARTICLE	IF	CITATIONS
13185	Molecular Dynamics Research of Spatial Orientation and Kinetic Energy of Active Site Collision of Carnosine under Weak Microwave Irradiation. <i>Journal of Physical Chemistry B</i> , 2022, 126, 7686-7700.	1.2	6
13186	Expanding the Knowledge of the Selective-Sensing Mechanism of Nitro Compounds by Luminescent Terbium Metal-Organic Frameworks through Multiconfigurational <i>ab Initio</i> Calculations. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7040-7050.	1.1	8
13187	Ti ₂ CT ₂ MXene as Anodes for Metal Ion Batteries: From Monolayer to Bilayer to Pillar Structure. <i>Langmuir</i> , 2022, 38, 11732-11742.	1.6	9
13188	Conformers of Vanillic Acid and Its Monohydrate: A Rotational Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6686-6694.	1.1	2
13189	Iridium-Catalyzed Stereoselective Transfer Hydrogenation of 1,5-Benzodiazepines. <i>Journal of Organic Chemistry</i> , 2022, 87, 12001-12018.	1.7	10
13190	Metal-Support Interactions in Molecular Single-Site Cluster Catalysts. <i>Journal of the American Chemical Society</i> , 2022, 144, 18459-18469.	6.6	8
13191	A Water-Stable and Red-Emissive Radical Cation for Mutp53 Cancer Therapy. <i>Angewandte Chemie</i> , 0, , .	1.6	0
13192	Stable borosilicate glass doped with CsPbBr ₃ quantum dots for efficient photodetectors. <i>Ceramics International</i> , 2023, 49, 1283-1290.	2.3	4
13193	Characterizing the Interactions of Dimethyl Sulfoxide with Water: A Rotational Spectroscopy Study. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6882-6889.	1.1	2
13194	The surface and encapsulated storage of H ₂ on Ga ₁₂ N ₁₂ . <i>International Journal of Hydrogen Energy</i> , 2022, 47, 33382-33390.	3.8	2
13195	Infrared intensities of B_{6C}^{2-} : a true challenge for DFT methods. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	0
13196	On closed-shell interactions between heavy main-group elements. <i>Journal of Computational Chemistry</i> , 2022, 43, 1985-1996.	1.5	2
13197	Linear Axially Chiral Conjugated Polymers Exhibiting Ultralong Low-Temperature Phosphorescence and Intense Circularly Polarized Luminescence. <i>Angewandte Chemie</i> , 0, , .	1.6	0
13198	Direct carboxylation of thiophene with CO ₂ in the solvent-free carboxylate-carbonate molten medium: Experimental and mechanistic insights. <i>Chinese Journal of Chemical Engineering</i> , 2022, 50, 264-282.	1.7	0
13199	Copper(I) iodide complex with 4-pyridinecarboxaldehyde ligand: Synthesis, spectroscopic characterisation, AIM and NCI analysis combined with molecular docking and antibacterial activity studies. <i>Journal of Molecular Structure</i> , 2023, 1273, 134279.	1.8	1
13200	Transient Absorption Spectroscopy of a Carbazole-Based Room-Temperature Phosphorescent Molecule: Real-Time Monitoring of Singlet-Triplet Transitions. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 9381-9389.	2.1	14
13201	Design, synthesis, and insecticidal activity of a novel series of flupyrimin analogs bearing 1-aryl-1H-pyrazol-4-yl subunits. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	0
13202	Designing of symmetrical A-D-A type non-fullerene acceptors by side-chain engineering of an indacenodithienothiophene (IDTT) core based molecule: A computational approach. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113904.	1.1	28

#	ARTICLE	IF	CITATIONS
13203	Interaction, bioaccessibility and stability of bovine serum albumin-gamma-oryzanol complex: Spectroscopic and computational approaches. <i>Food Chemistry</i> , 2023, 402, 134493.	4.2	5
13204	Synthesis, antibacterial, antifungal and computational study of (E)-4-(3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-3-oxoprop-1-en-1-yl)benzotrile. <i>Results in Chemistry</i> , 2022, 4, 100553.	0.9	13
13205	Liquid Crystal Nanoparticle Actuator by Polymer Surfactant-Assisted Assembly for Fabricating Bioinspired Smart Interface with Adjustable Light and Changeable Color. <i>ACS Applied Nano Materials</i> , 2022, 5, 15498-15506.	2.4	0
13206	Integrated Spectroscopic, Bio-active Prediction and Analytics of Isoquinoline Derivative for Breast Cancer Mitigation. <i>Chemistry Africa</i> , 2022, 5, 1979-1995.	1.2	30
13207	Solvent-driven micro/nanostructures of squaraine and croconaine dyes based on quinoxalinone for visual detection of nerve agent simulants. <i>Dyes and Pigments</i> , 2022, 208, 110824.	2.0	3
13208	The Linkage of Sulfonimidoyl Fluorides and Unactivated Alkenes via Hydrosulfonimidoylation. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	22
13209	The Linkage of Sulfonimidoyl Fluorides and Unactivated Alkenes via Hydrosulfonimidoylation. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	1
13210	Oxidative Radical NHC Catalysis: Divergent Difunctionalization of Olefins through Intermolecular Hydrogen Atom Transfer. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	30
13211	Atomic and Superatomic Orbital Interactions in In ₈ FeN _n Clusters. <i>Journal of Cluster Science</i> , 2023, 34, 1953-1964.	1.7	1
13212	Tuning the visible-NIR absorption of azulocyanine-based photosensitizers. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	1
13213	H ₂ and CO adsorption ability of cationic lithiated carbenes: A computational study. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 39917-39930.	3.8	1
13214	Influence of Pt decoration on the hydrogen storage performance of cup-stacked carbon nanotubes: A DFT study. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 39193-39203.	3.8	6
13215	Solvent effects on the interaction between alkali metal cations and 1,3-Diisopropoxycalix [4] arene-crown-6: Nuclear magnetic resonance spectroscopy and Independent Gradient Model Non-Covalent interactions analysis. <i>Journal of Molecular Liquids</i> , 2022, 367, 120534.	2.3	2
13216	Theoretical Insights into the Geometrical Evolution, Photoelectron Spectra, and Vibrational Properties of YGe _n ⁺ ($n = 6\text{--}20$) Anions: From Y-Linked to Y-Encapsulated Structures. <i>ACS Omega</i> , 2022, 7, 36330-36342.	1.6	2
13217	Dynamic Disulfide Bonds Contained Covalent Organic Framework Modified Separator as Efficient Inhibit Polysulfide Shuttling in Li-S Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 13638-13649.	3.2	7
13218	Effect of Ligand Structures on Ligand-Protected Gold Clusters: [Au ⁺ (p <i>m</i> -o-MBT)] ₈ Clusters. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7193-7201.	1.1	0
13219	In-situ growth of 2D magnesium hydroxide on zirconium-based metal organic frameworks for phosphate removal: An experimental and theoretical exploration of adsorption behavior. <i>Separation and Purification Technology</i> , 2023, 304, 122289.	3.9	7
13220	-Comparison of σ -hole aerogen-bonding interactions based on C ₂ H ₄ NgOX ₂ (Ng = Kr, Xe; X = F, Cl, Br) complexes. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	2

#	ARTICLE	IF	CITATIONS
13221	Synthesis, spectroscopic, topological, hirshfeld surface analysis, and anti-covid-19 molecular docking investigation of isopropyl 1-benzoyl-4-(benzoyloxy)-2,6-diphenyl-1,2,5,6-tetrahydropyridine-3-carboxylate. Heliyon, 2022, 8, e10831.	1.4	18
13222	Theoretical probing into complexation of Si-5LIO-1-Cm-3,2-HOPO with Uranyl. Theoretical Chemistry Accounts, 2022, 141, .	0.5	6
13223	Metal Confined in 2D Membranes for Molecular Recognition and Sieving towards Ethylene/Ethane Separation. Advanced Materials, 2022, 34, .	11.1	21
13224	Electrochemical behavior and interfacial bonding mechanism of new synthesized carbocyclic inhibitor for exceptional corrosion resistance of steel alloy: DFTB, MD and experimental approaches. Arabian Journal of Chemistry, 2022, 15, 104323.	2.3	13
13225	Synthesis, X-ray and DFT Studies of 6-halo-3-(hydroxymethyl)cinnolin-4(1H)-ones. Chemistry of Heterocyclic Compounds, 2022, 58, 432-437.	0.6	5

13226 Synthesis, X-Ray Diffraction, DFT and Hirshfeld Surface Studies of

#	ARTICLE	IF	CITATIONS
13239	Ionothermal Synthesis of Fully Conjugated Covalent Organic Frameworks for High Capacity and Ultrastable Potassium-Ion Batteries. <i>Advanced Materials</i> , 2022, 34, .	11.1	31
13240	FOX-7 based nitrogen rich green energetic salts: Synthesis, characterization, propulsive and detonation performance. <i>Chemical Engineering Journal</i> , 2023, 452, 139600.	6.6	14
13241	Bonding nature, nucleophilic reactivity and electron excitation of NLO active 2,6 dichloroindophenol sodium salt (polar and non polar solvents) with topology analysis- bacterial pathogens study. <i>Journal of Molecular Liquids</i> , 2022, 367, 120533.	2.3	7
13242	Structure, bonding, and interaction with molecular hydrogen of the β -D-glucopyranose-silver ⁺ (1:1) complex. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	2
13243	Structure-properties relationships of deep eutectic solvents formed between choline chloride and carboxylic acids: Experimental and computational study. <i>Journal of Molecular Structure</i> , 2023, 1273, 134283.	1.8	11
13244	MXene (Ti3T2CX)-reinforced thin-film polyamide nanofiltration membrane for short-chain perfluorinated compounds removal. <i>Chemical Engineering Research and Design</i> , 2022, 168, 275-284.	2.7	14
13245	Effect of Entrainer Thermodynamic Properties on the Separation of Ternary Mixtures Containing Two Minimum Boiling Azeotropes by Extractive Distillation. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 15273-15288.	1.8	13
13246	Experimental and computation studies of a Zn(II) coordination complex with isophthalic acid and benzimidazole as ligands. <i>Journal of Molecular Structure</i> , 2023, 1273, 134290.	1.8	1
13247	Insights into atomically dispersed reactive centers on g-C3N4 photocatalysts for water splitting. , 2023, 2, 100094.		18
13248	Critical role of tetracycline's self-promotion effects in its visible-light driven photocatalytic degradation over ZnO nanorods. <i>Chemosphere</i> , 2022, 309, 136691.	4.2	7
13249	New task-specific ionic liquids based on phenyl diazenyl methyl pyridinium cation: Energetic, electronic and optical properties exploration based on DFT calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 118, 108352.	1.3	2
13250	The effect of enantioselective chiral covalent organic frameworks and cysteine sacrificial donors on photocatalytic hydrogen evolution. <i>Nature Communications</i> , 2022, 13, .	5.8	59
13251	Color-tunable and high-quantum-yield afterglow of carbon dots by covalent fixation. <i>Journal of Luminescence</i> , 2022, 252, 119399.	1.5	5
13252	Edge carboxylation-induced charge separation dynamics of graphene quantum dot/cellulose nanocomposites. <i>Carbohydrate Polymers</i> , 2023, 299, 120190.	5.1	2
13253	Effective adsorption of Congo red dye by magnetic chitosan prepared by solvent-free ball milling. <i>Materials Chemistry and Physics</i> , 2022, 292, 126857.	2.0	15
13254	Chiral-Cage Carboranes for Circularly Polarized Luminescence and Aggregation-Induced Electrochemiluminescence. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	12
13255	Amino-group excites vitality in nitrogen-rich energetic salts of triazolium. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 0, , .	0.6	1
13256	An Electronic Structure Study of the Conversion from 1,2-diphenylacetylene to (E)-1,2-diphenylethene Using a Bidentate Ru(II) -NC Catalyst. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	0

#	ARTICLE	IF	CITATIONS
13257	Experimental and Theoretical Study on the Interactions between Dopamine Hydrochloride and Vitamin B6 Hydrochloride. Russian Journal of Physical Chemistry A, 2022, 96, 2299-2306.	0.1	1
13258	Theoretical Study for Evaluating and Discovering Organic Hydride Compounds as Potential Novel Methylation Reagents. ACS Omega, 0, , .	1.6	0
13260	Heteroleptic Dysprosium(III) Single-Molecule Magnets with Amidinate and Cyclopentadienyl Ligands. Crystal Growth and Design, 2022, 22, 6398-6404.	1.4	5
13262	Improved solubility and hygroscopicity of enoxacin by pharmaceutical salts formation with hydroxybenzoic acids via charge assisted hydrogen bond. Journal of Molecular Structure, 2023, 1273, 134272.	1.8	4
13263	Synthesis and structural investigation of mononuclear penta- and hexa-coordinated Co complexes of 8-hydroxyquinoline derived ligands. Journal of Molecular Structure, 2023, 1273, 134253.	1.8	0
13264	Conformational Landscape and Properties of Psilocybin: A Computational Approach. ChemistrySelect, 2022, 7, .	0.7	2
13265	Screening single metal atom supported on h-BN as the efficient adsorptive desulfurization adsorbent. Structural Chemistry, 2023, 34, 1105-1114.	1.0	1
13266	Chemiluminescent gels of G-quadruplexes in deep eutectic solvents. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 655, 130319.	2.3	5
13267	Alternating 1-Phenyl-2,2,2-Trifluoroethanol Conformational Landscape With the Addition of One Water: Conformations and Large Amplitude Motions. Journal of Physical Chemistry A, 2022, 126, 7250-7260.	1.1	10
13268	Interlayer adsorption of cationic dye on cationic surfactant-modified and unmodified montmorillonite. Journal of Hazardous Materials, 2023, 442, 130107.	6.5	38
13269	Computational study of novel pentacene derivatives: Prediction of structural, electronic, and optical properties. Journal of Physical Organic Chemistry, 2023, 36, .	0.9	0
13270	Molecular-based asphalt oxidation reaction mechanism and aging resistance optimization strategies based on quantum chemistry. Materials and Design, 2022, 223, 111225.	3.3	11
13271	Spectroscopic (FT-IR, FT-Raman) investigation, topological (QTAIM, RDC, ELF) analysis, drug-likeness and anti-inflammatory activity study on 2-methylaminobenzoic acid alkaloid. Journal of Molecular Structure, 2023, 1273, 134261.	1.8	7
13272	Oxidative Radical NHC Catalysis: Divergent Difunctionalization of Olefins through Intermolecular Hydrogen Atom Transfer. Angewandte Chemie, 2022, 134, .	1.6	1
13273	Mechanistic Study on Palladium-Catalyzed Cycloaddition of Vinyl ethylene Carbonates with $\hat{1},\hat{2}$ -Unsaturated Imines. Organometallics, 2022, 41, 2844-2853.	1.1	1
13274	Supramolecular and theoretical investigation of copper(II) complexes containing 2,2'-bipyridine and substituted chalcone ligands: Estimation of non-covalent interactions. Journal of Molecular Structure, 2023, 1273, 134271.	1.8	4
13275	The overlooked role of Co(OH) ₂ in Co ₃ O ₄ activated PMS system: Suppression of Co ²⁺ leaching and enhanced degradation performance of antibiotics with rGO. Separation and Purification Technology, 2023, 304, 122203.	3.9	13
13276	Intensification of High Boiling Point Organic Solvents on SO ₂ Absorption in Deep Eutectic Solvents Formed by Hydroxypyridine and 1-Butyl-3-methylimidazolium Chloride. Journal of Chemical & Engineering Data, 2022, 67, 3435-3442.	1.0	3

#	ARTICLE	IF	CITATIONS
13277	Crystal growth, crystal structure determination, and computational studies of a new mixed $(\text{NH}_4)_2\text{Mn}_x\text{Zn}_{1-x}(\text{SO}_4)_2(\text{H}_2\text{O})_6$ Tutton salt. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	5
13278	Hydrogen bonds interactions in biuret-water clusters: FTIR, X-ray diffraction, AIM, DFT, RDG, ELF, NLO analysis. <i>Journal of King Saud University - Science</i> , 2022, 34, 102350.	1.6	71
13279	Effect of co-toxicity of lead and nanoplastics on the flavonoid biosynthetic pathway in dandelion (<i>Taraxacum asiaticum</i> Dahlst). <i>Planta</i> , 2022, 256, .	1.6	8
13280	Paracetamol adsorption on C60 fullerene and its derivatives: In silico insights. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100769.	1.3	4
13281	Hofmann-MOF-derived CoFeNi nanoalloy@CNT as a magnetic activator for peroxymonosulfate to degrade benzophenone-1 in water. <i>Journal of Alloys and Compounds</i> , 2023, 937, 165189.	2.8	10
13282	Formal Pericyclic-Coupled Electron Transfer: I. Stepwise Formal Diels-Alder Cycloaddition Enabled by Addition-Coupled Electron Transfer. <i>ChemistrySelect</i> , 2022, 7, .	0.7	2
13283	Understanding electronic structures, chemical bonding, and fluxional behavior of $\text{Lu}_2\text{@C}_{2n}$ ($2n = 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 36, 38, 40, 42, 44, 46, 48, 50$) Endohedral Fullerenes. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 11511.	1.2	4
13284	Development of a novel poly-pseudorotaxane poly (m-phenylene isophthalamide) membrane with a biomimetic surface for effective oil-in-water emulsion separation. <i>Journal of Water Process Engineering</i> , 2022, 49, 103154.	2.6	0
13285	Experimental and Theoretical Studies on the Interaction of Dopamine Hydrochloride with Nicotinic Acid. <i>Journal of Solution Chemistry</i> , 0, , .	0.6	1
13286	Microsolvation of electrons by a handful of ammonia molecules. <i>Journal of Chemical Physics</i> , 2022, 157, 134301.	1.2	3
13287	Alkali-catalyzed hydrothermal oxidation treatment of triclosan in soil: Mechanism, degradation pathway and toxicity evaluation. <i>Science of the Total Environment</i> , 2023, 856, 159187.	3.9	3
13288	Metal-Halide Coordination Polymers with Excitation Wavelength- and Time-Dependent Ultralong Room-Temperature Phosphorescence. <i>Inorganic Chemistry</i> , 2022, 61, 16477-16483.	1.9	14
13289	Intermolecular copigmentation between anthocyanidin-3,5-O-diglucosides and three phenolic compounds: Insights from experimental and theoretical studies. , 2022, 1, 100111.		1
13290	Insight into the weak interaction between organic primary amine and propionic acid or phenol solvents in solvent extraction. <i>Journal of Molecular Liquids</i> , 2022, 367, 120524.	2.3	2
13291	Directional Self-Assembly of Ofloxacin and Syringic Acid: The First Salt Cocrystal of Ofloxacin with Phenolic Acid Displays Superior <i>In Vitro/Vivo</i> Biopharmaceutical Property and Enhanced Antibacterial Activity. <i>Crystal Growth and Design</i> , 0, , .	1.4	4
13292	Sensitivity of coupled cluster electronic properties on the reference determinant: Can Kohn-Sham orbitals be more beneficial than Hartree-Fock orbitals?. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	4
13293	The fluorescence mechanism of a probe based on benzothiazole group to detect HClO. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	2
13294	Comprehensive theoretical prediction of the stability and electronic properties of hydroxyurea and carmustine drugs on pristine and Chitosan-functionalized graphitic carbon nitride in vacuum and aqueous environment. <i>Vacuum</i> , 2023, 207, 111565.	1.6	6

#	ARTICLE	IF	CITATIONS
13295	Stabilized N coordinated Cu site in catalytic ozonation: The efficient generation of OH induced by surface hydroxyl groups based on the Lewis acid site. <i>Separation and Purification Technology</i> , 2023, 304, 122215.	3.9	9
13296	Natural Lignin: A Sustainable and Cost-Effective Electrode Material for High-Temperature Na-Clon Battery. <i>Energy and Environmental Materials</i> , 2024, 7, .	7.3	9
13297	Insight into the probe BTFMB responses to hydrogen peroxide switching on ESIPT reaction. <i>Chemical Physics Letters</i> , 2022, 807, 140067.	1.2	1
13298	Deciphering the cooperative effect of base and N-substituents on the origin of enantioselectivity switching for Mannich reactions of glycinate by carbonyl catalysts. <i>Journal of Catalysis</i> , 2022, 415, 1-11.	3.1	4
13299	Nonlinear optical activity of piperazine-1,4-dium bis(sulfanilate) compound. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113896.	1.1	8
13300	Theoretical structural analysis (FT-IR, FT-R), solvent effect on electronic parameters NLO, FMO, NBO, MEP, UV (IEFPCM model), Fukui function evaluation with pharmacological analysis on methyl nicotinate. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113890.	1.1	30
13301	Designing easily synthesizable non-fused small acceptors for organic solar cells. <i>Solar Energy</i> , 2022, 246, 23-35.	2.9	17
13302	Developing two thiocarbonylhydrazide modified glucose derivatives as high-efficiency green corrosion inhibitors for carbon steel. <i>Industrial Crops and Products</i> , 2022, 188, 115680.	2.5	12
13303	Near-infrared fluorescent probe with a large Stokes shift for bioimaging of β -galactosidase in living cells and zebrafish develop at different period. <i>Analytica Chimica Acta</i> , 2022, 1232, 340459.	2.6	6
13304	Coprecipitation of ferrihydrite, enoxacin, and citrate for their transformation. <i>Journal of Cleaner Production</i> , 2022, 376, 134241.	4.6	3
13305	DFT, solvation effects, reactivity and SERS analysis on structural, optical, and vibrational properties of a biomolecule of pyrimidine derivative adsorbed on metal clusters of Ag/Au/Cu. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100753.	1.3	9
13306	Triphenylamine derivatives functionalized di-ureasil hybrids for information encipherment. <i>Chemical Engineering Journal Advances</i> , 2022, 12, 100411.	2.4	1
13307	Role of trace TEMPO as electron shuttle in enhancing chloroquine phosphate elimination in UV-LED-driven persulfate activation process. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108641.	3.3	9
13308	Adsorption sites and electron transfer characteristics of methyl orange on three-dimensional hierarchical flower-like nanostructures of Co-Al-layered double hydroxides: Experimental and DFT investigation. <i>Separation and Purification Technology</i> , 2022, 303, 122282.	3.9	6
13309	Modelling the octanol-air partition coefficient of aromatic pollutants based on the solvation free energy and the dimer effect. <i>Chemosphere</i> , 2022, 309, 136608.	4.2	2
13310	Developing a robust thiadiazole derivative corrosion inhibitor for dynamic supercritical CO ₂ aqueous environment: Electrochemical tests and DFT calculations. <i>Corrosion Science</i> , 2022, 209, 110695.	3.0	18
13311	Anionic H-bonds improve the disorganization of starch in metal chloride hydrate-natural deep eutectic solvents. <i>Carbohydrate Polymers</i> , 2022, 298, 120150.	5.1	1
13312	Insights into the formation mechanism of aliphatic acid-choline chloride deep eutectic solvents by theoretical and experimental research. <i>Journal of Molecular Liquids</i> , 2022, 367, 120342.	2.3	7

#	ARTICLE	IF	CITATIONS
13313	Substituent effects on photophysical properties of ESIPT-based fluorophores bearing the 4-diethylaminosalicylaldehyde core. <i>Journal of Molecular Liquids</i> , 2022, 367, 120477.	2.3	18
13314	A conversion strategy to disaggregate asphaltenes via mild hydrotreatment: Theoretical and experimental investigation. <i>Chemical Engineering Science</i> , 2022, 264, 118106.	1.9	3
13315	Electrochemically activated peroxymonosulfate with mixed metal oxide electrodes for sulfadiazine degradation: Mechanism, DFT study and toxicity evaluation. <i>Chemosphere</i> , 2022, 309, 136695.	4.2	11
13316	Influence of stereoelectronic interactions on the ¹³ C NMR chemical shift in iodine-containing molecules. <i>Journal of Magnetic Resonance Open</i> , 2022, 12-13, 100080.	0.5	0
13317	Effect of Molecular Structure on the Difference of Lightning Impulse Discharge Between Mineral Oil and Natural Ester Using DFT Calculation. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2023, 30, 114-121.	1.8	1
13318	Rational design of efficient deep eutectic solvents for HCl absorption through their competitive H-bonding interactions. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
13319	An exchange interaction of the antiferromagnetic nature in benzoate bridged Mn(II) chains. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
13320	Unveiling the uncommon blue-excitable broadband yellow emission from self-trapped excitons in a zero-dimensional hybrid tellurium halide. <i>Journal of Materials Chemistry C</i> , 0, , .	2.7	2
13321	Selectivity mechanism of muscarinic acetylcholine receptor antagonism through <i>in silico</i> investigation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26269-26287.	1.3	0
13322	Benzothiadiazole-based fluorophores as efficient non-doped emitters for solution-processed organic light-emitting diodes. <i>New Journal of Chemistry</i> , 2022, 46, 22650-22662.	1.4	2
13323	Tuning the properties of graphene quantum dots by passivation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26232-26240.	1.3	6
13324	Iron(III) and aluminum(III) complexes of cyclopentazolate anions. <i>CrystEngComm</i> , 0, , .	1.3	0
13325	Insights into the binding of arginine to adenosine phosphate from mimetic complexes. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
13326	Theoretical and experimental insights into the properties of donor-acceptor type derivatives of quinoxaline and methanone containing different donor moieties. <i>New Journal of Chemistry</i> , 2022, 46, 20768-20776.	1.4	4
13327	Exploring inclusion complex of an anti-cancer drug (6-MP) with β -cyclodextrin and its binding with CT-DNA for innovative applications in anti-bacterial activity and photostability optimized by computational study. <i>RSC Advances</i> , 2022, 12, 30936-30951.	1.7	6
13328	Intermolecular amide and aldehyde interactions: rotational spectroscopy of the complexes of formaldehyde with 2-azetidinone and formamide. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 28012-28018.	1.3	4
13329	The combination of skeleton-engineering and periphery-engineering: a design strategy for organic doublet emitters. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26853-26862.	1.3	2
13330	Revealing the synergetic interaction between amino and carbonyl functional groups and their effect on the electronic and optical properties of carbon dots. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 27163-27172.	1.3	5

#	ARTICLE	IF	CITATIONS
13331	Designing dibenzosilole core based, A ₂ -A ₁ -A ₁ -A ₂ type donor molecules for promising photovoltaic parameters in organic photovoltaic cells. RSC Advances, 2022, 12, 29300-29318.	1.7	0
13332	Hydrogen bond networks in gas-phase complex anions. RSC Advances, 2022, 12, 29137-29142.	1.7	0
13333	Curing Degree Dependence of Dielectric Properties of Bisphenol-A-Based Epoxy Resin Cured With Methyl Hexahydrophthalic Anhydride. IEEE Transactions on Dielectrics and Electrical Insulation, 2022, 29, 2072-2079.	1.8	18
13334	Extraction of Au(III) from hydrochloric acid media using a novel amide-based ionic liquid. New Journal of Chemistry, 2022, 46, 19824-19833.	1.4	3
13335	Highly efficient ultralong organic phosphorescence induced by lone pair repulsions and noncovalent interactions. New Journal of Chemistry, 2022, 46, 20723-20728.	1.4	2
13336	Si ₅ -pentagonal rings and Y-shaped Si ₄ building blocks in Li ₃₂ Si ₁₈ system: similarities with the crystalline Zintl phase Li ₁₂ Si ₇ . Molecular Systems Design and Engineering, 0, , .	1.7	0
13337	Mechanism of [3+2] Annulations between Indole-2-formaldehydes and Isatins Mediated by N-Heterocyclic Carbene: A DFT Study. New Journal of Chemistry, 0, , .	1.4	0
13338	Revealing the sensing mechanism of a fluorescent pH probe based on a bichromophore approach. Physical Chemistry Chemical Physics, 2022, 24, 26731-26737.	1.3	4
13339	Rapid and highly selective colorimetric detection of mercury(II) ions in water sources based on a ribavirin functionalized AuNP sensor. Analytical Methods, 2022, 14, 4669-4679.	1.3	1
13340	Blue heteroleptic iridium(III) complexes for OLEDs: simultaneous optimization of color purity and efficiency. Journal of Materials Chemistry C, 2022, 10, 17965-17973.	2.7	1
13341	Interplay of unique N-H...N and H-H...O hydrogen bonding interactions in the heterodimers of nitromethane with acetylene and benzene as π -electron donors: experimental characterization at low temperatures under isolated conditions with computational corroboration. Physical Chemistry Chemical Physics, 2022, 24, 28411-28428.	1.3	1
13342	Planar pentacoordinate carbon in [XC ₇ H ₂] ²⁺ (X = Be and Mg) and its derivatives. Physical Chemistry Chemical Physics, 2022, 24, 27606-27611.	1.3	2
13343	Theoretical insights into the separation of Am(III)/Eu(III): designing ligands based on a preorganization strategy. Dalton Transactions, 2022, 51, 16659-16667.	1.6	8
13344	Metalloborosphenes with the stabilized classical fullerene-like borospherene B ₃₆ as electric field manipulated second-order nonlinear optical switches. New Journal of Chemistry, 2022, 46, 22246-22255.	1.4	2
13345	A broadly applicable quantitative relative reactivity model for nucleophilic aromatic substitution (S _N Ar) using simple descriptors. Chemical Science, 2022, 13, 12681-12695.	3.7	10
13346	Efficient deep red/near-infrared thermally activated delayed fluorescence emitters via molecular reconstruction: theoretical insights. Physical Chemistry Chemical Physics, 2022, 24, 26764-26775.	1.3	4
13347	Enhancement of tetrel bond involving tetrazole-TtR ₃ (Tt = C, Si; R = H, F). Promotion of SiR ₃ transfer by a triel bond. Physical Chemistry Chemical Physics, 2022, 24, 25895-25903.	1.3	3
13348	Accelerating PLQY and RISC rates in deep-blue TADF materials with the acridin-9(10H)-one acceptor by tuning the peripheral groups on carbazole donors. Journal of Materials Chemistry C, 2022, 10, 16524-16535.	2.7	5

#	ARTICLE	IF	CITATIONS
13349	Theoretical insights into single-pole quadruple-throw (SP4T) inorganic nonlinear optics molecular switch of Na(HCN) ₃ Na: from superalkali to superalkalides. <i>Journal of Materials Chemistry C</i> , 2022, 10, 16789-16802.	2.7	6
13350	Dissecting conjugation and electronic effects on the linear and non-linear optical properties of rhenium(λ) carbonyl complexes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 28069-28079.	1.3	2
13351	[Co(2,2'-bipy) ₃ Ag ₃] ₆ with a hole structure facilitates dye adsorption and photocatalytic reduction. <i>Dalton Transactions</i> , 2022, 51, 16784-16789.	1.6	3
13352	Reduced nucleophilicity: an intrinsic property of the Lewis base atom interacting with H in hydrogen-bonds with Lewis acids HX (X = F, Cl, Br, I, CN, CCH, CP). <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 25822-25833.	1.3	4
13353	Ultrafast charge transfer in a nonfullerene all-small-molecule organic solar cell: a nonadiabatic dynamics simulation with optimally tuned range-separated functional. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 27173-27183.	1.3	2
13354	A theoretical investigation of uranyl covalency <i>via</i> symmetry-preserving excited state structures. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1
13355	Computational mining of endohedral C ₇₀ electrides: tri-metal alkali and alkaline-earth encapsulation. <i>Dalton Transactions</i> , 2022, 51, 16836-16844.	1.6	1
13356	Ultrasensitive catechin electrochemical sensor based on uniform ordered mesoporous carbon hollow spheres (MCHSs) advanced carbon-based conductive materials. <i>Analyst</i> , The, 2022, 147, 5239-5247.	1.7	6
13357	Enhancement of DNAzymatic activity using iterative <i>in silico</i> maturation. <i>Journal of Materials Chemistry B</i> , 0, , .	2.9	0
13358	In-depth theoretical understanding of the chemical interaction of aromatic compounds with a gold nanoparticle. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 25327-25336.	1.3	2
13359	Quantum chemical modification of indaceno dithiophene-based small acceptor molecules with enhanced photovoltaic aspects for highly efficient organic solar cells. <i>RSC Advances</i> , 2022, 12, 28608-28622.	1.7	9
13360	The potential energy profile of the decomposition of 1,1-diamino-2,2-dinitroethylene (FOX-7) in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 26836-26847.	1.3	4
13361	Hydrogen bond reconstruction strategy for eutectic solvents that realizes room-temperature dissolution of cellulose. <i>Green Chemistry</i> , 2022, 24, 8760-8769.	4.6	9
13362	Origin of Humidity Influencing the Excited State Electronic Properties of Silicon Quantum Dots based Light-emitting Diodes. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
13363	First 1-hydroxy-1H-imidazole-based ESIPT emitter with an O-H \cdots O intramolecular hydrogen bond: ESIPT-triggered TICT and speciation in solution. <i>New Journal of Chemistry</i> , 0, , .	1.4	3
13364	Theoretical study on the structures, electronic properties, and aromaticity of thia[4]circulenes. <i>New Journal of Chemistry</i> , 2022, 46, 22703-22714.	1.4	3
13365	Interpenetrating dye-functionalized indium-organic frameworks for photooxidative cyanation and oxidative cyclization. <i>Journal of Materials Chemistry A</i> , 2022, 10, 24320-24330.	5.2	1
13366	First theoretical probe for efficient enhancement of optical nonlinearity <i>via</i> structural modifications into phenylene based π -A configured molecules. <i>RSC Advances</i> , 2022, 12, 31192-31204.	1.7	14

#	ARTICLE	IF	CITATIONS
13367	Computational design and molecular modeling of the interaction of nicotinic acid hydrazide nickel-based complexes with H ₂ S gas. RSC Advances, 2022, 12, 30365-30380.	1.7	29
13368	Supramolecular assembly in designing co-crystals of fumaric acid and pyrimidine/picolinate derivatives. Green Chemistry Letters and Reviews, 2022, 15, 825-836.	2.1	5
13369	Conformational Analysis and DFT Investigations of 1-(4-Fluorophenyl)Piperazine by ELF and LOL, Inhibitory activity against Alzheimer's Disease, and ADME Prediction. Sakarya University Journal of Science, 0, .	0.3	0
13370	S-scheme heterojunction/Schottky junction tandem synergistic effect promotes visible-light-driven catalytic activity. Nano Research, 2023, 16, 2152-2162.	5.8	9
13371	Involvement of Arsenic Atom of AsF ₃ in Five Pnictogen Bonds: Differences between X-ray Structure and Theoretical Models. Molecules, 2022, 27, 6486.	1.7	3
13372	A computational study of the inclusion of β -cyclodextrin and nicotinic acid: DFT, DFT-D, NPA, NBO, QTAIM, and NCI-RDG studies. Journal of Molecular Modeling, 2022, 28, .	0.8	6
13373	Exploring the Absorption Mechanisms of Imidazolium-Based Ionic Liquids to Epigallocatechin Gallate. International Journal of Molecular Sciences, 2022, 23, 12600.	1.8	0
13374	Thiadiazole-Based Covalent Organic Frameworks with a Donor-Acceptor Structure: Modulating Intermolecular Charge Transfer for Efficient Photocatalytic Degradation of Typical Emerging Contaminants. Environmental Science & Technology, 2022, 56, 16303-16314.	4.6	36
13375	Multiple Interpenetrating Metal-Organic Frameworks with Channel-Size-Dependent Behavior for Selective Gossypol Detection and Perovskite Quantum Dot Encapsulation. ACS Applied Materials & Interfaces, 2022, 14, 49945-49956.	4.0	13
13376	Investigations into the flotation of molybdenite in the presence of chalcopyrite using (3S,4S,5S,6R)-3,4,5,6-tetrahydroxyoxane-2-carboxylate acid as a novel selective depressant: An experimental and theoretical perspective. Journal of Molecular Liquids, 2022, 368, 120661.	2.3	3
13377	Probing the Structure-Property Relationships of Na ⁺ ·Cl ⁻ @C ₅₀ N ₅ H ₅ under the External Electric Field. Inorganic Chemistry, 2022, 61, 17646-17652.	1.9	1
13378	On the Role of Noncovalent Ligand-Substrate Interactions in Au(I) Catalysis: An Experimental and Computational Study of Protodeauration. ACS Catalysis, 2022, 12, 13158-13163.	5.5	4
13379	Theoretical calculations of formation and reactivity of <i>o</i> -quinomethide derivatives of resorcin[4]arene with reference to empirical data. Royal Society Open Science, 2022, 9, .	1.1	1
13380	Toward Advanced High-Performance Insensitive FOX-7-like Energetic Materials via Positional Isomerization. ACS Applied Materials & Interfaces, 2022, 14, 49847-49853.	4.0	14
13381	The Bonding Nature of Fe-CO Complexes in Heme Proteins. Inorganic Chemistry, 2022, 61, 17494-17504.	1.9	5
13382	Design of an open-shell nitrogen-centered diradicaloid with tunable stimuli-responsive electronic properties. Communications Chemistry, 2022, 5, .	2.0	7
13383	The Source of Proton in the Noyori-Ikariya Catalytic Cycle. ACS Catalysis, 2022, 12, 13149-13157.	5.5	3
13384	Photobiocatalytic Cascades for Acylating N-Heterocycles with Natural Amino Acids via the α -Keto Acids. Advanced Synthesis and Catalysis, 0, .	2.1	1

#	ARTICLE	IF	CITATIONS
13385	Design of Thermally Activated Delayed Fluorescence Materials with High Intersystem Crossing Efficiencies by Machine Learning-Assisted Virtual Screening. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 9910-9918.	2.1	7
13386	Synthesis of α,β -Unsaturated Ketones in Water: The Claisen-Schmidt Condensation Revisited. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 14271-14279.	3.2	4
13387	Computational Study on the Effect of Thienyl π -Donor on the Optical Response of Nonclassical Oligo-Pyrazinothienothiadiazole Biradicaloids. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7829-7839.	1.1	0
13388	Superstrong Chemical Bonding of Noble Gases with Oxidoboron (BO^{+}) and Sulfidoboron (BS^{+}). <i>Journal of Physical Chemistry A</i> , 2022, 126, 7888-7900.	1.1	3
13389	Multi-targeted fluorescent probes for detection of Zn(II) and Cu(II) ions based on ESIPT mechanism. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 287, 122051.	2.0	11
13390	Can Linear Conjugated Polymers Form Stable Helical Structures on the Carbon Nanotubes?. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 49189-49198.	4.0	4
13391	A Biomimetic Emitter Inspired from Green Fluorescent Protein. <i>Journal of Physical Chemistry B</i> , 2022, 126, 8771-8776.	1.2	0
13393	Piperazine-Linked Covalent Triazine Polymer as an Efficient Platform for the Removal of Toxic Mercury(II) Ions from Wastewater. <i>ACS Applied Polymer Materials</i> , 2022, 4, 8118-8126.	2.0	6
13394	First principle investigation of new dithienosilole-based dyes for DSSCs: effects of auxiliary acceptor groups. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	2
13395	Ranking the energy minima of the 20 natural amino acids using conceptual tools. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	0
13396	Redox-Triggered Switching of Conformational State in Triple-Decker Lanthanide Phthalocyaninates. <i>Molecules</i> , 2022, 27, 6498.	1.7	6
13397	A Theoretical Study of the C-X Bond Cleavage Mediated by Cob(II)Aloxime. <i>Molecules</i> , 2022, 27, 7283.	1.7	0
13398	Modular Cocrystallization of Customized Carboranylthiolate-Protected Copper Nanoclusters via Host-Guest Interactions. <i>ACS Nano</i> , 2022, 16, 18789-18794.	7.3	6
13399	Fast Prediction of Lipophilicity of Organofluorine Molecules: Deep Learning-Derived Polarity Characters and Experimental Tests. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 4928-4936.	2.5	13
13400	Understanding the origin of reactivity, mechanism and regioselectivity of the [3+2] cycloaddition reaction between nitrile imine and pyrrolopyrazine. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	1
13401	Efficient Degradation of High-Concentration Benzotriazole Wastewater via $\text{UV}/\text{H}_2\text{O}_2/\text{O}_3$ Operation: Degradation Mechanism, Toxicological Evaluation, and Economic Analysis. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 16431-16444.	1.8	2
13402	Nanopockets with a Thermoresponsive Nitrate Ionic Liquid for Highly Efficient Uranium Extraction at High Acidity. <i>ACS Applied Nano Materials</i> , 2022, 5, 14893-14901.	2.4	4
13403	Theoretical Investigation of Key Properties of the Pyrolysis of Methyl, Ethyl, and Dimethyl Dioxolane Isomers. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8326-8336.	1.1	2

#	ARTICLE	IF	CITATIONS
13404	Oxygen mediated oxidative couplings of flavones in alkaline water. <i>Nature Communications</i> , 2022, 13, .	5.8	5
13405	Visible photocatalytic degradation of tetrabromobisphenol A by CuO-modified Ce ₂ O ₃ : Mechanisms and DFT studies. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108878.	3.3	5
13406	Computational Insights on Periodicity in Bonding and Lewis Acidity and Basicity of the p-Block Trispyrazolylborate Complexes. <i>European Journal of Inorganic Chemistry</i> , 2023, 26, .	1.0	1
13407	First-Principles-Based Optimized Design of Fluoride Electrolytes for Sodium-Ion Batteries. <i>Molecules</i> , 2022, 27, 6949.	1.7	1
13408	Enantioselective Radical Hydroacylation of α,β -Unsaturated Carbonyl Compounds with Aldehydes by Triplet Excited Anthraquinone. <i>ACS Catalysis</i> , 2022, 12, 12984-12992.	5.5	19
13409	26.2: <i>Invited Paper:</i> Computational chemistry study of an aggregation-induced delayed fluorescence material: synthesis and properties. <i>Digest of Technical Papers SID International Symposium</i> , 2022, 53, 286-299.	0.1	0
13410	New gold(III) chlorophenyl terpyridine complex: Biomolecular interactions and anticancer activity against human oral squamous cell carcinoma. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	2
13411	Design of A-D-A-Type Organic Third-Order Nonlinear Optical Materials Based on Benzodithiophene: A DFT Study. <i>Nanomaterials</i> , 2022, 12, 3700.	1.9	7
13412	Comprehensive Empirical Model of Substitutional Influence on Hydrogen Bonding in Aromatic Schiff Bases. <i>International Journal of Molecular Sciences</i> , 2022, 23, 12439.	1.8	3
13413	Influence of the Active Site Flexibility on the Efficiency of Substrate Activation in the Active Sites of Bi-Zinc Metallo- β -Lactamases. <i>Molecules</i> , 2022, 27, 7031.	1.7	1
13414	A Tale of Two Sites: Neighboring Atomically Dispersed Pt Sites Cooperatively Remove Trace H ₂ in CO-Rich Stream. <i>Small</i> , 2022, 18, .	5.2	7
13415	Understanding the effectiveness of enzyme pre-reaction state by a quantum-based machine learning model. <i>Cell Reports Physical Science</i> , 2022, 3, 101128.	2.8	8
13416	Charge Transfer Doping of Carbon Nitride Films through Noncovalent Iodination for Enhanced Photoelectrochemical Performance: Combined Experimental and Computational Insights. <i>Small</i> , 2022, 18, .	5.2	2
13417	Enhanced Built-in Electric Field Promotes Photocatalytic Hydrogen Performance of Polymers Derived from the Introduction of B-N Coordination Bond. <i>Advanced Science</i> , 2022, 9, .	5.6	11
13418	2-Hydroxychalcone- β -Cyclodextrin Conjugate with pH-Modulated Photoresponsive Binding Properties. <i>Journal of Organic Chemistry</i> , 0, .	1.7	1
13419	Acceleration of Cathode Interfacial Kinetics by Liquid Organosulfides in Lithium Metal Batteries. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	10
13420	Butterfly-Shaped Nanographenes with Excellent Second-Order Nonlinear Optical Properties: The Synergy of B/N and Azulene. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	1
13421	Al ₂ C ₄ H ₂ Isomers with the Planar Tetracoordinate Carbon (ptC)/Aluminum (ptAl). <i>Atoms</i> , 2022, 10, 112.	0.7	3

#	ARTICLE	IF	CITATIONS
13422	The structure, stability, thermochemistry, and bonding in SO ₃ -(H ₂ O) _n (n = 1–7) clusters: a computational analysis. <i>Structural Chemistry</i> , 0, , .	1.0	1
13423	The structures and electronic properties of (LiF) _n (n = 2–18). <i>European Physical Journal D</i> , 2022, 76, .	0.6	3
13424	Theoretical insights into the roles of intermolecular interactions in BTATz-based solvate cocrystals. <i>Structural Chemistry</i> , 0, , .	1.0	0
13425	Preparation of polyether amine-bridged lignosulfonate for utilization as a nano dye dispersant. <i>International Journal of Biological Macromolecules</i> , 2022, 222, 2523-2534.	3.6	5
13426	Atroposelective Synthesis of Triaryl Imidopyranones with 1,2-Diaryloxanes by N-Heterocyclic Carbene Organocatalysis. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	22
13427	Coemissive luminescent nanoparticles combining aggregation-induced emission and quenching dyes prepared in continuous flow. <i>Nature Communications</i> , 2022, 13, .	5.8	11
13428	Copper-on-Magnetically Activated Carbon-Catalyzed Azide-Alkyne Click Cycloaddition in Water. <i>Catalysts</i> , 2022, 12, 1244.	1.6	3
13429	Enantioselective Total Synthesis of Dysiherbols A, C, and D. <i>Journal of the American Chemical Society</i> , 2022, 144, 19521-19531.	6.6	7
13430	Chiral Bis(tetrathiafulvalene)-1,2-cyclohexane-diamides. <i>Molecules</i> , 2022, 27, 6926.	1.7	1
13431	An investigation into the structural, electronic, and non-linear optical properties in CN (N = 20, 24, 26). <i>Tj ETQq1 1 0,784314</i>	0.8	3
13432	Coordination Switch Drives Selective C–S Bond Formation by the Non-heme Sulfoxide Synthases. <i>Angewandte Chemie</i> , 0, , .	1.6	0
13434	Flexible and Transparent SERS Substrates Composed of Au@Ag Nanorod Arrays for In Situ Detection of Pesticide Residues on Fruit and Vegetables. <i>Chemosensors</i> , 2022, 10, 423.	1.8	5
13435	C ₃ -Symmetric Propeller-like Phenanthridine Derivative with Multiple Write-In Modes for Programmable Anti-Counterfeiting. <i>Chemistry of Materials</i> , 2022, 34, 9492-9502.	3.2	7
13436	[N ₂ -I ₂ -N] ⁺ Type Halogen-Bonding-Driven Supramolecular Helical Polymers with Modulated Chirality. <i>ACS Nano</i> , 2022, 16, 19220-19228.	7.3	8
13437	Intramolecular Interactions in Derivatives of Uracil Tautomers. <i>Molecules</i> , 2022, 27, 7240.	1.7	2
13438	Face-Centered Cubic Silver Nanoclusters Consolidated with Tetradentate Formamidinate Ligands. <i>Journal of the American Chemical Society</i> , 2022, 144, 19365-19371.	6.6	10
13439	Effects of Lewis Basicity and Acidity on f-Hole Interactions in Carbon-Bearing Complexes: A Comparative Ab Initio Study. <i>International Journal of Molecular Sciences</i> , 2022, 23, 13023.	1.8	3
13440	Interaction of Glutamic Acid/Protonated Glutamic Acid with Amide and Water Molecules: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7750-7762.	1.1	2

#	ARTICLE	IF	CITATIONS
13441	Structural evolution and bonding characteristics of neutral Cs ₂ B _n clusters. <i>Molecular Physics</i> , 2022, 120, .	0.8	1
13442	Phase behavior and extraction mechanism of ethanol in alcohol ester mixture separated by deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2022, 368, 120694.	2.3	3
13443	Quantum nanomagnets in on-surface metal-free porphyrin chains. <i>Nature Chemistry</i> , 2023, 15, 53-60.	6.6	28
13444	Be ₂ C monolayer as an efficient adsorbent of toxic volatile organic compounds: theoretical investigation. <i>Molecular Physics</i> , 0, , .	0.8	0
13445	Unexpectedly significant stabilizing mechanism of iodous acid on iodic acid nucleation under different atmospheric conditions. <i>Science of the Total Environment</i> , 2023, 859, 159832.	3.9	10
13446	Dissociation reactions of hydrogen molecules at active sites on gold clusters: A <i>DFT</i> study. <i>Journal of the Chinese Chemical Society</i> , 0, , .	0.8	1
13447	On the origin and nature of internal methyl rotation barriers: an information-theoretic approach study. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	33
13448	Synthesis, spectroscopic studies, and single-crystal structures of two Δ supramolecular zinc(II) and nickel(II) complexes containing thiazole ring: Antimicrobial assays, time-dependent density functional theory calculations, and Hirshfeld surface analysis. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	5
13449	Dicationic ionic liquids (DILs) based on the phenyl and perfluoro-phenyl π -spacer-linked triazolium cations: a quantum chemical comparative study. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	3
13450	Carbazole-based donor materials with enhanced photovoltaic parameters for organic solar cells and hole-transport materials for efficient perovskite solar cells. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	4
13451	Highly Oxidized Germacranolides from <i>Elephantopus tomentosus</i> and the Configurational Revision of Some Previously Reported Analogues. <i>Journal of Natural Products</i> , 2022, 85, 2433-2444.	1.5	10
13452	Theoretical design and prediction of novel fluorene-based non-fullerene acceptors for environmentally friendly organic solar cell. <i>Arabian Journal of Chemistry</i> , 2023, 16, 104374.	2.3	2
13453	Quantum Chemical Calculation for Intermolecular Interactions of Alginate Dimer-Water Molecules. <i>Gels</i> , 2022, 8, 703.	2.1	5
13454	Quantum mechanics and molecular dynamics strategies to investigate self-aggregation of Quinolin-65. <i>Journal of Molecular Liquids</i> , 2022, 368, 120552.	2.3	4
13455	Anti-Symmetric Electromagnetic Interactions TM Response in Electron Circular Dichroism and Chiral Origin of Periodic, Complementary Twisted Angle in Twisted Bilayer Graphene. <i>Molecules</i> , 2022, 27, 6525.	1.7	1
13456	Synergism of 2-mercaptobenzimidazole and oleic imidazoline on corrosion inhibition of carbon steel in CO ₂ -saturated brine solutions. <i>Journal of Molecular Liquids</i> , 2022, 368, 120645.	2.3	7
13457	Constructing Nonaqueous Rechargeable Zinc-Ion Batteries with Zinc Trifluoroacetate. <i>ACS Applied Energy Materials</i> , 2022, 5, 12437-12447.	2.5	5
13458	Noncovalent Interactions in Halogenated Pyridinium Salts of the Weakly Coordinating Anion [Al(OTeF ₅) ₄] ⁺ . <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	2

#	ARTICLE	IF	CITATIONS
13459	Enhanced Degradation of Antibiotic by Peroxydisulfate Catalysis with CuO@CNT: Simultaneous H_2O_2 Oxidation and Electron-Transfer Regime. <i>Molecules</i> , 2022, 27, 7064.	1.7	1
13460	Impacts of polarizable continuum models on the SCF convergence and DFT delocalization error of large molecules. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	2
13461	Three Birds with One Stone: Tetramethylurea as Electrolyte Additive for Highly Reversible Zn-Metal Anode. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	62
13462	Design principles based on intramolecular interactions for hydroxyl-functionalized covalent organic frameworks. <i>Cell Reports Physical Science</i> , 2022, 3, 101114.	2.8	7
13463	Dicarboxylic Acid-Based Co-Crystals of Pyridine Derivatives Involving Structure Guiding Unconventional Synthons: Experimental and Theoretical Studies. <i>Crystals</i> , 2022, 12, 1442.	1.0	1
13464	Presentation of the simple and accurate models for estimating the individual hydrogen bond energies of Watson-Crick base pairs. <i>Structural Chemistry</i> , 0, , .	1.0	0
13465	Structure-Directing Interplay between Tetrel and Halogen Bonding in Co-Crystal of Lead(II) Diethyldithiocarbamate with Tetraiodoethylene. <i>International Journal of Molecular Sciences</i> , 2022, 23, 11870.	1.8	1
13466	Chiral Naphthalenediimides with High Efficiency Fluorescence and Circularly Polarized Luminescence in the Solid State for the Application in Organic Optoelectronics. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	2
13467	Mechanistic Insights into Cobalt-Catalyzed Regioselective C4-Alkenylation of 3-Acetylindole: A Detailed Theoretical Study. <i>Journal of Organic Chemistry</i> , 2022, 87, 14125-14136.	1.7	1
13468	Amino-modified polyvinyl alcohol fibers for the efficient removal of uranium from actual uranium-containing laundry wastewater. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2022, 331, 4489-4502.	0.7	1
13469	Mechanistic insights into CO_2 conversion chemistry of copper bis-(terpyridine) molecular electrocatalyst using accessible operando spectrochemistry. <i>Nature Communications</i> , 2022, 13, .	5.8	24
13470	Bottom-up design and assembly with superatomic building blocks. <i>Chinese Physics B</i> , 0, , .	0.7	0
13471	Selectively Identifying Exposed-over-Unexposed C-C Pairs in Human Telomeric i-Motif Structures with Length-Dependent Polymorphism. <i>Analytical Chemistry</i> , 2022, 94, 14994-15001.	3.2	1
13472	Antispasmodic activity of novel 2,4-dichloroanilinium perchlorate hybrid material: X-ray crystallography, DFT studies and molecular docking approach. <i>Journal of Molecular Structure</i> , 2023, 1274, 134440.	1.8	5
13473	New [1,3]thiazolo[3,2-b][1,2,4]triazol-7-ium cationic surfactant as a stabilizer of silver and gold nanoparticles. <i>Applied Nanoscience (Switzerland)</i> , 2023, 13, 5079-5090.	1.6	2
13474	Insights into the rheological properties, multi-scale structure and in vitro digestibility changes of starch- β -glucan complex prepared by ball milling. <i>International Journal of Biological Macromolecules</i> , 2023, 224, 1313-1321.	3.6	7
13475	Toward efficient functionalization of polystyrene backbone through ketene chemistry: Synthesis, characterization, and DFT study. <i>Polymers for Advanced Technologies</i> , 0, , .	1.6	0
13476	Nonsymmetric [Pt(C ^N *N ²)] Complexes: Aggregation-Induced Emission in the Solid State and in Nanoparticles Tuned by Ligand Structure. <i>Chemistry - A European Journal</i> , 0, , .	1.7	1

#	ARTICLE	IF	CITATIONS
13477	Theoretical investigation on interface interaction and properties of 3-nitro-1,2,4-triazol-5-one (NTO)/fluoropolymer polymer-bonded explosives (PBXs). <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	3
13478	Linear Regression Model for Predicting Allyl Alcohol C=O Bond Activity under Palladium Catalysis. <i>ACS Catalysis</i> , 2022, 12, 13921-13929.	5.5	6
13479	DFT analysis on the adsorption of melamine in Ga ₁₂ -N ₁₂ /P ₁₂ nanocages: solvent effects, SERS analysis, reactivity properties. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 8844-8855.	2.0	4
13480	Cation Bridge Mediating Homo- and Cross-Coupling in Copper-Catalyzed Reductive Coupling of Benzaldehyde and Benzophenone. <i>Inorganic Chemistry</i> , 2022, 61, 18033-18043.	1.9	3
13481	Classical vs. Non-Classical Cyclometalated Pt(II) Complexes. <i>Molecules</i> , 2022, 27, 7249.	1.7	4
13482	Thermodynamic Equilibrium–Nonequilibrium Competition in Nanofilaments for Achieving Complementary Electronic Synapses. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	1
13483	Distinguishing the Quantum Yield and Lifetime of Carbazole-Based Room-Temperature Phosphorescence Materials: QM/MM Study. <i>Annalen Der Physik</i> , 2022, 534, .	0.9	1
13484	Insights on sustainable fuels: a new benzimidazole derivative with potential as a diesel-biodiesel blend additive. <i>Biofuels</i> , 2023, 14, 279-292.	1.4	0
13485	Revealing and Tuning the Photophysics of C=N Containing Photothermal Molecules: Excited State Dynamics Simulations. <i>International Journal of Molecular Sciences</i> , 2022, 23, 11779.	1.8	0
13486	Coordination Switch Drives Selective C–S Bond Formation by the Non-Heme Sulfoxide Synthases**. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	10
13487	CHEMISORPTION OF C ₂ H ₂ ON C ₂₀ BOWL: A COMPUTATIONAL INVESTIGATION. <i>Journal of Structural Chemistry</i> , 2022, 63, 1600-1609.	0.3	1
13488	Acceleration of Nonradiative Charge Recombination Reactions at Larger Distances in Kinked Donor–Bridge–Acceptor Molecules. <i>Journal of Physical Chemistry B</i> , 2022, 126, 8851-8863.	1.2	0
13489	Boosting high initial coulombic efficiency of hard carbon by in-situ electrochemical presodiation. <i>Journal of Energy Chemistry</i> , 2023, 77, 310-316.	7.1	12
13490	Alkaline earthides based on 15-crown-5 ether with remarkable NLO response. <i>European Physical Journal Plus</i> , 2022, 137, .	1.2	4
13491	Theoretical research on the relationships between aromatic ligands and spectroscopic properties of Pt(II) complexes. <i>Molecular Physics</i> , 0, , .	0.8	0
13492	Polychlorinated Biphenyls Interactions with Water—Characterization Based on the Analysis of Non-Covalent Interactions and Energy Partitioning. <i>Sustainability</i> , 2022, 14, 12529.	1.6	0
13493	Acceleration of Cathode Interfacial Kinetics by Liquid Organosulfides in Lithium Metal Batteries. <i>Angewandte Chemie</i> , 0, , .	1.6	0
13494	Reactivity of sodium pentaphospholide Na[cycloP ₅] towards C≡E (E = C, N, P) triple bonds.. <i>Chemistry - A European Journal</i> , 0, , .	1.7	3

#	ARTICLE	IF	CITATIONS
13495	Dithienylethene-Containing Cyclometalated Platinum(II) Complexes with Tunable Photochromic and Photophysical Properties. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	1
13496	N-Halamine-modified mesoporous silica for water disinfection. <i>Materials Chemistry and Physics</i> , 2023, 293, 126936.	2.0	4
13497	Enhancement of intrinsic optical transitions in silicon nanocrystals by state localization. <i>Physical Review B</i> , 2022, 106, .	1.1	2
13498	Theoretical Investigation of Regiodivergent Addition of Anilines and Phenolates to <i>p</i> -Benzoquinone Ring. <i>ACS Omega</i> , 0, , .	1.6	0
13499	Self-Assembly of a Graphene Oxide Liquid Crystal for Water Treatment. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 47549-47559.	4.0	1
13500	Anchoring I_{3}^{+} via Charge-Transfer Interaction by a Coordination Supramolecular Network Cathode for a High-Performance Aqueous Dual-Ion Battery. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 47716-47724.	4.0	4
13502	Insights into the structure and growth of Lu-doped germanium clusters: comparing density functional theory calculations with photoelectron spectroscopy experiments. <i>Molecular Physics</i> , 2022, 120, .	0.8	4
13503	Studies on the structural and electronic characteristics of alkaline-earth metal Mg_{n+1} and $BaMg_n$ ($n=2-10$) clusters and their anions. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	1
13504	Catalytic Desaturation and β -Fluorination of Aliphatic Amides Enabled by an Oxidative-Promoted Bond Destabilization. <i>ACS Catalysis</i> , 2022, 12, 12964-12972.	5.5	5
13505	Insight into stabilities and magnetism of $EuGe_n$ ($n=1-20$) nanoclusters: an assessment of electronic aromaticity. <i>Journal of Materials Science</i> , 2022, 57, 19338-19355.	1.7	5
13506	The role of alkali metal cations and platinum-surface hydroxyl in the alkaline hydrogen evolution reaction. <i>Nature Catalysis</i> , 2022, 5, 923-933.	16.1	79
13507	Facet effect of hematite on the hydrolysis of phthalate esters under ambient humidity conditions. <i>Nature Communications</i> , 2022, 13, .	5.8	12
13508	New Theoretical Insights about Anticorrosive Effects and Adsorption Mechanism of Some β -Amino Acids on Al Surface: DFT, MEP, FMO, NBO, QSAR, Fukui Functions and Monte Carlo Simulation. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2022, 58, 1054-1070.	0.3	3
13509	Spectroscopic and computational approach to study the interacting mechanism of drug-adenine complex. <i>Spectroscopy Letters</i> , 0, , 1-28.	0.5	3
13510	Identifying the role of excited-state proton transfer and photoinduced electron transfer in detecting hypochlorous acid for a benzothiazole-based colorimetric fluorescent probe. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	2
13511	First Hyperpolarizabilities of Intramolecular Charge-Transfer Architectures Based on Acenaphthene Derivatives in Gas, Solution, and Solid States. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7432-7441.	1.1	3
13512	Thionation toward High-Contrast ACQ-DIE Probes by Reprogramming the Aqueous Segregation Behavior: Enlightenment from a Sulfur-Substituted G-Quadruplex Ligand. <i>Analytical Chemistry</i> , 2022, 94, 15231-15239.	3.2	5
13513	Site-selective multi-emitter gold-silver metallopolymers: A novel class of self-assembled materials. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	1

#	ARTICLE	IF	CITATIONS
13514	Theoretical Study on the Electro-Reduction of Carbon Dioxide to Methanol Catalyzed by Cobalt Phthalocyanine. <i>Inorganic Chemistry</i> , 2022, 61, 16549-16564.	1.9	10
13515	Can a chemical bond be exclusively covalent or ionic?. <i>Journal of Chemical Sciences</i> , 2022, 134, .	0.7	2
13516	Side substitution on benzothiadiazole-based hole transporting materials with a D ⁺ A ⁻ D molecular configuration for efficient perovskite solar cells. <i>Current Applied Physics</i> , 2022, , .	1.1	0
13517	Simultaneous Recognition and Separation of Organic Isomers Via Cooperative Control of Pore ⁺ Inside and Pore ⁻ Outside Interactions. <i>Advanced Science</i> , 2022, 9, .	5.6	5
13518	Ultrafast photoinduced dynamics of a donor-(π)bridge-acceptor based merocyanine dye. <i>Scientific Reports</i> , 2022, 12, .	1.6	1
13519	Aromaticity and antiaromaticity in monoheterocyclic three ⁺ membered rings: Application of natural bond orbital theory. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	3
13520	Atroposelective Synthesis of Triaryl π -Pyranones with 1,2 ⁺ Diaxes by π -Heterocyclic Carbene Organocatalysis. <i>Angewandte Chemie</i> , 0, , .	1.6	0
13521	Carbon-atom hybridization tunes the halogen-bond strength in the series of DABCO ⁺ C ₂ H ₂ ⁿ I ₂ ⁿ (n = 0, 1, 2) cocrystals. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 591-596.	0.2	2
13522	A warm-white light-emitting diode based on single-component emitter aromatic carbon nitride. <i>Nature Communications</i> , 2022, 13, .	5.8	19
13523	Computational Investigation into Heteroleptic Photoredox Catalysts Based on Nickel(II) Tris-Pyridinethiolate for Water Splitting Reactions. <i>ACS Organic & Inorganic Au</i> , 0, , .	1.9	1
13524	Toward High-Performance Quinoxaline Based Non-fullerene ⁺ Small Molecule Acceptors for Organic Solar Cells. <i>Electronic Materials Letters</i> , 2023, 19, 38-54.	1.0	4
13525	Toward Understanding the Effect of Fluoride Ions on the Solvation Structure in Lithium Metal Batteries: Insights from First-Principles Simulations. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 48762-48769.	4.0	3
13526	Synthesis, structural, computational, electronic spectra, wave function properties and molecular docking studies of (Z)-4-(((5-methylfuran-2-yl)methylene)amino)-N-(thiazol-2-yl)benzenesulfonamide. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100786.	1.3	24
13527	Theoretical Insight into B ⁺ C Chemical Bonding in Closo-Borate [B _n H _n CH ₃] ⁺ (n = 6, 10, 12) and Monocarborane [CB _n H _n CH ₃] ⁺ (n = 5, 9, 11) Anions. <i>Inorganics</i> , 2022, 10, 186.	1.2	2
13528	Schiff Bases Derived from 2 ⁺ Amino ⁺ 6 ⁺ methylbenzothiazole, 2 ⁺ Amino ⁺ 5 ⁺ chloropyridine and 4 ⁺ Chlorobenzaldehyde: Structure, Computational Studies and Evaluation of ⁺ Biological Activity. <i>ChemistrySelect</i> , 2022, 7, .	0.7	8
13529	2-thioxo -3N-(2-ethoxyphenyl) -5 [4 ⁺ -methyl -3 ⁺ N-(2 ⁺ -ethoxyphenyl) thiazol-2 ⁺ (3 ⁺ H)-ylidene] thiazolidin-4-one: Growth, spectroscopic behavior, single-crystal investigation, Hirshfeld surface analysis, DFT/TD-DFT computational studies and NLO evaluation. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2023, 198, 199-214.	0.8	3
13530	Fluorescence quenching, DFT, NBO, and TD-DFT calculations on 1, 4-bis [2-benzothiazolyl vinyl] benzene (BVB) and meso-tetrakis (4-sulfonatophenyl) porphyrin (TPPS) in the presence of silver nanoparticles. <i>Structural Chemistry</i> , 2023, 34, 1265-1277.	1.0	3
13531	Diazulenylmethyl Cations with a Silicon Bridge: A ⁺ Extended Cationic Motif to Form ⁺ Aggregates with Near-Infrared Absorption and Emission. <i>Journal of the American Chemical Society</i> , 2022, 144, 20385-20393.	6.6	24

#	ARTICLE	IF	CITATIONS
13532	Controllable Synthesis and Synergistic Antioxidation Mechanism of Poly(<i>p</i> -methoxyphenol-phenylamine) in Biodegradable Vegetable-Based Lubricating Oils. <i>Industrial & Engineering Chemistry Research</i> , 0, , .	1.8	0
13533	Theoretical Simulation on Regulating the Magnetic Coupling Properties of Diradical Artificial Bases. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7820-7828.	1.1	2
13534	Unveiling the Aggregation-Induced Emission (AIE) Mechanism and the Effect of Substituents on Luminescence Properties for Salicylaldehyde Azine Derivatives with Intramolecular Hydrogen Bond. <i>Journal of Physical Chemistry C</i> , 2022, 126, 18429-18438.	1.5	6
13535	Molecular Electronic Study of Spiro-[cyclopenta[1,2- <i>b</i> :5,4- <i>i</i>]-dithiophene-4,9-fluorene] Derivatives: Route to Decent Hole-Transporting Materials. <i>Journal of Physical Chemistry C</i> , 2022, 126, 18238-18250.	1.5	0
13536	Computation of Förster Resonance Energy Transfer in Lipid Bilayer Membranes. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8070-8081.	1.1	2
13537	Design Principles for the Acceptor Units in Donor-Acceptor Conjugated Polymers. <i>ACS Omega</i> , 2022, 7, 38969-38978.	1.6	7
13538	Open-Cage Fullerene as Molecular Container for F ⁺ , Cl ⁺ , Br ⁺ and I ⁺ . <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	12
13539	Open-Cage Fullerene as Molecular Container for F ⁺ , Cl ⁺ , Br ⁺ and I ⁺ . <i>Angewandte Chemie</i> , 0, , .	1.6	2
13540	Corralarenes: A Family of Conjugated Tubular Hosts. <i>Journal of the American Chemical Society</i> , 2022, 144, 20351-20362.	6.6	17
13541	Antiviral Disaccharide Lead Compounds against SARS-CoV-2 through Computer-Aided High-Throughput Screen. <i>ChemBioChem</i> , 2022, 23, .	1.3	2
13542	Natural dihydroisobenzofuran derivatives as a template for promising radical scavengers: theoretical insights into structure-activity relationships, thermochemistry and kinetics. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	3
13543	BH ₄ ⁺ Ng ⁺ (Ar ⁿ): Viable Compounds with a B-Ng Covalent Bond. <i>ChemPhysChem</i> , 2023, 24, .	1.0	2
13544	Neutral Boryl Radicals in a Mixed-Valent B(III)-B(II) Adducts. <i>Chemistry - A European Journal</i> , 0, , .	1.7	2
13545	A study on singlet oxygen generation for tetracycline degradation via modulating the size of Fe ₂ O ₃ nanoparticle anchored on g-C ₃ N ₄ nanotube photocatalyst. <i>Nano Research</i> , 2023, 16, 2236-2244.	5.8	8
13546	Pharmaceutical Salts of Piroxicam and Meloxicam with Organic Counterions. <i>Crystal Growth and Design</i> , 2022, 22, 6504-6520.	1.4	5
13547	Combining PD-L1 blockade with immunogenic cell death induced by AIE photosensitizer to improve antitumor immunity. <i>Biomaterials</i> , 2022, 291, 121899.	5.7	18
13548	BiPO ₄ /BiOCl/g-C ₃ N ₄ heterojunction based photoelectrochemical sensing of dopamine in serum samples. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 656, 130456.	2.3	11
13549	Complexes of carbon dioxide with methanol and its monohalogen-substituted: beyond the tetrel bond. <i>Chemical Physics Letters</i> , 2022, , 140158.	1.2	2

#	ARTICLE	IF	CITATIONS
13550	Sequential C ¹³ H Methylation Catalyzed by the B ₁₂ -Dependent SAM Enzyme TokK: Comprehensive Theoretical Study of Selectivities. Chemistry - A European Journal, 2023, 29, .	1.7	3
13551	Mixed-Precision Implementation of the Density Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2022, 18, 7260-7271.	2.3	2
13552	The influence of leveler Brilliant Green on copper superconformal electroplating based on electrochemical and theoretical study. Journal of Industrial and Engineering Chemistry, 2023, 118, 78-90.	2.9	9
13553	Thiolate-Bridged Heterodinuclear Manganese-Cobalt Complexes with Bridging Hydride Ligands. Organometallics, 2023, 42, 133-145.	1.1	1
13554	Comprehensive study on thermal decomposition mechanism and interaction of 3-Nitro-1,2,4-Triazol-5-One/Poly-3-nitromethyl-3-methyloxetane plastic bonded explosives. Journal of Analytical and Applied Pyrolysis, 2022, 168, 105753.	2.6	4
13555	Quantum Chemical Investigations on the Hydrogen-Bonded Interactions of Bioactive Molecule N ² -(4-Methoxysalicylidene) Arginine Hemihydrate. Polycyclic Aromatic Compounds, 0, , 1-22.	1.4	0
13556	HPLC, fluorescence spectroscopy, UV spectroscopy and DFT calculations on the mechanism of scavenging •OH radicals by Hypericin. Journal of Molecular Structure, 2023, 1274, 134472.	1.8	5
13557	Stimulation calculation of desulfurization mechanisms dominated by free radicals reactions during pyrolysis of thiophenes under water vapor atmosphere. Computational and Theoretical Chemistry, 2022, 1217, 113912.	1.1	0
13558	Theoretical studies, spectroscopic investigation, molecular docking, molecular dynamics and MMGBSA calculations with 2-hydrazinoquinoline. Journal of Molecular Structure, 2023, 1274, 134482.	1.8	5
13559	Exploring electronic structure and spectral properties of nitrogen-doped boron clusters		
13560	Simple Approach for Synthesizing a Fluorinated Polymer Donor Enables Promoted Efficiency in Polymer Solar Cells. ACS Applied Energy Materials, 2022, 5, 14250-14261.	2.5	1
13561	Insights of hydrogen adsorption and dissociation on Ni doped Mg ₄ clusters: A DFT study. Computational and Theoretical Chemistry, 2022, 1217, 113907.	1.1	5
13562	Theoretical investigation on interactions between N-methylpyrrolidone-FeCl ₃ and components in model oil: The role of S-Fe coordination in thiophene removal. Journal of Molecular Liquids, 2022, 368, 120719.	2.3	4
13563	Geometries and electronic structures of Pr _n Al (n=20-40) cages: A DFT study. Computational and Theoretical Chemistry, 2022, 1217, 113922.	1.1	0
13564	Bright Organic Mechanoluminescence and Remarkable Mechanofluorochromism from Circularly Polarized TADF Enantiomers with Aggregation-Induced Emission Properties. Chemistry - A European Journal, 0, , .	1.7	0
13565	Theoretical Investigations on MIL-100(M) (M=Cr, Sc, Fe) with High Adsorption Selectivity for Nitrogen and Carbon Dioxide over Methane. Chemistry - an Asian Journal, 2023, 18, .	1.7	2
13566	A Detailed Study of Electronic and Dynamic Properties of Noble Gas-Oxygen Molecule Adducts. Molecules, 2022, 27, 7409.	1.7	1
13567	Understanding Two Variation Patterns of Organic Contaminant Degradation with pH in the Fe _{VI} System under Acidic Conditions. ACS ES&T Engineering, 2023, 3, 64-72.	3.7	13

#	ARTICLE	IF	CITATIONS
13568	Realizing compatibility of high voltage cathode and poly (ethylene oxide) electrolyte in all-solid-state lithium batteries by bilayer electrolyte design. <i>Chemical Engineering Journal</i> , 2023, 454, 140104.	6.6	5
13569	Achieving 34.3% External Quantum Efficiency for Red Thermally Activated Delayed Fluorescence Organic Light-Emitting Diode by Molecular Isomer Engineering. <i>Advanced Optical Materials</i> , 2023, 11, .	3.6	24
13570	Effect of choline chloride based deep eutectic solvents on the aqueous solubility of 4-hydroxycoumarin drug: Measurement and correlation. <i>Journal of Molecular Liquids</i> , 2022, 368, 120650.	2.3	1
13571	Reactivities of silane coupling agents in the silica/rubber composites: Theoretical insights into the relationships between energy barriers and electronic characteristics. <i>Journal of Computational Chemistry</i> , 2023, 44, 581-593.	1.5	1
13572	Aptamer-Gated Mesoporous Silica Nanoparticles for N Protein Triggered Release of Remdesivir and Treatment of Novel Coronavirus (2019-nCoV). <i>Biosensors</i> , 2022, 12, 950.	2.3	2
13573	Adsorption properties of metal functionalized fullerene (C ₅₉ Au, C ₅₉ Hf) Tj ETQq1 1 0.784314 rgBT /Overlook hydroxyurea (HXU): insight from theoretical computation. <i>Zeitschrift Fur Physikalische Chemie</i> , 2022, 236, 1515-1546.	1.4	44
13574	A stability analysis of choline chloride: urea deep eutectic solvent using density functional theory. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113921.	1.1	7
13575	Triaryl Carbonium Ion-Pair-Mediated Cooperative Aerobic Dehydrogenation of N-Heterocycles. <i>ACS Catalysis</i> , 2022, 12, 14123-14129.	5.5	6
13576	Pyrrolidine-2,5-dione-derived ionic liquids promoted efficient transformation of flue gas CO ₂ into β -alkylidene cyclic carbonates at room temperature. <i>Journal of CO₂ Utilization</i> , 2022, 65, 102227.	3.3	2
13577	Trimetallic Chalcogenide Species: Synthesis, Structures, and Bonding. <i>Molecules</i> , 2022, 27, 7473.	1.7	2
13578	A theoretical investigation into the effect of solvent on crystal morphology of 1-methyl-3,4,5-trinitro-1H-pyrazole (MTNP). <i>Journal of Crystal Growth</i> , 2023, 601, 126952.	0.7	3
13579	In-situ immobilization mechanism of lead and cadmium species by pyrolytic char in MSW pyrolysis process: Effect of chlorine group. <i>Journal of Analytical and Applied Pyrolysis</i> , 2022, 168, 105750.	2.6	2
13580	Electrochemical Diazidation of Alkenes Catalyzed by Manganese Porphyrin Complexes with Second-Sphere Hydrogen-Bond Donors. <i>ACS Catalysis</i> , 2022, 12, 14106-14112.	5.5	8
13581	Donor or Acceptor: Molecular Engineering Based on dibenzo[a,c]phenazine Backbone for Highly Efficient Thermally-Activated Delayed Fluorescence Organic Light-Emitting Diodes. <i>Advanced Optical Materials</i> , 2023, 11, .	3.6	8
13582	Insights into the structural, electronic and spectral properties of gas-phase GaMgn+ (n=12) clusters. <i>Optik</i> , 2022, 270, 170093.	1.4	1
13583	Palladium/PCPhosCatalyzed Asymmetric Heck/TsujiTrost Reactions of AminoTethered 1,3Cyclohexadiene with Aryl and Alkenyl Halides. <i>Angewandte Chemie</i> , 0, , .	1.6	0
13584	Electronic and structure conformational analysis (HOMO-LUMO, MEP, NBO, ELF, LOL, AIM) of hydrogen bond binary liquid crystal mixture: DFT/TD-DFT approach. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113920.	1.1	11
13585	Structural, Theoretical Analysis, and Molecular Docking of Two Benzamide Isomers. Halogen Bonding and Its Role in the Diverse Ways of Coupling with Protein Residues. <i>Chemical and Pharmaceutical Bulletin</i> , 2022, 70, 782-790.	0.6	2

#	ARTICLE	IF	CITATIONS
13586	A versatile artificial metalloenzyme scaffold enabling direct bioelectrocatalysis in solution. <i>Science Advances</i> , 2022, 8, .	4.7	2
13587	Interheteromolecular Hyperconjugation Boosts (De)hydrogenation for Reversible H ₂ Storage. <i>ChemSusChem</i> , 2023, 16, .	3.6	3
13588	B3Al4+: A Three-Dimensional Molecular Reuleaux Triangle. <i>Molecules</i> , 2022, 27, 7407.	1.7	4
13589	Surface enhanced Raman spectra (SERS) and computational study of gemcitabine drug adsorption on to Au/Ag clusters with different complexes: Adsorption behavior and solvent effect (IEFPCM) of Anticancer agent. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113914.	1.1	5
13590	Development and characterization of an amorphous curcumin-Eudragit®E100 solid dispersions with improved solubility, stability, and pharmacokinetic properties. <i>Pharmaceutical Development and Technology</i> , 2022, 27, 965-974.	1.1	6
13591	Photodegradation of a mixture of five pharmaceuticals commonly found in wastewater: Experimental and computational analysis. <i>Environmental Research</i> , 2023, 216, 114659.	3.7	15
13592	Study of interaction between different solvents and neurotransmitters dopamine, l-adrenaline, and l-noradrenaline using LED, QTAIM and AIMD. <i>Journal of Molecular Liquids</i> , 2022, 368, 120708.	2.3	9
13593	Palladium/PCyPhos-Catalyzed Asymmetric Heck/Tsuji-Trost Reactions of Amino-ethered 1,3-cyclohexadiene with Aryl and Alkenyl Halides. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	7
13594	Circularly polarized luminescence of pinene-modified tetradentate platinum(II) enantiomers containing fused 5/6/6 metallocycles. <i>Heliyon</i> , 2022, , e11358.	1.4	0
13595	Geometric Structure, Electronic, and Spectral Properties of Metal-free Phthalocyanine under the External Electric Fields. <i>ACS Omega</i> , 2022, 7, 41266-41274.	1.6	3
13596	Modeling of pristine, Ir- and Au-decorated C60 fullerenes as sensors for detection of hydroxyurea and nitrosourea drugs. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108802.	3.3	40
13597	Structural microheterogeneity and hydrogen bonding properties in the mixtures of two ionic liquids with a common imidazolium cation. <i>Journal of Molecular Liquids</i> , 2022, 368, 120594.	2.3	8
13598	Ultra-low-permittivity, high hydrophobic, and excellent thermally stable fluoroelastomer/polyimide composite films employing dielectric reduction. <i>European Polymer Journal</i> , 2022, 181, 111667.	2.6	4
13599	Intra-ring proton transfer effect on the Structure-NLO property relationships of phthalocyanine derivatives. <i>Journal of Molecular Liquids</i> , 2022, 368, 120652.	2.3	4
13600	The effect of metal silver(I) salt on CO ₂ conversion to α -alkylidene cyclic carbonates: A DFT study. <i>Journal of CO₂ Utilization</i> , 2022, 66, 102267.	3.3	1
13601	Application for the porous structure of cellulose separators: Ionic conduction path in lithium-ion battery. <i>Journal of Electroanalytical Chemistry</i> , 2022, 926, 116937.	1.9	1
13602	Comparative DFT study on the H ₂ adsorption and the sensing properties of BN-, BP-, AlN-, and AlP-decorated graphene nanoflakes. <i>Diamond and Related Materials</i> , 2022, 130, 109510.	1.8	3
13603	Effect of hydroxyl functional groups on SO ₂ adsorption by activated carbon. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108727.	3.3	4

#	ARTICLE	IF	CITATIONS
13604	Solvents evaluation for extraction of polycyclic aromatics from FCC diesel: Experimental and computational thermodynamics. <i>Chemical Engineering Science</i> , 2022, 264, 118205.	1.9	5
13605	Density functional theory investigation on the interaction of F2 with (4,0) SWCNT and X-doped (4,0) SWCNT for gas sensor application (X=ÅB, S, Si, N, and Al). <i>Diamond and Related Materials</i> , 2022, 130, 109463.	1.8	2
13606	Reasons of low formaldehyde adsorption capacity on activated carbon: Multi-scale simulation of dynamic interaction between pore size and functional groups. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108723.	3.3	12
13607	Heterologous expression of family GH11 <i>Aspergillus niger</i> xylanase B (AnXylB11) in <i>Pichia pastoris</i> and competitive inhibition by riceXIP: An experimental and simulation study. <i>Colloids and Surfaces B: Biointerfaces</i> , 2022, 220, 112907.	2.5	0
13608	Effect of inorganic salt concentration and types on electrophoretic migration of oil droplets in oil-in-water emulsion: A molecular dynamics study. <i>Journal of Molecular Liquids</i> , 2022, 367, 120549.	2.3	5
13609	NLO properties and electronegativity characteristics of superalkalis doped all-cis-1,2,3,4,5,6-hexafluorocyclohexane complexes. <i>Optik</i> , 2022, 271, 170139.	1.4	5
13610	Visualization of UV and ECD spectra of E&Z isomers of N-(4-Å-Hydroxy-cinnamoyl)-Å-hydroxyanthranilic acid. <i>Computational Biology and Chemistry</i> , 2022, 101, 107777.	1.1	5
13611	Highly stable macro-porous N-donor CyMe4-BTPhen/SiO2-P adsorbent for efficient selective extraction of actinides from HLLW: An experimental, mechanism, theoretical study. <i>Environmental Nanotechnology, Monitoring and Management</i> , 2022, 18, 100749.	1.7	0
13612	Degradation of UV-P mediated by hydroxyl radical, sulfate radical and singlet oxygen in aquatic solution: DFT and experimental studies. <i>Environmental Pollution</i> , 2022, 315, 120416.	3.7	4
13613	Experimental and theoretical study on the extraction of keratin from human hair using protic ionic liquids. <i>Journal of Molecular Liquids</i> , 2022, 368, 120626.	2.3	4
13614	Three birds with one stone: Microphase separation induced by densely grafted short chains in ion conducting membranes. <i>Journal of Membrane Science</i> , 2022, 664, 121119.	4.1	3
13615	Insight into the effect of anions on cycloaddition of CO2 catalyzed by carboxylate anion-based ionic liquids: A theoretical study by QM and MD. <i>Journal of Molecular Liquids</i> , 2022, 368, 120629.	2.3	1
13616	Molecular insights into azeotrope separation in the methyl tert-butyl ether production process using ChCl-based deep eutectic solvents. <i>Chemical Engineering Science</i> , 2022, 264, 118179.	1.9	13
13617	Separation of ethyl acetate-isopropanol using low transition temperature mixtures: Vapor-liquid equilibrium experiments and quantum chemical calculation. <i>Journal of Molecular Liquids</i> , 2022, 367, 120589.	2.3	0
13618	Thermal hazard characteristics and essential mechanism study of 1-hydroxybenzotriazole: Thermodynamic study combined DFT simulation. <i>Chemical Engineering Research and Design</i> , 2022, 168, 713-722.	2.7	3
13619	Benzothiazole-based Schiff bases as novel AIE(E)gens: Mechanistic insights into distinction between dimethylphenylamine and triphenylamine fragments in double bond-bridged D-A system. <i>Dyes and Pigments</i> , 2023, 208, 110849.	2.0	2
13620	Combined computational and experimental investigation on the Fenton reagent catalysed hydroxylation of benzene. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2022, 141, 104576.	2.7	0
13621	Assessing nanoparticle-surfactant-salt synergistic effects on droplet-Å-droplet electrocoalescence by molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , 2022, 367, 120570.	2.3	12

#	ARTICLE	IF	CITATIONS
13622	Excellent ultrafast broadband optical limiting of functionalized twistacenes based on two-photon absorption-induced excited state absorption. <i>Dyes and Pigments</i> , 2023, 208, 110842.	2.0	1
13623	Dicyanomethylene-functionalized s-indacene-based D- π -A- π -D dyes exhibiting large near-infrared two-photon absorption cross-section. <i>Dyes and Pigments</i> , 2023, 208, 110864.	2.0	2
13624	Molecular insight into the polymorphism-dependent organic phosphorescence. <i>Dyes and Pigments</i> , 2023, 208, 110853.	2.0	3
13625	Studies on the thermal degradation mechanism of polyethylene terephthalate and its 2-carboxy ethyl (phenyl) phosphinic acid copolymers. <i>Polymer Degradation and Stability</i> , 2022, 206, 110185.	2.7	6
13626	On the structure of cetylpyridinium perchlorate: A combined XRD, NMR, IR and DFT study. <i>Journal of Molecular Liquids</i> , 2022, 368, 120659.	2.3	4
13627	A novel sustained-release formulation of 5-fluorouracil-phenylalanine cocrystal self-assembled by cocrystal-entrapped micelle strategy displays enhanced antitumor efficacy. <i>Journal of Molecular Liquids</i> , 2022, 368, 120665.	2.3	1
13628	DFT Insights into the mechanism of Ru(II) Catalyzed C7-selective amidation of N-pivaloylindole. <i>Journal of Organometallic Chemistry</i> , 2022, 982, 122534.	0.8	1
13629	Excellent capture of Pb(II) and Cu(II) by hierarchical nanoadsorbent Fe ₃ O ₄ @SiO ₂ @PAA-SO ₃ H: A combined experimental and theoretical study. <i>Chemosphere</i> , 2022, 309, 136791.	4.2	5
13630	Theoretical study of multi-coordinated Xe(AuF) (n=4): Intriguing bond-bending isomerism. <i>Chemical Physics</i> , 2023, 565, 111743.	0.9	1
13631	Solvent-free 3D layered energetic metal organic framework: Structure, stability, and its laser response. <i>Journal of Solid State Chemistry</i> , 2023, 317, 123607.	1.4	4
13632	Designing a novel metal-organic framework@covalent organic framework composite for the selective removal of fluoroquinolones: Adsorption behaviors and theoretical investigation. <i>Applied Surface Science</i> , 2023, 609, 155433.	3.1	12
13633	A double network conductive gel with robust mechanical properties based on polymerizable deep eutectic solvent. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 656, 130349.	2.3	11
13634	Molecular insights into the role of O ₂ in reversed C ₂ H ₆ /C ₂ H ₄ separation on metal-organic frameworks. <i>Separation and Purification Technology</i> , 2023, 304, 122332.	3.9	3
13635	Data-mining based assembly of promising metal-organic frameworks on Xe/Kr separation. <i>Separation and Purification Technology</i> , 2023, 304, 122357.	3.9	5
13636	New insight into poor flotation recovery of fine molybdenite: An overlooked phase transition from 2H to 1T MoS ₂ . <i>Separation and Purification Technology</i> , 2023, 304, 122286.	3.9	16
13637	Effect of surface modification on optical and electronic properties of graphene quantum dots. <i>Applied Surface Science</i> , 2023, 609, 155379.	3.1	21
13638	Photostable aggregation-induced emission of iridium(III) complex realizing robust and high-resolution imaging of latent fingerprints. <i>Sensors and Actuators B: Chemical</i> , 2023, 375, 132898.	4.0	14
13639	Synthesis and spectral studies of Ni(â€¦) complexes involving functionalized dithiocarbamates and triphenylphosphine: X-ray crystal structure, thermal stability, Hirshfeld surface analysis, DFT and biological evaluation. <i>Inorganica Chimica Acta</i> , 2023, 545, 121271.	1.2	3

#	ARTICLE	IF	CITATIONS
13640	Phase behavior and molecular insights on the separation of dimethyl carbonate and methanol azeotrope by extractive distillation using deep eutectic solvents. Separation and Purification Technology, 2023, 305, 122489.	3.9	12
13641	Enhanced photocatalytic toluene oxidation performance induced by two types of cooperative fluorine doping in polymeric carbon nitride with the first-principles calculations. Journal of Colloid and Interface Science, 2023, 630, 452-459.	5.0	4
13642	Modulation of halogen-bonded 2D self-assemblies of benzothiadiazole derivative: Concentration and solvent effects. Applied Surface Science, 2023, 609, 155256.	3.1	3
13643	Optical response properties of some metal cluster supported host-guest systems. , 2023, , 123-137.		0
13644	Molecular electrides: An overview of their structure, bonding, and reactivity. , 2023, , 275-295.		0
13645	Femtosecond transient absorption spectroscopy on the thermally activated delayed fluorescence of bis[4-(9-H-carbazole)phenyl] sulfone. Journal of Luminescence, 2023, 253, 119459.	1.5	1
13646	Preparation of ZIF-67@DTMS NPs/Epoxy composite coating and its anti-corrosion performance for Q235 carbon steel in 3.5wt% NaCl solution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2023, 656, 130370.	2.3	13
13647	Investigation of non-covalent interactions in Polypyrrole/Polyaniline/Carbon black ternary complex for enhanced thermoelectric properties via interfacial carrier scattering and π - π stacking. Journal of Colloid and Interface Science, 2023, 630, 46-60.	5.0	10
13648	Zintl cluster as a building block of superalkali, superhalogen, and superatom. , 2023, , 333-344.		0
13649	Anchoring the late first row transition metals with B12P12 nanocage to act as single atom catalysts toward oxygen evolution reaction (OER). Materials Science in Semiconductor Processing, 2023, 153, 107164.	1.9	25
13650	Exploring the separation mechanism of Gemini surfactant in scheelite froth flotation at low temperatures: Surface characterization, DFT calculations and kinetic simulations. Separation and Purification Technology, 2023, 305, 122358.	3.9	12
13651	Enhancement of polysiloxane/epoxy resin compatibility through an electrostatic and van der Waals potential design strategy. Polymer Testing, 2023, 117, 107820.	2.3	10
13652	Crystal structure, in vitro cytotoxicity, DNA binding and DFT calculations of new copper (II) complexes with coumarin-amide ligand. Journal of Inorganic Biochemistry, 2023, 238, 112030.	1.5	8
13653	Demystifying viscous isoalkanes as the organic solvent in interfacial polymerization for manufacturing desalination membranes. Desalination, 2023, 545, 116166.	4.0	3
13654	Effects of polystyrene nanoplastics with different functional groups on the accumulation and toxicity of Pb on dandelion. Chemosphere, 2023, 310, 136874.	4.2	13
13655	Mechanism of photo-assisted atomic layer etching of chlorinated Si(111) surfaces: Insights from DFT/TDDFT calculations. Materials Science in Semiconductor Processing, 2023, 153, 107169.	1.9	3
13656	Synergistic and efficient degradation of acid red 73 by UV/O ₃ /PDS: Kinetic studies, free radical contributions and degradation pathways. Environmental Research, 2023, 216, 114449.	3.7	6
13657	Polyetherimide membrane with tunable porous morphology for safe lithium metal-based batteries. Chemical Engineering Journal, 2023, 453, 139804.	6.6	16

#	ARTICLE	IF	CITATIONS
13658	Uncovering the dependence of ESIPT behaviors and fluorescence properties of two new benzothiazole-based fluorophores on solvent polarity: A TD-DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 286, 121991.	2.0	8
13659	NaOH-modified biochar supported Fe/Mn bimetallic composites as efficient peroxymonosulfate activator for enhance tetracycline removal. <i>Chemical Engineering Journal</i> , 2023, 454, 139949.	6.6	35
13660	Synthesis, characterization and biological evaluation of two cyclometalated iridium(III) complexes containing a glutathione S-transferase inhibitor. <i>Journal of Inorganic Biochemistry</i> , 2023, 238, 112050.	1.5	5
13661	Fe ³⁺ -enhanced zero valent iron/peroxymonosulfate (ZVI/PMS) process for the transformation of iopamidol during coagulation and reduction of iodinated disinfection by-products. <i>Chemical Engineering Journal</i> , 2023, 453, 139723.	6.6	9
13662	Quantum computational, spectroscopic, topological investigations and molecular docking studies on piperazine derivatives: A comparative study on Ethyl, Benzene and Furan sulfonyl Piperazine. <i>Journal of Molecular Structure</i> , 2023, 1274, 134324.	1.8	3
13663	Crystal structure, intermolecular interactions and NLO properties for imidazolium hydrogen sulfate ionic liquid. <i>Journal of Molecular Structure</i> , 2023, 1273, 134307.	1.8	6
13664	Solubility, solvent effect, preferential solvation and DFT computations of 5-nitrosalicylic acid in several aqueous blends. <i>Journal of Chemical Thermodynamics</i> , 2023, 177, 106936.	1.0	1
13665	Insight for the synthesis and crystal structure of diazatetraasterane derivatives: Experimental and theoretical studies. <i>Journal of Molecular Structure</i> , 2023, 1273, 134316.	1.8	0
13666	The molecular nature of the eliminating azeotropy of dimethyl carbonate-ethanol system by ionic liquid entrainer. <i>Separation and Purification Technology</i> , 2023, 305, 122420.	3.9	2
13667	Synthesis of novel pyridinium based compounds and their possible application in dye-sensitized solar cells. <i>Journal of Molecular Structure</i> , 2023, 1274, 134433.	1.8	2
13668	New insights into the excited state of an A-D-A quadrupolar molecule strongly hydrogen bonded to molecules of methanol and hexafluoro isopropanol. <i>Journal of Molecular Structure</i> , 2023, 1273, 134294.	1.8	4
13669	Antihypotensive potency of p-syneprhine: Spectral analysis, molecular properties and molecular docking investigation. <i>Journal of Molecular Structure</i> , 2023, 1273, 134233.	1.8	18
13670	(E)-2-styrylanthracene-9,10-dione derivatives as novel fluorescent probes: synthesis, photophysical properties and application in mitochondria imaging. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 286, 121988.	2.0	0
13671	Insight into the retardation of retrogradation of chestnut starch by heat-moisture treatment with flavonoids. <i>Food Chemistry</i> , 2023, 404, 134587.	4.2	6
13672	Catalytic activity enhancement by P and S co-doping of a single-atom Fe catalyst for peroxymonosulfate-based oxidation. <i>Chemical Engineering Journal</i> , 2023, 453, 139890.	6.6	13
13673	Different positions of cyano substitution controlled directionality of ESIPT processes with two asymmetric proton acceptors system: A TD-DFT study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 436, 114353.	2.0	6
13674	Selective adsorption mechanism of copper from nickel electrolytes by tert-butyl 2-(N-octyl-2-picolylamino) acetate functionalized chelating resin: A DFT study. <i>Applied Surface Science</i> , 2023, 610, 155385.	3.1	1
13675	New insight into the mechanism of symmetry-breaking charge separation induced high-valent iron(â€¦) for highly efficient photodegradation of organic pollutants. <i>Applied Catalysis B: Environmental</i> , 2023, 321, 122066.	10.8	7

#	ARTICLE	IF	CITATIONS
13676	Solvent effect on ESIPT process of N-(8-Quinoly) salicylaldimine: A DFT/TD-DFT calculation. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 436, 114335.	2.0	7
13677	Upcycling contaminated biomass into metal-supported heterogeneous catalyst for electro-Fenton degradation of thiamethoxam: Preparation, mechanisms, and implications. Chemical Engineering Journal, 2023, 453, 139814.	6.6	10
13678	Solvent interaction and dynamics of neurotransmitters aspartic acid and glutamic acid with water and ethanol. Journal of Molecular Structure, 2023, 1273, 134347.	1.8	9
13679	Citric acid modified ultrasmall copper peroxide nanozyme for in situ remediation of environmental sulfonyleurea herbicide contamination. Journal of Hazardous Materials, 2023, 443, 130265.	6.5	16
13680	Chemical bonding and aromaticity analyses of petroporphyrins with vanadium or nickel. Fuel, 2023, 333, 126344.	3.4	3
13681	Influence of the coordination metal on the thermal properties of double selenates: Theoretical insights and experimental study. Journal of Molecular Structure, 2023, 1274, 134411.	1.8	1
13682	An investigation on 3-hydroxybenzaldehyde for exploring terahertz low-frequency vibration modes with quasi-harmonic approximation method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2023, 287, 122046.	2.0	0
13683	Extraction-adsorption coupled desulfurization of fuel oil by novel functionalized porous liquids. Chemical Engineering Journal, 2023, 453, 139935.	6.6	14
13684	Inhibiting effect investigation of ammonium dihydrogen phosphate on oxidative pyrolysis characteristics of bituminous coal. Fuel, 2023, 333, 126352.	3.4	17
13685	Experimental and quantum chemical calculations investigations of morpholine-based ionic liquids as extractants for efficient extraction of nitrogen heterocyclic neutral compounds. Fuel, 2023, 333, 126446.	3.4	6
13686	Synthesis, structural and exploration of non-covalent interactions of the palladium complex with the crystalline water molecule: A comprehensive quantum chemical approach. Journal of Molecular Structure, 2023, 1274, 134419.	1.8	4
13687	One-pot non-covalent heterogenization and aromatization of poly(ionic liquids) for metal-/cocatalyst-free and atmospheric CO ₂ conversion. Applied Catalysis B: Environmental, 2023, 322, 122125.	10.8	12
13688	Combination of peroxymonosulfate and Fe(III) for enhanced degradation of sulfamethoxazole: The overlooked roles of high-valent iron species. Chemical Engineering Journal, 2023, 453, 139742.	6.6	22
13689	Comparative DFT-D3 assessment of fluorogenic supramolecular interaction of naphthalene moiety location on new dibenzodiaza-crown ether macrocycles with C ₆₀ . Journal of Molecular Structure, 2023, 1273, 134343.	1.8	1
13690	Simultaneous strengthening and toughening lignin/cellulose nanofibril composite films: Effects from flexible hydrogen bonds. Chemical Engineering Journal, 2023, 453, 139770.	6.6	31
13692	Y ₈ C ₄ cluster: a boron-carbon molecular wheel with dodeca-coordination number in plane. Physical Chemistry Chemical Physics, 2022, 24, 28548-28553.	1.3	1
13693	Ultra High Reversible Hydrogen Storage Capacity of Li ₄ B ₂ Cluster: A Quantum Chemical Study. Physical Chemistry Chemical Physics, 0, , .	1.3	1
13694	Preparation and redistribution mechanism of dimethyldichlorosilane catalyzed by the AlCl ₃ /ZSM-5(5T)@MIL-53(Al) core-shell catalyst. New Journal of Chemistry, 2022, 46, 23282-23291.	1.4	2

#	ARTICLE	IF	CITATIONS
13695	A π -extended benzothiadiazole derivative for high-efficiency TADF-sensitized π -,uorescent organic light-emitting diode. <i>Chemical Communications</i> , 0, , .	2.2	3
13696	The organic co-crystals formed using naphthalenediimide-based triangular macrocycles and coronene: intermolecular charge transfers and nonlinear optical properties. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 29747-29756.	1.3	5
13697	Effects of nitric acid concentration for nitration of fused [1,2,5]oxadiazolo[3,4- <i>d</i>]pyrimidine-5,7-diamine. <i>Dalton Transactions</i> , 2022, 51, 17987-17993.	1.6	2
13698	Doping C ₆₀ (OH) to Regulate the Crosslink Network and Energy Band Structures of Epoxy Resin and Allow for Electronic Directional Drive in C ₆₀ (OH)/EP. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2023, 30, 230-237.	1.8	5
13699	Effective tuning of magnetic anisotropy in distorted pentagonal bipyramidal Ni(η^5) complexes <i>via</i> substitution of axial coligands. <i>Dalton Transactions</i> , 0, , .	1.6	2
13700	Examining the gas-phase homodimers of 3,3,3-trifluoro-1,2-epoxypropane using quantum chemistry and microwave spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 28495-28505.	1.3	3
13701	Apples to apples comparison of standardized to unstandardized principal component analysis of methods that assign partial atomic charges in molecules. <i>RSC Advances</i> , 2022, 12, 31617-31628.	1.7	3
13702	Electrical Properties of Insulating Liquids Based on Molecular Properties Calculated by Density Functional Theory. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2022, 29, 2274-2282.	1.8	5
13703	Improvement of the fluorescent sensing biomarker 3-nitrotyrosine for a new luminescent coordination polymer by size regulation. <i>CrystEngComm</i> , 2022, 24, 8286-8293.	1.3	5
13704	Actinide-doped boron clusters: from borophenes to borospherenes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 29705-29711.	1.3	2
13705	Sumanene-functionalised bis(terpyridine) μ -ruthenium(η^5) complexes showing photoinduced structural change and cation sensing. <i>Inorganic Chemistry Frontiers</i> , 2022, 10, 211-217.	3.0	4
13706	Theoretical exploration of molecular packing and the charge transfer mechanism of organic solar cells based on PM6:Y6. <i>Journal of Materials Chemistry A</i> , 2022, 10, 25611-25619.	5.2	6
13707	Antioxidant mechanisms and products of four 4,5,7-trihydroxyflavonoids with different structural types. <i>RSC Medicinal Chemistry</i> , 2023, 14, 173-182.	1.7	3
13708	Synthesis, nonlinear optical analysis and DFT studies of D π - π -D and A π - π -A configured Schiff bases derived from bis-phenylenediamine. <i>RSC Advances</i> , 2022, 12, 32185-32196.	1.7	8
13709	Ultra-small NIR J-aggregates of BODIPY for potent phototheranostics. <i>Biomaterials Science</i> , 2022, 11, 195-207.	2.6	5
13710	Carbazole and dibenzo[<i>b</i>], <i>d</i>]furan-based hole transport materials with high thermal stability. <i>New Journal of Chemistry</i> , 2022, 46, 22633-22638.	1.4	3
13711	Torsion effect of the imide ring on the performance of transparent polyimide films with methyl-substituted phenylenediamine. <i>Polymer Chemistry</i> , 2022, 13, 6606-6613.	1.9	8
13712	Discovery of resonance-enhanced emission effect and its application in the design of fluorescent molecules. <i>Journal of Materials Chemistry C</i> , 2022, 10, 17695-17702.	2.7	2

#	ARTICLE	IF	CITATIONS
13713	Impacts of noncovalent interactions involving sulfur atoms on protein stability, structure, folding, and bioactivity. <i>Organic and Biomolecular Chemistry</i> , 2022, 21, 11-23.	1.5	5
13714	Adjusting the Balance between Hydrogen and Chalcogen Bonds. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 111763.	1.3	5
13715	Broad wavelength sensitive coumarin sulfonium salts as photoinitiators for cationic, free radical and hybrid photopolymerizations. <i>Progress in Organic Coatings</i> , 2023, 174, 107272.	1.9	9
13716	The anti-TMV potency of the tobacco-derived fungus <i>Aspergillus versicolor</i> and its active alkaloids, as anti-TMV activity inhibitors. <i>Phytochemistry</i> , 2023, 205, 113485.	1.4	13
13717	First-principles study of chalcogen-bonded self-assembly structures on silicene: Some insight into the fabrication of molecular architectures on surfaces through chalcogen bonding. <i>Chemical Physics</i> , 2023, 565, 111763.	0.9	0
13718	Strengthened adsorption films of double antibiotic medicines skeletons-based dendrimers on copper surface: Molecular dynamics simulation and intensified anti effects of algae, bacteria and corrosion. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 656, 130501.	2.3	4
13719	Regulatory mechanism of a novel non-aqueous absorbent for CO ₂ capture using 2-amino-2-methyl-1-propanol: Low viscosity and energy efficient. <i>Journal of CO₂ Utilization</i> , 2023, 67, 102277.	3.3	20
13720	Temperature-controlled electrochemical sensor based on environmentally responsive polymer/BiPO ₄ /BiOCl/multi-walled carbon nanotube composite for the detection of catechol in water. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 657, 130543.	2.3	5
13721	Ab initio study of the low-lying states of PS molecule. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2023, 295, 108415.	1.1	1
13722	Dual-emitting Mn(II) and Zn(II) halide complexes with 9,10-dihydro-9-oxa-10-phosphaphenanthrene-10-oxide as ligand. <i>Inorganica Chimica Acta</i> , 2023, 545, 121285.	1.2	9
13723	Mercuriphilic interactions in heterometallic Ru-Hg carbonyl clusters. <i>Inorganica Chimica Acta</i> , 2023, 545, 121281.	1.2	0
13724	Structural and antimicrobial property changes of veterinary antibiotics in thermal treatment. <i>Environmental Pollution</i> , 2023, 316, 120519.	3.7	0
13725	Balance of sulfur doping content and conductivity of hard carbon anode for high-performance K-ion storage. <i>Energy Storage Materials</i> , 2023, 54, 668-679.	9.5	25
13726	Shear flow induced specific ion interfacial effect on enhanced difference in mass transfer in the boundary layer. <i>Chemical Engineering Journal</i> , 2023, 454, 140199.	6.6	1
13727	A theoretical study on the influence of N-containing heterocyclic ligands on the luminescence mechanisms (phosphorescence or TADF) of Au (III) complexes. <i>Organic Electronics</i> , 2023, 113, 106676.	1.4	0
13728	Theoretical study on the origin of the dual phosphorescence emission from organic aggregates at room temperature. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 287, 122077.	2.0	6
13729	In-situ growth of ZIF-8 nanocrystals on biochar for boron adsorption. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 657, 130504.	2.3	9
13730	Pyridine-based covalent organic framework for efficient and selective removal of Hg(II) from water: Adsorption behavior and adsorption mechanism investigations. <i>Chemical Engineering Journal</i> , 2023, 454, 140154.	6.6	23

#	ARTICLE	IF	CITATIONS
13731	Hydrogen bond network reconstruction of lignite for efficient moisture removal via deep-eutectic-solvent-assisted hydrothermal treatment. <i>Fuel</i> , 2023, 334, 126653.	3.4	7
13732	Insights into atrazine degradation by thermally activated persulfate: Evidence from dual C&H isotope analysis and DFT simulations. <i>Chemical Engineering Journal</i> , 2023, 454, 140207.	6.6	7
13733	Novel insights on the graphene oxide nanosheets induced demulsification and emulsification of crude oil-in-water emulsion: A molecular simulation study. <i>Fuel</i> , 2023, 333, 126529.	3.4	3
13734	Construction of covalent organic frameworks with alternating rigid and flexible units and their controlled release of active sites. <i>Chemical Engineering Journal</i> , 2023, 454, 140119.	6.6	2
13735	Understanding adsorption mechanisms of mercury over unburned carbon. <i>Fuel</i> , 2023, 333, 126399.	3.4	6
13736	Photolysis of fungicide triadimefon: A combined experimental and theoretical investigation on homolytic C O and C N bonds dissociation mechanisms. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 436, 114402.	2.0	2
13737	Free radical mechanism of toxic organic compound formations from o-chlorophenol. <i>Journal of Hazardous Materials</i> , 2023, 443, 130367.	6.5	4
13738	Activation of persulfate by vanadium oxide modified carbon nanotube for 17 β -estradiol degradation in soil: Mechanism, application and ecotoxicity assessment. <i>Science of the Total Environment</i> , 2023, 858, 159760.	3.9	7
13739	Optical properties, bioimaging and theoretical calculation of a Zn(II) complex based on triphenylamine derivative. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 286, 122012.	2.0	1
13740	Spectroscopic, reactivity analysis and docking studies of 3-(adamantan-1-yl)-4-(4-fluorophenyl)-1-[(4-phenylpiperazin-1-yl)methyl]-4,5-dihydro-1H-1,2,4-triazole-5-thione: 1.8 DFT and MD simulations. <i>Journal of Molecular Structure</i> , 2023, 1274, 134418.		3
13741	Ozone mechanism, kinetics, and toxicity studies of halophenols: Theoretical calculation combined with toxicity experiment. <i>Science of the Total Environment</i> , 2023, 858, 160101.	3.9	6
13742	Ligands-triggered evolution of catalytic intermediates during periodate activation via soluble Mn(II) for organic contaminants's abatement. <i>Applied Catalysis B: Environmental</i> , 2023, 322, 122093.	10.8	17
13743	The anti-snake activity of <i>Nectandra angustifolia</i> flavonoids on phospholipase A2: In vitro and in silico evaluation. <i>Journal of Ethnopharmacology</i> , 2023, 302, 115889.	2.0	3
13744	Investigation and design of efficient intramolecular charge transfer dyes with DBTP-based dual-electron-donor structure. <i>Materials Science in Semiconductor Processing</i> , 2023, 154, 107203.	1.9	0
13745	Exploration of electronic and non-linear optical properties of novel 4-Aryl-2-methylpyridine based compounds synthesized via high-yielding Pd(0) catalysed reaction. <i>Journal of Molecular Structure</i> , 2023, 1274, 134469.	1.8	2
13746	Insight into synergistic effects of oxygen and nitrogen dual-dopants in carbon catalysts on selective catalytic reduction of NOx with NH3: A combined computational and experimental verification. <i>Chemical Engineering Journal</i> , 2023, 454, 140098.	6.6	10
13748	End-group modification of terminal acceptors on benzothiadiazole-based BT2F-IC4F molecule to establish efficient organic solar cells. <i>Journal of Molecular Liquids</i> , 2022, 368, 120770.	2.3	31
13749	Supramolecular assemblies involving energetically significant unconventional $\pi(\text{CN})\cdots\pi$ and anion- π (nitrile) contacts in Zn(II) coordination compounds: Antiproliferative evaluation and theoretical studies. <i>Journal of Molecular Structure</i> , 2023, 1274, 134568.	1.8	2

#	ARTICLE	IF	CITATIONS
13750	Molecular-Level Designed Polymer Electrolyte for High-Voltage Lithium-Metal Solid-State Batteries. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	23
13751	Suppressed recombination loss in organic photovoltaics adopting a planar mixed heterojunction architecture. <i>Nature Energy</i> , 2022, 7, 1076-1086.	19.8	128
13752	A DFT Computational and Synthetic Study of New Curcuminoidpropargyl Adducts with Pseudo-Cofacial Aryl Rings. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0
13753	Synthesis, Spectroscopic (FTIR, FT-Raman and UV-Vis), Structural Investigation, Hirshfeld, AIM, NBO, Chemical Reactivity, In-Vitro and In-Silico Analysis of N-(2-Hydroxyphenyl)-4-Toluenesulfonamide. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 8005-8036.	1.4	2
13754	Study on the Mechanism of Sodium Dodecylbenzene Sulfonate Oxidation by Electro-Fenton System. <i>Water, Air, and Soil Pollution</i> , 2022, 233, .	1.1	1
13755	Solvent polarity, structural and electronic properties with different solvents and biological studies of 3,3,5-triphenylfuran-2(3H)-one- cancers of the blood cells. <i>Journal of Molecular Liquids</i> , 2022, 368, 120674.	2.3	7
13756	Theoretical Study on the Structures, Electronic Properties, and Aromaticity of Thiophene Analogues of Anti-Kekulene. <i>Chemistry</i> , 2022, 4, 1546-1560.	0.9	2
13757	Carbonyl heterocycle modified mesoporous carbon nitride in photocatalytic peroxydisulfate activation for enhanced ciprofloxacin removal: Performance and mechanism. <i>Journal of Hazardous Materials</i> , 2023, 444, 130412.	6.5	9
13758	Topological Analysis of the Electron Density of Molecules with Bridging Hydrogens To Tackle the Chemical Structure Monolith. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	0
13759	Photo-Induced Reaction of Cp*Ru(η^5 -H) ₄ RuCp* with Arenes Resulting in Irreversible Formation of η^5 -Cyclohexadiene Complexes. <i>Organometallics</i> , 2022, 41, 3750-3761.	1.1	1
13760	Alkyl-Substituted N,S-Embedded Heterocycloarenes with a Planar Aromatic Configuration for Hosting Fullerenes and Organic Field-Effect Transistors. <i>Journal of the American Chemical Society</i> , 2022, 144, 21521-21529.	6.6	15
13761	Dual-Function Presodiation with Sodium Diphenyl Ketone towards Ultra-Stable Hard Carbon Anodes for Sodium-Ion Batteries. <i>Angewandte Chemie</i> , 0, , .	1.6	0
13762	Silver Dependent Enantiodivergent Gold(I) Catalysed Asymmetric Intramolecular Hydroamination of Alkenes: A Theoretical Study. <i>Catalysts</i> , 2022, 12, 1392.	1.6	1
13763	Novel Organotin(IV) Complexes of 2-[4-Hydroxy-3-((2-hydroxyethylimino)methyl)phenylazo]benzoic Acid: Synthesis, Structure, Noncovalent Interactions and In Vitro Antibacterial Activity. <i>Crystals</i> , 2022, 12, 1582.	1.0	10
13764	A Comprehensive Study of N-Butyl-1H-Benzimidazole. <i>Molecules</i> , 2022, 27, 7864.	1.7	4
13765	Synthesis of coplanar quaternary ammonium salts with excellent electrochemical properties based on an anthraquinone skeleton and their application in copper plating. <i>Electrochimica Acta</i> , 2023, 437, 141541.	2.6	2
13766	A crystalline and stable microporous framework based on the dative B \rightarrow N bonds. <i>Chem</i> , 2023, 9, 242-252.	5.8	13
13767	Theoretical Exploration of Peculiar Sandwich-Type Clusters Formed by the Coordination of E ₃ ²⁺ (E = Si, Ge, Sn) Zintl Clusters: Structural Properties, Active Sites, and Hydrogen Storage. <i>Langmuir</i> , 2022, 38, 14485-14496.	1.6	3

#	ARTICLE	IF	CITATIONS
13768	Novel Insight into the Molecular Frustration of IFLPs Based on Boron-Functionalized Pyrimidines for CO ₂ Sequestration. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8633-8644.	1.1	6
13769	Exploration of Non Covalent Interactions, Structural, Vibrational, Chemical Reactivity and NLO Properties of 1, 2-Diphenyl-2-Methoxyethanone Oxime: A Theoretical Approach. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-29.	1.4	0
13770	Cellulose Regeneration in Imidazolium-Based Ionic Liquids and Antisolvent Mixtures: A Density Functional Theory Study. <i>ACS Omega</i> , 2022, 7, 42170-42180.	1.6	3
13771	Mechanistic Insights into the Selective Synthesis of 4H-Pyran Derivatives On-Water Using Naturally Occurring Alginate from <i>Sargassum muticum</i> : Experimental and DFT Study. <i>Gels</i> , 2022, 8, 713.	2.1	0
13772	Separation of Lactic Acid Based on Amide-Based Hydrophobic Deep Eutectic Solvents: Insights from Experiments and Molecular Dynamics Simulations. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 15589-15598.	3.2	9
13773	Development of highly-efficient OD/1D/OD dual Z-scheme CdS/ZnWO ₄ /ZnS heterojunction photocatalysts in pollutant removal and involved mechanism. <i>Applied Surface Science</i> , 2023, 611, 155681.	3.1	46
13774	The Interplay between ESIPT and TADF for the 2,2'-Bipyridine-3,3'-diol: A Theoretical Reconsideration. <i>International Journal of Molecular Sciences</i> , 2022, 23, 13969.	1.8	8
13775	Five Cocrystal Forms of Antitumor Drug Temozolomide with <i>p</i> -Hydroxybenzoic Acid: Structure, Computational Analysis, Characterizations, Stability, and Transformation. <i>Crystal Growth and Design</i> , 2022, 22, 7195-7206.	1.4	2
13776	Computational assessment of herbal medicine-derived compounds as potential inhibitors of SARS-CoV-2 main protease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 9602-9613.	2.0	1
13777	Dual-Function Presodiation with Sodium Diphenyl Ketone towards Ultra-Stable Hard Carbon Anodes for Sodium-Ion Batteries. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	57
13778	Silver-doped nickel thiolates as electrocatalysts for heterogeneous CO ₂ reduction. <i>Science China Materials</i> , 2023, 66, 407-412.	3.5	4
13779	Broad-specificity indirect competitive enzyme-linked immunosorbent assay for aristolochic acids: Computer-aided hapten design and molecular mechanism of antibody recognition. <i>Science of the Total Environment</i> , 2023, 859, 159941.	3.9	5
13780	Structural growth, stability and electronic characteristics of Al-Sc clusters. <i>Computational and Theoretical Chemistry</i> , 2022, 1218, 113942.	1.1	0
13782	Conversion of lignin oil and hemicellulose derivative into high-density jet fuel. <i>Journal of Energy Chemistry</i> , 2023, 77, 452-460.	7.1	24
13783	Quantitatively regulating the ketone structure of triazine-based covalent organic frameworks for efficient visible-light photocatalytic degradation of organic pollutants: Tunable performance and mechanisms. <i>Journal of Hazardous Materials</i> , 2023, 444, 130366.	6.5	12
13784	An experimental and theoretical study on the effects of amine chain length on CO ₂ absorption performance. <i>AIChE Journal</i> , 2023, 69, .	1.8	8
13785	Conformational Flexibility-Controlled Piezochromic Behavior of Organic Fluorophores. <i>Chemistry of Materials</i> , 2022, 34, 10711-10720.	3.2	4
13786	An ultra-sensitive luteolin sensor based on Co-doped nitrogen-containing carbon framework/MoS ₂ @MWCNTs composite for natural sample detection. <i>Electrochimica Acta</i> , 2023, 438, 141534.	2.6	18

#	ARTICLE	IF	CITATIONS
13787	Effects of Ionic Liquids on the Stabilization Process of Gold Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2022, 126, 9617-9631.	1.2	3
13788	Direct Conversion of N ₂ and O ₂ to Nitric Oxide at Room Temperature Initiated by Double Aromaticity in the Y ₂ BO ⁺ Cation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 10697-10704.	2.1	3
13789	Intrinsic Light-Activated Oxidase Mimicking Activity of Conductive Polyaniline Nanofibers: A Class of Metal-Free Nanozyme. <i>ACS Applied Bio Materials</i> , 2022, 5, 5518-5531.	2.3	5
13790	The interaction mechanism between molten SiO ₂ -Al ₂ O ₃ -CaO slag and graphite with different crystal orientations: Experiment and Ab initio molecular dynamics simulation. <i>Ceramics International</i> , 2023, 49, 8295-8301.	2.3	3
13791	New Ferrocene-Based Metalloligand with Two Triazole Carboxamide Pendant Arms and Its Iron(II) Complex: Synthesis, Crystal Structure, 57Fe Mössbauer Spectroscopy, Magnetic Properties and Theoretical Calculations. <i>Inorganics</i> , 2022, 10, 199.	1.2	1
13792	Mechanistic effects of graphitization degrees and surface oxygen heteroatoms on VOCs adsorptive separation: Experimental and theoretical perspective. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108985.	3.3	5
13793	Uncovering the optimal pyrolysis temperature of NH ₂ -MIL-88B-derived FeOX/Fe@porous carbon composites for the ultrasensitive electrochemical detection of baicalin in natural plant samples. <i>Carbon</i> , 2023, 202, 125-136.	5.4	13
13794	Enhanced activation of peroxymonosulfate by a floating FeMo ₃ O _x /C ₃ N ₄ photocatalyst under visible-light assistance for oxytetracycline degradation: Performance, mechanisms and comparison with H ₂ O ₂ activation. <i>Environmental Pollution</i> , 2023, 316, 120668.	3.7	13
13795	Atomic chemical environment of tungsten in coal: Implication for the evolution of the germanium coal deposits. <i>Ore Geology Reviews</i> , 2022, 150, 105196.	1.1	1
13796	Theoretical Insights into the Metal-Nonmetal Interaction Inside M ₂ O@C ₂ v(31922)-C ₈₀ (M = Sc or Gd). <i>ACS Omega</i> , 0, , .	1.6	0
13797	Ab Initio Study of Metal Oxo-Trimer Nanoporous MOF Building Units for the Catalytic Conversion of CO ₂ to Methanol. <i>ACS Applied Nano Materials</i> , 2022, 5, 17750-17757.	2.4	2
13798	Electronic Structure Analysis and Synthesis of Nitroso N-Heterocyclic Imines. <i>ChemistrySelect</i> , 2022, 7, .	0.7	1
13799	Predicting Small Molecule Activation including Catalytic Hydrogenation of Dinitrogen Promoted by a Dual Lewis Acid. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	3
13800	Low-Temperature Production of Glyceric Acid from Biomass-Based Sugar via the Cooperative Roles of MgO and NaBF ₄ . <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 16689-16701.	1.8	2
13801	Photophysical Exploration of Zn(II) Polypyridine Photosensitizers in Two-Photon Photodynamic Therapy: Insights from Theory. <i>Inorganic Chemistry</i> , 2022, 61, 18729-18742.	1.9	4
13802	Structure, Stability, Electronic and Magnetic Properties of FemBin (m + n = 2 × 4) Clusters: A DFT Study. <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 2466-2475.	0.1	2
13803	Pyridine Carboxamides Based on Sulfobetaines: Design, Reactivity, and Biological Activity. <i>Molecules</i> , 2022, 27, 7542.	1.7	3
13804	Antiaromatic Sapphyrin Isomer: Transformation into Contracted Porphyrinoids with Variable Aromaticity. <i>Angewandte Chemie</i> , 0, , .	1.6	0

#	ARTICLE	IF	CITATIONS
13805	Unraveling the Mechanistic Pathway for the Dual Fluorescence in Green Fluorescent Protein (GFP) Chromophore Analogue: A Detailed Theoretical Investigation. <i>Journal of Physical Chemistry B</i> , 2022, 126, 9930-9944.	1.2	2
13806	Contrastive study on organic contaminated soils remediated using dielectric barrier discharge (DBD) plasma. <i>Separation and Purification Technology</i> , 2023, 306, 122576.	3.9	10
13807	Three for the Price of One: Concomitant N^{\ominus} , O^{\ominus} , and F^{\ominus} Halogen Bonds in the Same Crystal Structure. <i>Molecules</i> , 2022, 27, 7550.	1.7	3
13808	Chalcogen bond-assisted syn-locked scaffolds: DFT analysis and biological implications of novel tubulin inhibitors. <i>Biochemical and Biophysical Research Communications</i> , 2023, 638, 134-139.	1.0	0
13809	Quantum Computational, Spectroscopic, Hirshfeld Surface Analysis of 3-Picoline (Monomer and) Polycyclic Aromatic Compounds, 2023, 43, 7828-7852.	1.4	1
13810	Mechanism of highly efficient electrochemical degradation of antibiotic sulfadiazine using a layer-by-layer GNPs/PbO ₂ electrode. <i>Environmental Research</i> , 2023, 217, 114778.	3.7	11
13811	Fluorine Substitution Tunes the Nanofiber Chirality of Supramolecular Hydrogels to Promote Cell Adhesion and Proliferation. <i>Advanced Fiber Materials</i> , 2023, 5, 377-387.	7.9	14
13812	Construction of Carbon Dots with Wavelength-Tunable Electrochemiluminescence and Enhanced Efficiency. <i>Analytical Chemistry</i> , 2022, 94, 16510-16518.	3.2	10
13813	Mechanism Analysis of Ethanol Production from Cellulosic Insulating Paper Based on Reaction Molecular Dynamics. <i>Polymers</i> , 2022, 14, 4918.	2.0	1
13814	Constructing molecular bridge for high-efficiency and stable perovskite solar cells based on P3HT. <i>Nature Communications</i> , 2022, 13, .	5.8	30
13815	On the possibility of using the Ti@Si ₁₆ superatom as a novel drug delivery carrier for different drugs: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, , 108378.	1.3	1
13816	Amine-Reactive BODIPY Dye: Spectral Properties and Application for Protein Labeling. <i>Molecules</i> , 2022, 27, 7911.	1.7	2
13817	PyMM: An Open-Source Python Program for QM/MM Simulations Based on the Perturbed Matrix Method. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 33-41.	2.3	5
13818	Featuring a new computational protocol for the estimation of intensity and overall quantum yield in lanthanide chelates with applications to Eu(III) mercapto-triazole Schiff base ligands. <i>Optical Materials: X</i> , 2022, 16, 100216.	0.3	4
13819	Prominent Spatial Structure and Synergistic Linkage Effects in Bimetallic Titanium Olefin Polymerization Catalysts. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 17017-17026.	1.8	1
13820	Efficient degradation of organic pollutants using peroxydisulfate activated by magnetic carbon nanotube. <i>Water Science and Technology</i> , 2022, 86, 2611-2626.	1.2	4
13821	Screening method and mechanism of ionic liquid as extractant in fuel extraction desulfurization process. <i>Journal of Chemical Technology and Biotechnology</i> , 2023, 98, 669-678.	1.6	1
13822	Chalcogen Bond as a Factor Stabilizing Ligand Conformation in the Binding Pocket of Carbonic Anhydrase IX Receptor Mimic. <i>International Journal of Molecular Sciences</i> , 2022, 23, 13701.	1.8	7

#	ARTICLE	IF	CITATIONS
13823	Fundamental Variable and Density Representation in Multistate DFT for Excited States. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 7403-7411.	2.3	7
13824	Alkali-Metal-Free Coinage Metalides: Specific Pairing and Location of Doping Atoms Bring Forth High Stability and Considerable Nonlinear Optical Response. <i>Organometallics</i> , 0, , .	1.1	1
13825	Study on Gas Chromatography Retention Time Variation of Acetic Acid Combined with Quantum Chemical Calculation. <i>Chromatographia</i> , 2023, 86, 3-11.	0.7	1
13826	An account of noncovalent interactions in homoleptic palladium(II) and platinum(II) complexes within the DFT framework: A correlation between geometries, energy components of symmetry-adapted perturbation theory and NCI descriptors. <i>Heliyon</i> , 2022, 8, e11408.	1.4	5
13827	Cost-effective Vat Orange 3-derived Organic Cathodes for Electrochemical Energy Storage. <i>Batteries and Supercaps</i> , 0, , .	2.4	2
13828	Exploration on dual emission mechanism of CPzP and CPzPO with thermally activated delayed fluorescence. <i>Molecular Physics</i> , 0, , .	0.8	0
13829	Interactions between Extracellular DNA and Perfluoroalkyl Acids (PFAAs) Decrease the Bioavailability of PFAAs in Pakchoi (<i>Brassica chinensis</i> L.). <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 14622-14632.	2.4	3
13830	Photocatalytic Selective Oxidation of Toluene into Benzaldehyde on Mixed-Valence Vanadium Oxide V ₆ O ₁₃ Catalyst with Density Functional Theory. <i>Catalysis Letters</i> , 0, , .	1.4	0
13831	Assembling properties of 3,6-dinitropyrazolo[4,3-c]pyrazole-based energetic compounds. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	2
13832	Structural and spectroscopic analysis, solvent effect on the molecular properties and molecular docking of trans-2-(4-(dimethylamino) styryl)-benzothiazole. <i>Chemical Physics Letters</i> , 2023, 810, 140192.	1.2	3
13833	Effects of Fluorinated Aromatic Spacer in AgBi Double Perovskite for X-ray Detector. <i>Journal of Physical Chemistry C</i> , 2022, 126, 19417-19423.	1.5	6
13834	Analysis of the structure and chemical bonding of C ₅ H ₅ ScB ₄ O: a density functional study. <i>Chemical Physics</i> , 2022, , 111768.	0.9	0
13835	Revealing the photoelectric performance and multistep electron transfer mechanism in D-A- π -A dyes coupled with a chlorophyll derivative for co-sensitized solar cells. <i>Journal of Molecular Liquids</i> , 2022, 368, 120797.	2.3	5
13836	Oligomer formation from the gas-phase reactions of Criegee intermediates with hydroperoxide esters: mechanism and kinetics. <i>Atmospheric Chemistry and Physics</i> , 2022, 22, 14529-14546.	1.9	3
13837	Reduced energetic disorder enables over 14% efficiency in organic solar cells based on completely non-fused-ring donors and acceptors. <i>Science China Chemistry</i> , 2022, 65, 2604-2612.	4.2	14
13838	Effects of Heavy Iodine Atoms and Expanded Conjugation on Charge Transfer Dynamics in Carboxylic Acid BODIPY Derivatives as Triplet Photosensitizers. <i>ChemPhysChem</i> , 2023, 24, .	1.0	3
13839	Radical scavenging capacity, UV activity, and molecular docking studies of 2 ^E , 5 ^E , 3, 4-Tetrahydrochalcone: An insight into the photoprotection. <i>Chemical Physics Impact</i> , 2022, 5, 100126.	1.7	1
13840	Intramolecular Assembly of Nitrobiazoles and an Ether Bridge: Toward Energetic Materials with Enhanced Energy and Safety. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 52951-52959.	4.0	7

#	ARTICLE	IF	CITATIONS
13841	Experimental Detection and Simulation of Terahertz Spectra of Aqueous L-Arginine. <i>Biosensors</i> , 2022, 12, 1029.	2.3	1
13842	Intramolecular H-Bonds in an Organocatalyst Enabled an Asymmetric Michael/Alkylation Cascade Reaction to Construct Spirooxindoles Incorporating a Densely Substituted Cyclopropane Motif. <i>Organic Letters</i> , 2022, 24, 8553-8558.	2.4	3
13843	Unprecedented Prediction of a B ₁₆₀ Cluster Stuffed by Dual-Icosahedron B ₁₂ . <i>ACS Omega</i> , 0, , .	1.6	2
13844	Dehydroepiandrosterone Cocrystals with Improved Solubility and Bioavailability. <i>Pharmaceutics</i> , 2022, 14, 2478.	2.0	3
13845	The critical role of dimethylamine in the rapid formation of iodic acid particles in marine areas. <i>Npj Climate and Atmospheric Science</i> , 2022, 5, .	2.6	12
13846	Mechanistic insights into reductive deamination with hydrosilanes catalyzed by B(C ₆ F ₅) ₃ : A DFT study. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	0
13847	Insights into the Active Catalyst Formation from Dinuclear Palladium Acetate in Pd-Catalyzed Coupling Reactions: A DFT Study. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8562-8576.	1.1	3
13848	A novel bright additive for copper electroplating: electrochemical and theoretical study. <i>Ionics</i> , 2023, 29, 363-375.	1.2	7
13849	Thermal degradation and flame retardancy prediction of Fe, Al, and Cu-based metal-organic framework and polyethylene terephthalate nanocomposites using DFT calculation. <i>Polymer</i> , 2022, 263, 125496.	1.8	4
13850	Mechanistic insights into the effects of alkali metal ion on ZSM-11 zeolite synthesis and its catalytic alkylation performance. <i>Microporous and Mesoporous Materials</i> , 2023, 347, 112352.	2.2	3
13851	Computationally rational design of metal- π -involving halogen bonds with π - π covalency: Structures and bonding analysis. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	0
13852	Investigating the X-aminopyridine (X = 2 and 3) molecules sensing by Al ₁₂ N ₁₂ and B ₁₂ N ₁₂ fullerene-like nanocages: DFT, QTAIM, RDC and TD-DFT insights. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 9721-9731.	2.0	1
13853	Antiaromatic Sapphyrin Isomer: Transformation into Contracted Porphyrinoids with Variable Aromaticity. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	4
13854	A Density Functional Theory Study on Rechargeable Mg-ion Batteries: C ₂₀ Fullerene as a Promising Anode Material. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0
13855	Synthesis, Molecular and Supramolecular Structures of Symmetric Dinuclear Cd(II) Azido Complex with bis-Pyrazolyl s-Triazine Pincer Ligand. <i>Symmetry</i> , 2022, 14, 2409.	1.1	3
13856	N-protected pyrroles as synthons for variants of core-modified N-confused calixphyrins: Spectroscopic and theoretical characterization. <i>Journal of Porphyrins and Phthalocyanines</i> , 0, , A-I.	0.4	0
13857	CaBO ₂ F: A novel deep-UV structural template with high nonlinear optical performance induced by electron delocalization. <i>Science China Materials</i> , 0, , .	3.5	10
13858	Tetranuclear Copper Complexes with Bulky Aminoalcohol Ligands as Catalysts for Oxidative Phenoxazinone Synthase-like Coupling of Aminophenol: A Combined Experimental and Theoretical Study. <i>Catalysts</i> , 2022, 12, 1408.	1.6	3

#	ARTICLE	IF	CITATIONS
13859	DFT Studies on the Early-Transition-Metal-Catalyzed Polymerization of Polar Monomers with a Methylene Spacer between Vinyl and Functional Groups. <i>Organometallics</i> , 2022, 41, 3514-3521.	1.1	2
13860	Molecular stacking pattern effects in heterojunction of D_{18} : Y_6 organic solar cell. <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	1
13861	Poly(ether imide) Porous Membrane Developed by a Scalable Method for High-Performance Lithium-Sulfur Batteries: Combined Theoretical and Experimental Study. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 52794-52805.	4.0	11
13862	Grafting of Tetraphenylethylene on Silica Surface, Characterizations, and Their Chromatographic Performance as Reversed-Phase Stationary Phases. <i>Langmuir</i> , 2022, 38, 14400-14408.	1.6	6
13863	Microscopic Study on the Performance Optimization of Porous Ionic Liquids for CO_2 Capture by Selection of Crown Ether Solvents. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 15263-15272.	3.2	2
13864	Stereo-Recognition of Hydrogen Bond and Its Implications for Lignin Biomimetic Synthesis. <i>Biomacromolecules</i> , 0, , .	2.6	1
13865	Rational design of dithieno[2,3-D:2',3'-D ¹ ,3 ¹ -D ¹]-benzo[1,2-B:4,5-B ¹] dithiophene based small molecule donor for plausible performance organic solar cell. <i>Optical and Quantum Electronics</i> , 2023, 55, .	1.5	8
13866	A Theoretical Perspective to Decipher the Origin of High Hydrogen Storage Capacity in Mn(II) Metal-Organic Framework. <i>ChemPhysChem</i> , 0, , .	1.0	0
13867	Synthesis of new bis(thiosemicarbazone) derivatives and DFT analysis of antioxidant characteristics in relation to HAT and SET reactions. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100789.	1.3	1
13868	Novel Feleucin-K3-Derived Peptides Modified with Sulfonyl-AA Building Blocks Targeting <i>Pseudomonas aeruginosa</i> and Methicillin-Resistant <i>Staphylococcus aureus</i> Infections. <i>Journal of Medicinal Chemistry</i> , 2023, 66, 1254-1272.	2.9	4
13869	Evidence of charge donation through synergistic effect of bioconjugated silver nanoparticles with flavanols accomplishing augmented antimicrobial and antioxidant activities. <i>Journal of Molecular Liquids</i> , 2022, , 120754.	2.3	1
13870	Molecular modeling and DFT studies of diazenylphenyl derivatives as a potential HBV and HCV antiviral agents. <i>Chemical Physics Impact</i> , 2022, 5, 100122.	1.7	29
13871	Adsorption behavior and sensing properties of toxic gas molecules onto Pt _n Be (n = 5, 7, 10) clusters: A DFT benchmark study. <i>Materials Today Communications</i> , 2022, 33, 104851.	0.9	1
13872	Study of the dynamics of the interaction of glycine and GABA with water and ethanol using theoretical tools. <i>Journal of Molecular Liquids</i> , 2022, 368, 120721.	2.3	5
13873	Molecular mechanism of ion channel protein TMEM16A regulated by natural product of narirutin for lung cancer adjuvant treatment. <i>International Journal of Biological Macromolecules</i> , 2022, 223, 1145-1157.	3.6	5
13874	Alkali metal (Na and Li) doped C18 nanocluster with boosted electronic and nonlinear optical properties. <i>Optik</i> , 2022, 271, 170185.	1.4	3
13875	Point-defect engineering on phosphorene quantum dots for DNA bases adsorption and sensor performance. <i>Materials Today Communications</i> , 2022, 33, 104868.	0.9	0
13876	The first marine dual-drug cocrystal of cytarabine with 5-fluorouracil having synergistic antitumor effects shows superior biopharmaceutical peculiarities by oral administration. <i>International Journal of Pharmaceutics</i> , 2022, 629, 122386.	2.6	2

#	ARTICLE	IF	CITATIONS
13877	Mechanistic insight into separation of benzene and cyclohexane by extractive distillation using deep eutectic solvent as entrainer. <i>Journal of Molecular Liquids</i> , 2022, 368, 120780.	2.3	7
13878	A General Twisted Intramolecular Charge Transfer Triggering Strategy by Protonation for Zero-Background Fluorescent Turn-On Sensing. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 10871-10881.	2.1	3
13879	Investigation of the Structure of Atomically Dispersed Ni ⁶¹ Sites in Ni and N-Doped Carbon Electrocatalysts by ⁶¹ Ni Mössbauer Spectroscopy and Simulations. <i>Journal of the American Chemical Society</i> , 2022, 144, 21741-21750.	6.6	2
13880	Generalized Energy-Based Fragmentation Approach for the Electronic Emission Spectra of Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 7630-7638.	2.3	4
13881	Quest of new molecular frameworks for photoinduced carbon monoxide-releasing molecules: a computational prospective. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	2
13882	Theoretical study of cyano-promoted intramolecular aza-Diels-Alder reaction. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	0
13883	A new green alternative solvent for extracting echinacoside and acteoside from <i>Cistanche deserticola</i> based on ternary natural deep eutectic solvent. <i>Journal of Industrial and Engineering Chemistry</i> , 2023, 118, 499-510.	2.9	6
13884	Photocatalytic direct borylation of carboxylic acids. <i>Nature Communications</i> , 2022, 13, .	5.8	12
13885	Theoretical Study of Complexes of Tetravalent Actinides with DOTA. <i>Symmetry</i> , 2022, 14, 2451.	1.1	0
13886	Different reaction mechanisms of SO ₄ ²⁻ and OH with organic compound interpreted at molecular orbital level in Co(II)/peroxymonosulfate catalytic activation system. <i>Water Research</i> , 2023, 229, 119392.	5.3	77
13887	Density functional theory study of the influence of activating and deactivating groups on Naphthalene. <i>Results in Chemistry</i> , 2022, 4, 100669.	0.9	11
13888	Eutectic solvents formed by (+)-DTTA and L-menthol as novel chiral recognition and separation media for enantioselective extraction of valsartan enantiomers. <i>Journal of Molecular Liquids</i> , 2022, 368, 120818.	2.3	2
13889	Synthesis, Characterization, DFT Study and Antifungal Activities of Some Novel 2-(Phenyldiazenyl)phenol Based Azo Dyes. <i>Materials</i> , 2022, 15, 8162.	1.3	2
13890	Label-free, rapid and ratiometric detection of tetracyclines via guest stacking-induced emission triggered by MXene-derived nanosensors. <i>Sensors and Actuators B: Chemical</i> , 2023, 377, 133026.	4.0	5
13891	Ultrafast excited state dynamics of two non-emissive flavonoids that undergo excited state intramolecular proton transfer in solution. <i>Chemical Physics Letters</i> , 2023, 811, 140189.	1.2	1
13893	Theoretical investigation of the Zn ²⁺ detection mechanism based on the quinoline derivative of the Schiff-base receptor. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 287, 122123.	2.0	5
13894	Rational design strategies for nonconventional luminogens with efficient and tunable emission in dilute solution. <i>Chemical Engineering Journal</i> , 2023, 454, 140469.	6.6	6
13895	Insertion Reaction of Me ₃ SiN ₃ with Bis(germylene). <i>Inorganic Chemistry</i> , 2022, 61, 19067-19074.	1.9	3

#	ARTICLE	IF	CITATIONS
13896	Theoretical Study on Spectrum and Luminescence Mechanism of Indocyanine Green Dye Based on Density Functional Theory (DFT). <i>Journal of Chemistry</i> , 2022, 2022, 1-8.	0.9	1
13897	Alkali and Transition Metal Doped 15-crown-5 with Enhanced Non-linear Optical Response: A DFT Study. <i>Journal of Computational Biophysics and Chemistry</i> , 0, , .	1.0	1
13898	Molecular investigation of interplay mechanism between polydopamine and graphene oxide: The effect of oxidation degree on the adsorption behavior of polydopamine. <i>Applied Surface Science</i> , 2023, 611, 155759.	3.1	6
13899	Computational study on the prototropic tautomerism between simple oxo-, thio-, carbon-, aza-hydrazones, and their respective azines. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	1
13900	Versatile hydrogen-bonded organic framework (HOF) platform for simultaneous detection and efficient removal of heavy metal ions. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108983.	3.3	5
13901	Structure and conformations of 3-methylcatechol: A rotational spectroscopic and theoretical study. <i>Journal of Molecular Spectroscopy</i> , 2022, 390, 111715.	0.4	3
13902	Di- π - π Stacking of Pyrenidecaphyrin(1.1.0.0.0.1.1.0.0.0) and Its Bis- π -Organopalladium Complexes: Synthesis and Chiroptical Properties. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	8
13903	Exploring the fluorination effect mechanism on charge transport in organic solar cells. <i>Solar Energy</i> , 2022, 248, 160-170.	2.9	6
13904	Sebaceous gland-inspired self-lubricated de-icing coating by continuously secreting lubricants. <i>Progress in Organic Coatings</i> , 2023, 174, 107311.	1.9	2
13905	Z-scheme transfer pathway assisted photoelectrocatalyst Zn ₂ SnO ₄ /rGO/Ag/AgBr for organic pollutants treatment. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 657, 130552.	2.3	6
13906	Rational regulating pore structures of covalent organic frameworks for sulfur hexafluoride capture and separation. <i>Separation and Purification Technology</i> , 2023, 306, 122595.	3.9	2
13907	Experimental and theoretical study on efficient CO ₂ absorption coordinated by molecules and ions of DBN and 1,2,4-triazole formed deep eutectic solvents. <i>Fuel</i> , 2023, 334, 126709.	3.4	13
13908	Solvent-driven self-assembly of two novel di- and tetra-nuclear Cu(II) bis(salamo)-based complexes. <i>Journal of Molecular Structure</i> , 2023, 1274, 134554.	1.8	40
13909	Sulfication-induced non-radiative electron-hole recombination dynamics in graphene quantum dots for tuning photocatalytic performance. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 287, 122117.	2.0	3
13910	Nonflammable dual-salt localized high-concentration electrolyte for graphite/LiNi _{0.8} Co _{0.1} Mn _{0.1} O ₂ lithium-ion batteries: Li ⁺ solvation structure and interphase. <i>Journal of Power Sources</i> , 2023, 555, 232392.	4.0	5
13911	Synergistic enhancement of efficiency and stability of perovskite solar cells via dual interface modification. <i>Applied Surface Science</i> , 2023, 611, 155745.	3.1	3
13912	Quantum DFT methods to explore the interaction of 1-Adamantylamine with pristine, and P, As, Al, and Ga doped BN nanotubes. <i>Scientific Reports</i> , 2022, 12, .	1.6	5
13913	Understanding the transformations of nanoplastic onto phospholipid bilayers: Mechanism, microscopic interaction and cytotoxicity assessment. <i>Science of the Total Environment</i> , 2023, 859, 160388.	3.9	7

#	ARTICLE	IF	CITATIONS
13914	Diâ€²,7â€²pyrenidecaphyrin(1.1.0.0.0.1.1.0.0.0) and Its Bisâ€²Organopalladium Complexes: Synthesis and Chiroptical Properties. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	2
13915	What is the role of phytochemical compounds as capping agents for the inhibition of aggregation in the green synthesis of metal oxide nanoparticles? A DFT molecular level response. <i>Inorganic Chemistry Communication</i> , 2023, 147, 110243.	1.8	8
13916	Inherently chiral belt-shaped conjugated macrocycles with strong fluorescence and circularly polarized luminescence. <i>Chemical Communications</i> , 2022, 59, 227-230.	2.2	5
13917	High proton conductivity modulated by active protons in 1D ultra-stable metalâ€²organic coordination polymers: a new insight into the coordination interaction/ability of metal ions. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 1238-1254.	3.0	3
13918	Intrinsic influence of selenium substitution in thiophene and benzo-2,1,3-thiadiazole on the electronic structure, excited states and photovoltaic performances evaluated using theoretical calculations. <i>New Journal of Chemistry</i> , 2023, 47, 1797-1807.	1.4	5
13919	Locating the hydrogen atoms in endohedral clusterfullerenes by density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 2451-2461.	1.3	2
13920	Why does thionating a carbonyl molecule make it a better electron acceptor?. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1342-1348.	1.3	3
13921	Solvent-mediated precipitating synthesis and optical properties of polyhydrido Cu₁₃nanoclusters with four vertex-sharing tetrahedrons. <i>Chemical Science</i> , 2023, 14, 994-1002.	3.7	11
13922	(Pre)association as a crucial step for computational prediction and analysis of the catalytic activity of Î¶-hole donating organocatalysts. <i>Organic Chemistry Frontiers</i> , 2022, 10, 169-180.	2.3	8
13923	Bis-TTF-Ge derivatives: promising linear and nonlinear optical properties, a theoretical investigation. <i>New Journal of Chemistry</i> , 2023, 47, 1234-1246.	1.4	8
13924	The hydrogen storage capacities of 4d transition metals in various boron systems. <i>Journal of Energy Storage</i> , 2023, 57, 106216.	3.9	3
13925	Sodium complexes as precise tools for cutting polymer chains. Exploration of PLA degradation by unique cooperation of sodium centers. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 1076-1090.	3.0	2
13926	A series of <i>N</i>-trinitromethyl-substituted polynitro-pyrazoles: high-energy-density materials with positive oxygen balances. <i>RSC Advances</i> , 2022, 12, 33304-33312.	1.7	2
13927	Palladium-catalyzed generation of CO from formic acid for alkoxy-carbonylation of internal alkenes involves a PTSA-assisted NHâ€²Pd mechanism: a DFT mechanistic study. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 2294-2303.	1.3	2
13928	Partner Effect in Accelerating Pincer-Co Catalyzed Nitrile Hydroboration Reactions. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
13929	The nature of stability and adsorption interactions of binary Au-Li clusters with bridge adsorption structures. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
13930	Impacts of external fields on aromaticity and acidity of benzoic acid: a density functional theory, conceptual density functional theory and information-theoretic approach study. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 2595-2605.	1.3	6
13931	Solvent dependent triplet state delocalization in a co-facial porphyrin heterodimer. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 30051-30061.	1.3	2

#	ARTICLE	IF	CITATIONS
13932	Competition between ultralong organic phosphorescence and thermally activated delayed fluorescence in dichloro derivatives of 9-benzoylcarbazole. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 29437-29450.	1.3	2
13933	Synthesis, Antifungal Activity and Molecular Docking Study of 1,3,4-Thiadiazole-Urea Compounds Containing <i>gem</i> -Dimethylcyclopropane Ring Structure. <i>Chinese Journal of Organic Chemistry</i> , 2022, 42, 3784.	0.6	1
13934	Merging the AuCu ₃ - and BaAl ₄ -based structure motifs: flux-assisted synthesis, crystal, and electronic structure of Ca ₂ Pt ₇ XP ₄ phosphide platinides (X = Al, Ti, and Zn). <i>Dalton Transactions</i> , 2022, 51, 18583-18592.	1.6	3
13935	Uncovering the role of non-covalent interactions in solid-state photoswitches by non-spherical structure refinements with NoSpherA2. <i>Faraday Discussions</i> , 0, 244, 370-390.	1.6	3
13936	Multichannel charge transfer enhanced radiative decay and RISC in TADF materials containing multiple donors and acceptors. <i>Journal of Materials Chemistry C</i> , 2022, 10, 18189-18199.	2.7	2
13937	pH and light dual stimuli-responses of mixed system of 2-hydroxyl-propanediyl-bis(dimethyldodecyl) Tj ETQq _{1,1} 0.7843 ₁₄ rgBT	1.7	0
13938	Theoretical investigation of C1-C4 hydrocarbons adsorption and separation in a porous metal-organic framework. <i>RSC Advances</i> , 2022, 12, 34053-34065.	1.7	0
13939	Insights into chalcone analogues with potential as antioxidant additives in diesel-biodiesel blends. <i>RSC Advances</i> , 2022, 12, 34746-34759.	1.7	3
13940	Fulvic acid-polyphosphate composite embedded in ZnO nanorods (FA@PP@ZnO) for efficient P/Zn nutrition for peas (<i>Pisum sativum</i> L.). <i>RSC Advances</i> , 2022, 12, 33008-33020.	1.7	1
13941	Solvent effect on the production of spherical lignin nanoparticles. <i>Green Chemistry</i> , 2023, 25, 993-1003.	4.6	10
13942	A theoretical study of the ligand-controlled palladium-catalysed regioselective synthesis of dibenzosilole derivatives. <i>Dalton Transactions</i> , 2023, 52, 737-746.	1.6	3
13943	Amplification of dissymmetry factors by dihedral angle engineering in donor-acceptor type circularly polarized luminescence materials. <i>Journal of Materials Chemistry C</i> , 2023, 11, 893-897.	2.7	5
13944	A TD-DFT study of a class of fluorescent probes for detection of typical oxidants. <i>Organic and Biomolecular Chemistry</i> , 2023, 21, 315-322.	1.5	2
13945	First ternary tungsten tellurate (WTe ₂ O ₇) with unique crystal structure type. <i>Dalton Transactions</i> , 2023, 52, 2243-2254.	1.6	2
13946	Construction of surface oxygen vacancies by bimetallic doping combined with ellagic acid modification to enhance the photocatalytic degradation of ethinyl estradiol by TiO ₂ . <i>Chemical Engineering Journal</i> , 2023, 455, 140929.	6.6	10
13947	Synthetic perylenequinone as anchoring center of sulfur and catalyst for polysulfides conversion. <i>Chemical Engineering Journal</i> , 2023, 455, 140847.	6.6	5
13948	Building a Rigid-Soft Coupling Interphase by Reduction-Oxidation Collaborative Approach with Lithium Difluorobis(oxalato) Phosphate Additives. <i>Journal of Materials Chemistry A</i> , 0, , .	5.2	1
13949	Wide-range color-tunable polycyclo-heteraborin multi-resonance emitters containing B-N covalent bonds. <i>Chemical Science</i> , 2023, 14, 979-986.	3.7	8

#	ARTICLE	IF	CITATIONS
13950	Overlooked potential of <i>N,N</i> -bidentate directing-groups in Ni-catalyzed C-H functionalization of benzamides. <i>Chemical Communications</i> , 2023, 59, 482-485.	2.2	1
13951	DFT and molecular docking study of the effect of a green solvent (water and DMSO) on the structure, MEP, and FMOs of the 1-ethylpiperazine-1,4-dium bis(hydrogenoxalate) compound. <i>Journal of Molecular Liquids</i> , 2023, 369, 120851.	2.3	26
13952	Predicting adsorption behavior of Triacanthine anticancer drug with pure B12N12 nano-cage: A theoretical study. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100812.	1.3	4
13953	Boron-based tubular BeB ₁₂ and quasi-planar BeB ₁₂ clusters: structural transformation and chemical bonding. <i>New Journal of Chemistry</i> , 2023, 47, 2736-2746.	1.4	3
13954	Controllable construction of red thermally activated delayed fluorescence molecules based on a spiro-acridine donor. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1032-1044.	1.3	5
13955	Structural evolution and electronic properties of neutral and anionic TiAsi (A =) Tj ETQq1 1 0.784314 rgBT /Overl <i>Chemical Physics</i> , 2022, 25, 529-539.	1.3	0
13956	Screening, packing systematics, Hansen solubility parameters and desolvation of resmetirom (MGL-3196) solvates. <i>Journal of Molecular Liquids</i> , 2023, 369, 120857.	2.3	7
13957	Facile synthesis of thermally stable tetrazolo[1,5- <i>b</i>][1,2,4]triazine substituted energetic materials: synthesis and characterization. <i>Dalton Transactions</i> , 2023, 52, 747-753.	1.6	8
13958	Influence of solvation on the spectral, molecular structure, and antileukemic activity of 1-benzyl-3-hydroxy-2-methylpyridin-4(1H)-one. <i>Journal of Molecular Liquids</i> , 2023, 370, 121045.	2.3	10
13959	Peroxymonosulfate activation by iron-carbon composite derived from coal gasification slag for sulfamethoxazole removal: Performance evaluation and mechanism insight. <i>Chemical Engineering Journal</i> , 2023, 456, 140996.	6.6	13
13960	Adsorption and electronic properties of pristine and Al-doped C60 fullerenes using N2O molecule: A theoretical study. <i>Journal of Molecular Liquids</i> , 2023, 369, 120855.	2.3	4
13961	Theoretical investigation on intermolecular interactions, co-crystal structure, thermal decomposition mechanism, and shock properties of 3-nitro-1,2,4-triazol-5-one (NTO) and ammonium perchlorate. <i>CrystEngComm</i> , 2023, 25, 671-682.	1.3	4
13962	Theoretical exploration to the significance of $n(S)/n(O) \hat{=} \hat{=} f^*$ (C-COOMe) stereoelectronic interactions. <i>New Journal of Chemistry</i> , 2022, 47, 384-391.	1.4	0
13963	Interaction of imidazolium based ionic liquid electrolytes with carbon nitride electrodes in supercapacitors; a step forward for understanding electrode-electrolyte interaction. <i>Journal of Molecular Liquids</i> , 2023, 369, 120955.	2.3	20
13964	Thermophysical modelling of transport and optical properties of 1-propanol+1,3-diaminopropane or 1,2-diaminopropane or 1-amino-2-propanol binary liquid mixture at T=298.15-318.15 K: Molecular interaction analysis by density functional theory (DFT) and graph theoretical approach (GTA). <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2023, 142, 104641.	2.7	9
13965	Using molecular dynamics simulations to study the non-thermal effects of microwave radiation on the mechanism of char gasification. <i>Renewable Energy</i> , 2023, 202, 784-796.	4.3	4
13966	How to active ethanolamine for selective hydrogenation by imidazolium-based cation and conjugated π bond. <i>Molecular Catalysis</i> , 2023, 535, 112809.	1.0	0
13967	A density functional theory (DFT) on the leaching process of weathered crust elution-deposited rare earth ore with lixiviants. <i>Minerals Engineering</i> , 2023, 191, 107980.	1.8	0

#	ARTICLE	IF	CITATIONS
13968	Quinoxaline-fused octaphyrin(2.0.0.0.2.0.0.0). A rudimentary chemosensor. <i>Chemical Communications</i> , 2023, 59, 708-711.	2.2	2
13969	Balance the rapid release of insecticide microcapsules using double-layer shielding effect when the foliar application. <i>Chemical Engineering Journal</i> , 2023, 455, 140899.	6.6	8
13970	A dual-response mitochondria-targeted NIR fluorescent probe with large Stokes shift for monitoring viscosity and HOCl in living cells and zebrafish. <i>Analyst</i> , The, 2022, 148, 38-46.	1.7	7
13971	Atoms in molecules theory, electrostatic potential surface and frontier molecular orbital analyses on water multimers and pyridine " Water hydrogen bonded complexes. <i>Computational and Theoretical Chemistry</i> , 2023, 1219, 113960.	1.1	1
13972	Theoretical investigation of intermolecular interactions between CNT, SiCNT and SiCGeNT nanomaterials with vinyl chloride molecule: A DFT, NBO, NCI, and QTAIM study. <i>Diamond and Related Materials</i> , 2023, 131, 109602.	1.8	7
13973	Constructing optimally hierarchical HY zeolite for the synthesis of high-energy-density tricyclic hydrocarbon fuel. <i>Molecular Catalysis</i> , 2023, 535, 112871.	1.0	2
13974	Mechanistic insight into surface oxygen species of the polyoxometalate-supported Pd single-atom catalysts for highly efficient CO oxidation. <i>Molecular Catalysis</i> , 2023, 534, 112802.	1.0	0
13975	Exploring the underlying oxygen reduction reaction electrocatalytic activities of pyridinic-N and pyrrolic-N doped graphene quantum dots. <i>Molecular Catalysis</i> , 2023, 535, 112880.	1.0	3
13976	Visible-light-induced selective defluoroalkylations of polyfluoroarenes with alcohols. <i>Chemical Science</i> , 2023, 14, 916-922.	3.7	11
13977	Schiff bases from chlorine substituted anilines and salicylaldehyde: Synthesis, characterization, fluorescence, thermal features, biological studies and electronic structure investigations. <i>Journal of Molecular Liquids</i> , 2023, 370, 121055.	2.3	35
13978	An exploration of excited-state properties of three hydroxyanthraquinone compounds from the marine crinoid <i>Pterometra venusta</i> . <i>Chemical Physics Letters</i> , 2023, 811, 140230.	1.2	0
13979	Intramolecular charge transfer effect for highly efficient deep red and near infrared thermally activated delayed fluorescence. <i>Materials Horizons</i> , 2023, 10, 945-951.	6.4	7
13980	Direct solidification of switchable-hydrophilicity salicylic acid: A design for the on-site dispersive liquid-liquid microextraction of benzoylurea insecticides in water and honey samples. <i>Journal of Chromatography A</i> , 2023, 1688, 463710.	1.8	7
13981	New lead-iodide formates with a strong second-harmonic generation response and suitable birefringence obtained by the substitution strategy. <i>Chemical Science</i> , 2022, 14, 136-142.	3.7	3
13982	A semi-conductive organic cathode material enabled by extended conjugation for rechargeable aqueous zinc batteries. <i>Energy and Environmental Science</i> , 2023, 16, 89-96.	15.6	42
13983	An off-on-off fluorescence probe based on a pyrazole derivative for Al ³⁺ and Fe ³⁺ detection. <i>New Journal of Chemistry</i> , 2023, 47, 751-757.	1.4	6
13984	Oligothiophene electron donor and electron acceptor for all small molecule organic solar cells with efficiency over 9%. <i>Chemical Engineering Journal</i> , 2023, 456, 141006.	6.6	6
13985	A theoretical study on the methanol to propene mechanism catalyzed by a phosphorus-modified acidic FAU zeolite. <i>New Journal of Chemistry</i> , 2023, 47, 1740-1759.	1.4	2

#	ARTICLE	IF	CITATIONS
13986	Influence of oxidation on the magnetism of small Co oxide clusters probed by Sternâ€“Gerlach deflection. <i>Physical Chemistry Chemical Physics</i> , 2022, 25, 171-182.	1.3	0
13987	Sulfamethoxazole: Molecular docking and crystal structure prediction. <i>Results in Chemistry</i> , 2023, 5, 100716.	0.9	3
13988	A novel photoelectrochemical sensor based on flower-like SnS ₂ , sea urchin-like AgBiS ₂ and graphene oxide nanocomposite film for efficient and sensitive detection of acetaminophen in lake water samples. <i>Analytica Chimica Acta</i> , 2023, 1239, 340681.	2.6	14
13989	Enclathration of Mn(II)(H ₂ O) ₆ guests and unusual Cu ⁺ O bonding contacts in supramolecular assemblies of Mn(II) Co-crystal hydrate and Cu(II) Pyridinedicarboxylate: Antiproliferative evaluation and theoretical studies. <i>Polyhedron</i> , 2023, 230, 116243.	1.0	2
13990	An <i>in situ</i> formed copolymer electrolyte with high ionic conductivity and high lithium-ion transference number for dendrite-free solid-state lithium metal batteries. <i>Journal of Materials Chemistry A</i> , 2023, 11, 1966-1977.	5.2	17
13991	A pincer-shaped binary molecular wheel B ₇ Mg ₄ ⁺ cluster: hybrid in-plane heptacoordination, double π aromaticity, and electronic transmutation. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
13992	New charge-transfer complexes of 1,2,5-chalcogenadiazoles with tetrathiafulvalenes. <i>CrystEngComm</i> , 2023, 25, 391-402.	1.3	3
13993	The reactivity of antimony and bismuth <i>N</i> , <i>C</i> , <i>N</i> -pincer compounds toward K[BEt ₃ H] $\hat{=}$ the formation of heterocyclic compounds <i>vs</i> elementâ€“element bonds <i>vs</i> stable terminal Sbâ€“H bonds. <i>Dalton Transactions</i> , 2022, 52, 218-227.	1.6	1
13994	Extracellular polymeric substances enhance dissolution and microbial methylation of mercury sulfide minerals. <i>Environmental Sciences: Processes and Impacts</i> , 2023, 25, 44-55.	1.7	5
13995	Probing the mechanism of adaptive aromaticity in metallapyridiniums. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 934-941.	3.0	2
13996	Physical image of amino acid interaction on graphene surface: Scientific fundamental for biological identification and detection from first-principles. <i>Diamond and Related Materials</i> , 2023, 131, 109571.	1.8	2
13997	π - π stacking in the polymorphism of 2-(naphthalenylamino)-nicotinic acids and a comparison with their analogues. <i>CrystEngComm</i> , 2023, 25, 432-443.	1.3	1
13998	Design of Deep-Ultraviolet Nonlinear Optical Materials Based on Fundamental Building Blocks with Excellent Microscopic Properties. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
13999	Theoretical study of the thermally activated delayed fluorescence (TADF) combined with aggregation-induced emission (AIE) molecular solid-state effect on the luminescence mechanism. <i>Chemical Physics Letters</i> , 2023, 811, 140257.	1.2	2
14000	Phenylethynylanthracene based pushâ€“pull molecular systems: tuning the photophysics through <i>para</i> -substituents on the phenyl ring. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
14001	AIEgens for dual second harmonic generation and fluorescence $\hat{=}$ turn-onâ€“imaging of membrane and photodynamic therapy in cancer cells. <i>Materials Chemistry Frontiers</i> , 2023, 7, 502-513.	3.2	3
14002	Origin of high piezoelectricity of a bismuth-based organicâ€“inorganic hybrid crystal. <i>Journal of Materials Chemistry C</i> , 2023, 11, 1401-1408.	2.7	2
14003	Synthesis, structural, spectral, computational, docking and biological activities of Schiff base 5-bromosalicylaldehyde and sulfadiazine. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100823.	1.3	22

#	ARTICLE	IF	CITATIONS
14004	Theoretical investigations on P-stabilized boryl cation radicals: from the Aufbau principle to SOMO→HOMO conversion. Dalton Transactions, 2023, 52, 384-393.	1.6	2
14005	Theoretical investigation of borane compounds mimicking transition metals for N ₂ fixation and activation. Physical Chemistry Chemical Physics, 0, , .	1.3	1
14006	Theoretical study of Ga-doped magnesium mineral based on the atomic cluster level: Gas-phase GaMgn-(n=12) DFT investigation. Chemical Physics Letters, 2023, 811, 140218.	1.2	0
14007	Environmentally affable and highly efficient donor material based on cyclopentadithiophene (CPDT) framework for remarkable organic solar cells. Optical Materials, 2023, 135, 113316.	1.7	11
14008	Molecularly understanding and regulating carrier injection behavior of ETL/perovskite towards high performance PeLEDs. Chemical Engineering Journal, 2023, 456, 141077.	6.6	5
14009	Dielectric relaxation, dipole moment, electronic characterization and non-covalent interaction behavior of valeramide and halo-phenol in non-polar liquid: A density functional theory-based approach. Journal of Molecular Liquids, 2023, 370, 121027.	2.3	10
14010	Insight into poly(1,3-dioxolane)-based polymer electrolytes and their interfaces with lithium Metal: Effect of electrolyte compositions. Chemical Engineering Journal, 2023, 455, 140931.	6.6	2
14011	Simultaneous removal of Arsenic(III) and Chromium(VI) over ZnFe ₂ O ₄ {100}/{111} Z-scheme photocatalyst: Facet-dependent active site and overlooked As(III)/Cr(VI) complex. Journal of Cleaner Production, 2023, 383, 135493.	4.6	7
14012	Alanine rich amphiphilic peptides as green substitutes for hydrate inhibitors: A molecular simulation study. Journal of Molecular Liquids, 2023, 370, 121008.	2.3	22
14013	Cu(ⁱ)-catalysed asymmetric intramolecular tandem oxaziridination/rearrangement reaction: theoretical insight into the mechanism, enantioselectivity, ligand effect, and comparison with the corresponding Lewis-acid-promoted reaction. Organic Chemistry Frontiers, 0, , .	2.3	0
14014	Relativistic Modulation of Supramolecular Halogen/Copper Interactions and Phosphorescence in Cu(I) Pyrazolate Cyclotrimers. Dalton Transactions, 0, , .	1.6	2
14015	Spodium bonding to anticrown-Hg ₃ boosts phosphorescence of cyclometalated-Pt ^{II} complexes. Inorganic Chemistry Frontiers, 2023, 10, 493-510.	3.0	6
14016	Fluoroalkoxyaluminate-based ionic liquids as electrolytes for sodium-ion batteries. Journal of Molecular Liquids, 2023, 369, 120919.	2.3	5
14017	Electronic structures of zwitterionic and protonated forms of glycine betaine in water: Insights into solvent effects from ab initio simulations. Journal of Molecular Liquids, 2023, 369, 120871.	2.3	5
14018	Theoretical prediction of superatomic orbitals in spherical trihedral metallo-borosphenes Be ₃ B ₁₂ +1/+2. Results in Physics, 2023, 44, 106162.	2.0	0
14019	Facile fabrication of hierarchically porous melamine foam@COF composite for sample treatment of non-targeted food safety analysis and oil/water separation. Chemical Engineering Journal, 2023, 455, 140900.	6.6	24
14020	Efficient enrichment of iodine by supported ionic liquid with three effective adsorption sites: Heteroatoms, fused aromatic rings and ionic bond. Chemical Engineering Journal, 2023, 456, 140979.	6.6	20
14021	In situ prepared all-fluorinated polymer electrolyte for energy-dense high-voltage lithium-metal batteries. Energy Storage Materials, 2023, 55, 642-651.	9.5	6

#	ARTICLE	IF	CITATIONS
14022	A bimetallic Ag ₁₅ Cu ₁₂ (S ₆ C ₆ H ₁₁) ₁₈ (CH ₃ COO) ₃ nanocluster featuring an irregular Ag ₁₂ kernel. Dalton Transactions, 2023, 52, 971-976.		
14023	Metal-organic framework-derived ZrO ₂ on N/S-doped porous carbons for mechanistic and kinetic inspection of catalytic H ₂ O ₂ homolysis. Carbon, 2023, 203, 630-649.	5.4	10
14024	Synthesis, spectroscopic, SC-XRD/DFT and non-linear optical (NLO) properties of chromene derivatives. RSC Advances, 2022, 13, 464-477.	1.7	6
14025	Structural and electronic properties of Ln ₂ Si ₆ q: (Sm, Eu, Yb; q = 1) clusters. Chemical Physics, 2023, 566, 111782.	0.9	6
14026	Synthesis, computational, experimental antimicrobial activities and theoretical molecular docking studies of (E)-4-((4-hydroxy-3-methoxy-5-nitrobenzylidene) amino)-N-(thiazole-2-yl) benzenesulfonamide. Journal of the Indian Chemical Society, 2023, 100, 100824.	1.3	18
14027	Mechanistic insight into the effects of alkali metal ions on the formation of NO precursors during the pyrolysis of 2,5-diketopiperazine. Fuel, 2023, 334, 126773.	3.4	3
14028	Understanding the role of host-guest interactions in enhancing oil recovery through β -cyclodextrin and adamantane modified copolymer. Journal of Molecular Liquids, 2023, 369, 120841.	2.3	8
14029	A benzotriazole-coumarin derivative as a turn-on fluorescent probe for highly efficient and selective detection of homocysteine and its bioimaging application. Microchemical Journal, 2023, 185, 108293.	2.3	1
14030	Spectroscopic evidence of a Xe ⁺ Xe bond in the linear Xe ₂ Au ⁺ Xe ion. Chemical Communications, 2022, 59, 179-182.	2.2	1
14031	In vivo monitoring an important plant immune signaling molecule salicylic acid by rhodamine-engineered probes and their density functional theory (DFT) calculations. Arabian Journal of Chemistry, 2023, 16, 104476.	2.3	2
14032	Internal acylation-induced AIE/AIEE switch of pyrimido[2,1-b][1,3]benzothiazoles (PBTs): Restriction of access to dark state caused by distortion of 4H-pyrimidine ring. Dyes and Pigments, 2023, 210, 110982.	2.0	2
14033	Hydrogen evolution reaction of Be _n + H ₂ O (n = 5-9) based on density functional theory. Physical Chemistry Chemical Physics, 2022, 25, 570-579.	1.3	3
14034	Theoretical study on the structure and properties of Au-Au interlocking gold(I) thiolate [2]catenanes. New Journal of Chemistry, 0, , .	1.4	0
14035	Theoretical prediction on the hydrolysis rate of the new types of nerve agents: A density functional study. Toxicology Reports, 2023, 10, 27-31.	1.6	3
14036	Efficient and accurate density-based prediction of macromolecular polarizabilities. Physical Chemistry Chemical Physics, 2023, 25, 2131-2141.	1.3	7
14037	Molecular insight into nano-heterogeneity of localized high-concentration electrolyte: Correlation with lithium dynamics and solid-electrolyte interphase formation. Journal of Power Sources, 2023, 557, 232545.	4.0	3
14038	Perylene imide derivatives: Structural modification of imide position, aggregation caused quenching mechanism, light-conversion quality and photostability. Dyes and Pigments, 2023, 210, 110948.	2.0	7
14039	Au, Ag and Cu Doped BNNT for ethylene oxide gas detection: A density functional theory study. Sensors and Actuators A: Physical, 2023, 350, 114109.	2.0	5

#	ARTICLE	IF	CITATIONS
14040	Highly efficient deep-blue electrofluorescence with optimized excited state composition and "hot-exciton" channel. <i>Dyes and Pigments</i> , 2023, 210, 111002.	2.0	11
14041	Liquid-liquid equilibrium experiment and mechanism analysis of menthol-based deep eutectic solvents extraction for separation of fuel additive tert-butanol. <i>Environmental Research</i> , 2023, 218, 115043.	3.7	5
14042	A novel regulable enantioselective platform based on porphyrin tubular cage assemblies with controllable handedness. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 658, 130627.	2.3	1
14043	Single crystal investigation, spectroscopic, DFT studies, and in-silico molecular docking of the anticancer activities of acetylacetonate coordinated Re(I) tricarbonyl complexes. <i>Inorganica Chimica Acta</i> , 2023, 546, 121335.	1.2	7
14044	Efficient regulation of active layer morphology and interfacial charge-transfer process by porphyrin-based additive in organic solar cells. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 659, 130818.	2.3	1
14045	Carbon dots nanophotosensitizers with tunable reactive oxygen species generation for mitochondrion-targeted type I/II photodynamic therapy. <i>Biomaterials</i> , 2023, 293, 121953.	5.7	30
14046	HCl removal and recovery using choline chloride-glycerol deep eutectic solvent in rotor-stator reactor: Molecular mechanism, experimental and modeling studies. <i>Fuel</i> , 2023, 334, 126818.	3.4	7
14047	Effect of iron on heterogeneous reduction reaction of NO by char: A combined experimental and theoretical study. <i>Combustion and Flame</i> , 2023, 248, 112579.	2.8	4
14048	Atmospheric microplastics and nanoplastics as vectors of primary air pollutants - A theoretical study on the polyethylene terephthalate (PET) case. <i>Environmental Pollution</i> , 2023, 318, 120860.	3.7	12
14049	Theoretical investigation of turn-off mechanism of a new fluorescence probe L. <i>Chemical Physics Letters</i> , 2023, 812, 140256.	1.2	1
14050	High drug carrying efficiency of boron-doped Triazine based covalent organic framework toward anti-cancer tegafur; a theoretical perspective. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 113990.	1.1	18
14051	Ultra-high NH ₃ absorption by triazole cation-functionalized ionic liquids through multiple hydrogen bonding. <i>Separation and Purification Technology</i> , 2023, 307, 122825.	3.9	9
14052	Novel phenoxo-bridged di- and tri-nuclear Cu(II) salamo-like complexes driven by various counter-anions. <i>Inorganica Chimica Acta</i> , 2023, 546, 121336.	1.2	50
14053	Adsorbing CNCl on pristine, C-, and Al-doped boron nitride nanotubes: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 113980.	1.1	7
14054	Application of dual-solvent extraction for separating a low-temperature coal tar: A detailed experimental and quantum chemical study. <i>Fuel</i> , 2023, 334, 126654.	3.4	3
14055	A novel AIEE pillar[5]arene-based conjugated oligomer as paraquat fluorescence turn-off sensor. <i>Dyes and Pigments</i> , 2023, 210, 111027.	2.0	4
14056	A ratiometric fluorescent probe 4-(benzothiazol-2-yl)-2-hydroxy benzaldehyde for detecting malononitrile: Theoretical investigation on the ICT and ESIPT mechanism. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 113978.	1.1	4
14057	Enhanced bone regeneration via ZIF-8 decorated hierarchical polyvinylidene fluoride piezoelectric foam nanogenerator: Coupling of bioelectricity, angiogenesis, and osteogenesis. <i>Nano Energy</i> , 2023, 106, 108076.	8.2	13

#	ARTICLE	IF	CITATIONS
14058	The formation mechanism of highly oxygenated organic molecules produced by toluene in the urban atmosphere. <i>Atmospheric Environment</i> , 2023, 295, 119555.	1.9	2
14059	Study on spectral properties of butyl hydroxytoluene: Experiment and theoretical calculation. <i>Inorganic Chemistry Communication</i> , 2023, 148, 110283.	1.8	1
14060	NiN4S-doped single walled carbon nanotube as an ultrafast H ₂ gas sensor: A DFT simulation. <i>Inorganic Chemistry Communication</i> , 2023, 148, 110334.	1.8	3
14061	2-Amino-2-methyl-1-propanol regulated triethylenetetramine-based nonaqueous absorbents for solid-liquid phase-change CO ₂ capture: Formation of crystalline powder products and mechanism analysis. <i>Separation and Purification Technology</i> , 2023, 307, 122722.	3.9	11
14062	A comparative study on the physicochemical properties of the nanostructured triazolium based ionic liquids composed of [5F-PhMTZ] ⁺ cation and various anions with their non-fluorinated cation analogues. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 113984.	1.1	1
14063	Ag ⁺ ion in choline chloride and glycerol mixture: Evaluation of electrochemical properties and molecular modelling approaches. <i>Journal of Molecular Liquids</i> , 2023, 371, 121053.	2.3	4
14064	Adsorption of naphthalene and its derivatives onto high-density polyethylene microplastic: Computational, isotherm, thermodynamic, and kinetic study. <i>Environmental Pollution</i> , 2023, 318, 120919.	3.7	5
14065	The oxidation mechanism and kinetics of limonic acid by hydroxyl radical in atmospheric aqueous phase. <i>Atmospheric Environment</i> , 2023, 294, 119527.	1.9	0
14066	Reversing adsorption and separation of 1-phenylethanol and acetophenone in organic phase via β -ketoenamine-linked covalent organic frameworks. <i>Chemical Engineering Journal</i> , 2023, 454, 140531.	6.6	3
14067	Synthesis, single crystal characterization and anti-AD activities of a novel complex of Cu(II) with in situ formed protonated chrysin derivative ligand. <i>Journal of Inorganic Biochemistry</i> , 2023, 239, 112086.	1.5	2
14068	A quantum-chemical study of boro-fullerenes B ₆₀ H ₆₀ , B ₆₀ F ₃₀ H ₃₀ , and B ₆₀ F ₆₀ . <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 113987.	1.1	0
14069	Theoretical investigation of the electronic absorption spectra of the glucosides. <i>Biophysical Chemistry</i> , 2023, 293, 106945.	1.5	0
14070	The catalytic performance enhanced via π -electron cloud interaction of polymerized cobalt phthalocyanine/3D-graphene as bifunctional oxygen catalysts for Zn-air battery. <i>Journal of Power Sources</i> , 2023, 556, 232471.	4.0	7
14071	Insight into boron-doped biochar as efficient metal-free catalyst for peroxydisulfate activation: Important role of -O-B-O- moieties. <i>Journal of Hazardous Materials</i> , 2023, 445, 130479.	6.5	36
14072	Experimental spectroscopy, eco-friendly solvents effect on transitions, reactive sites and biological research on methyl gallate α -MTT assay (cytotoxicity). <i>Journal of Molecular Liquids</i> , 2023, 371, 121092.	2.3	4
14073	Systematic investigation of structure and electronic properties of Cs doped anionic Bn clusters. <i>Computational Materials Science</i> , 2023, 218, 111931.	1.4	0
14074	Highly-efficient selective recognition and rapid enrichment of chrysin by magnetic surface molecularly imprinted polymer. <i>Food Chemistry</i> , 2023, 405, 134993.	4.2	17
14075	Revealing self-aggregation mechanism of asphaltenes during oxidative aging using quantum mechanical calculations. <i>Journal of Molecular Liquids</i> , 2023, 371, 121063.	2.3	3

#	ARTICLE	IF	CITATIONS
14076	Unraveling photo-induced proton transfer mechanism and proposing solvent regulation manner for the two intramolecular proton-transfer-site BH-BA fluorophore. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 288, 122141.	2.0	10
14077	One-pot simultaneous extraction and enzymatic hydrolysis to prepare glycyrrhetic acid via ionic liquid-based two-phase systems. <i>Separation and Purification Technology</i> , 2023, 307, 122763.	3.9	3
14078	Uncovering the effect of atom substitution on ESIPT direction and Luminescent property of the asymmetric two proton acceptor compound: A TD-DFT study. <i>Journal of Molecular Structure</i> , 2023, 1276, 134693.	1.8	2
14079	Research on the hydrothermal regeneration of powdered activated coke in wastewater treatment. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109120.	3.3	4
14080	Nonaqueous amino-phenolic dual-functionalized ionic liquid absorbents for reversible CO ₂ capture: Phase change behaviors and mechanism. <i>Separation and Purification Technology</i> , 2023, 308, 122986.	3.9	9
14081	Complexation mechanism of crown ether with indium in the presence of KI: Toward efficient recovery of indium from secondary resources. <i>Separation and Purification Technology</i> , 2023, 308, 122936.	3.9	2
14082	Structure and dynamics of 38-atom Ag-Pt nanoalloys using ANN based-interatomic potential. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 113985.	1.1	2
14083	Cyclodextrin as a green anti-agglomerant agent in oil-in-water emulsion containing asphalt. <i>Fuel</i> , 2023, 335, 127041.	3.4	29
14084	Effects of external field wavelength and solvation on the photophysical property and optical nonlinearity of 1,3-thiazolium-5-thiolates mesoionic compound. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 289, 122227.	2.0	4
14085	Intra- and intermolecular charge transfer control of symmetric A1-A2-A1 ladder-like small molecules/g-C ₃ N ₄ heterojunctions for efficient photocatalytic sterilization and degradation from visible to near-infrared. <i>Applied Surface Science</i> , 2023, 612, 155854.	3.1	3
14086	Promotional effect of nitrogen-doped and pore structure for the direct synthesis of hydrogen peroxide from hydrogen and oxygen by Pd/C catalyst at ambient pressure. <i>Arabian Journal of Chemistry</i> , 2023, 16, 104452.	2.3	1
14087	Cocrystallization with nutrient ferulic acid towards reducing the dissolubility behaviors of antifungal drug 5-fluorocytosine: An integrated theoretical and experimental case research. <i>Journal of Molecular Structure</i> , 2023, 1275, 134601.	1.8	6
14088	Effective removal of Hg ²⁺ and Cd ²⁺ in aqueous systems by Fe-Mn oxide modified biochar: A combined experimental and DFT calculation. <i>Desalination</i> , 2023, 549, 116306.	4.0	14
14089	Theoretical and experimental study of new deep eutectic solvents for extraction of perfluorinated iodoalkanes. <i>Arabian Journal of Chemistry</i> , 2023, 16, 104469.	2.3	4
14090	Molecular glasses based on 1,8-naphthalimide and triphenylamine moieties as bipolar red fluorescent OLED emitters with conventional versus TADF hosting. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 288, 122185.	2.0	6
14091	Theoretical investigation on FRET strategy of ratio metric fluorescent probe sensing hydrogen sulfide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 289, 122223.	2.0	5
14092	A novel fluorescent probe with high sensitivity for sequential detection of CN ⁻ and Al ³⁺ in highly aqueous medium and its applications in living cell bioimaging. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 437, 114488.	2.0	7
14093	Recognition mechanism of imidazo[1,5- <i>b</i>]pyridine-based fluorescence probe towards thiophenols with multi-mechanisms of PET and ESIPT. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 437, 114477.	2.0	5

#	ARTICLE	IF	CITATIONS
14094	Preparation of magnetic porous graphene oxide by intercalating rigid molecule and subsequent magnetization for enhancing pharmaceuticals removal from water. <i>Materials Today Communications</i> , 2023, 34, 105119.	0.9	1
14095	Tuning hybridized local and charge transfer emission in pyrene derivatives by incorporating phenanthroimidazole to realize high exciton harvest in blue organic light-emitting diodes. <i>Dyes and Pigments</i> , 2023, 210, 111008.	2.0	3
14096	Structure property relationship of two pyrazole derivatives: Insights from crystal structure and computational studies. <i>Journal of Molecular Structure</i> , 2023, 1276, 134771.	1.8	1
14097	Toward the design of inorganic-organic hybrid Ir(III) complexes containing borazine and benzene ligands with excellent second-order NLO responses: An appropriate substitution and π -conjugated extension. <i>Journal of Molecular Liquids</i> , 2023, 371, 121081.	2.3	3
14098	Olefin coordination versus weak agostic C-H-M interactions in Sandwich-Type complexes of the split (3 λ^+ 2) Five-Electron donor hydrocarbon ligand Tricyclo[5.2.1.0]-deca-3,8-dien-5-yl (dicp) related to cyclopentadiene dimer. <i>Inorganica Chimica Acta</i> , 2023, 547, 121338.	1.2	0
14099	Crystal engineering of Pb(II)-salen coordination polymer enforced for the selective fluorescence NACs sensing activity in a dispersed aqueous medium: A combined experimental and theoretical DFT monologue. <i>Journal of Molecular Structure</i> , 2023, 1276, 134717.	1.8	9
14100	Molecular level insight into the different interaction intensity between microplastics and aromatic hydrocarbon in pure water and seawater. <i>Science of the Total Environment</i> , 2023, 862, 160786.	3.9	9
14101	Design and structural analysis of centrosymmetric and non-centrosymmetric Zn(II) complexes by the host-guest complexation method. <i>Journal of Molecular Structure</i> , 2023, 1275, 134716.	1.8	1
14102	Molecular simulation investigations on interaction properties of the teriflunomide-chitosan complex in aqueous solution. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 174, 111171.	1.9	19
14103	Super-amphiphilic graphene promotes peroxy monosulfate-based emulsion catalysis for efficient oil purification. <i>Journal of Hazardous Materials</i> , 2023, 445, 130469.	6.5	5
14104	Surface hydroxyl-riched calcium carbonate and copper oxide composites for Fenton-like removal of bisphenol A. <i>Separation and Purification Technology</i> , 2023, 308, 122912.	3.9	6
14105	Synthesis, spectral, crystal structure, DFT and Hirshfeld surface analysis of Zn(II) complexes involving dithiocarbamate and imine ligands and usage as precursor to prepare ZnS for photodegradation of dyes. <i>Journal of Molecular Structure</i> , 2023, 1276, 134805.	1.8	2
14106	Switching the ESIPT and TICT process of DP-HPPI via intermolecular hydrogen bonding. <i>Journal of Molecular Structure</i> , 2023, 1277, 134800.	1.8	5
14107	Inhibitory mechanism of phenolic compounds in rapeseed oil on α -amylase and α -glucosidase: Spectroscopy, molecular docking, and molecular dynamic simulation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 289, 122251.	2.0	8
14108	An insight to the role of perchlorate counter ions and different non-covalent interactions in the solid state structures of mono-anionic malonic acid bridged trinuclear mixed valence cationic complexes of cobalt with tetradentate N ₂ O ₂ donor ligands. <i>Inorganica Chimica Acta</i> , 2023, 547, 121324.	1.2	4
14109	Integrated investigation for extractive denitrogenation of fuel oils with Eco-friendly Piperazine-Based ionic liquids. <i>Fuel</i> , 2023, 337, 127187.	3.4	7
14110	Effect of oxygen functional groups on competitive adsorption of benzene and water on carbon materials: Density functional theory study. <i>Science of the Total Environment</i> , 2023, 863, 160772.	3.9	18
14111	Anthracene separation from analogous polycyclic aromatic hydrocarbons using the naphthalene-based solvents. <i>Fuel</i> , 2023, 335, 127029.	3.4	1

#	ARTICLE	IF	CITATIONS
14112	Sensor behavior of transition-metals (X=Ag, Au, Pd, and Pt) doped Zn11-X-O12 nanostructured materials for the detection of serotonin. <i>Materials Today Communications</i> , 2023, 34, 105048.	0.9	13
14113	Theoretical study on thermally activated delayed fluorescent molecules based on space charge transfer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 288, 122131.	2.0	1
14114	Evaluation of the difference in adsorption of sodium alginate as an efficient and non-toxic arsenopyrite depressant on the surface of arsenopyrite and chalcopyrite. <i>Applied Surface Science</i> , 2023, 613, 156016.	3.1	12
14115	A highly selective and sensitive hydrogen sulfide scavenger along with its imaging in cells and zebrafish. <i>Sensors and Actuators B: Chemical</i> , 2023, 379, 133169.	4.0	3
14116	Multifunctional semiconducting carbon nitrides enabling sequential fluorescent sensing of telomerase activity and internal self-checking. <i>Sensors and Actuators B: Chemical</i> , 2023, 378, 133170.	4.0	2
14117	Solubility modeling, dissolution and solvation thermodynamics, and solute-solvent interactions of diflufenican in aqueous aprotic and protic cosolvents. <i>Journal of Chemical Thermodynamics</i> , 2023, 179, 106981.	1.0	2
14118	Solvent conditions effect on the excited state intramolecular proton transfer mechanism and photophysical property of 1-hydroxy-2-acetonaphthone: A DFT/TD-DFT analysis. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 437, 114437.	2.0	1
14119	AIEE active stilbene based fluorescent sensor with red-shifted emission for vapor phase detection of nitrobenzene and moisture sensing. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 437, 114459.	2.0	15
14120	Adsorption behavior of methylene blue on graphene and hexagonal boron nitride monolayers in aqueous solution: A first-principles treatment. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 174, 111151.	1.9	2
14121	Intensification of NO ₂ removal in sulfite solutions with reusable copper chloride: Mechanism and process parameters. <i>Separation and Purification Technology</i> , 2023, 308, 122996.	3.9	0
14122	Breaking the bottleneck of organic light conversion agents: Preparation, performance evaluation and intrinsic mechanism. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 288, 122161.	2.0	3
14123	Adsorption mechanism of ammonia nitrogen and phenol on lignite surface: Molecular dynamics simulations and quantum chemical calculations. <i>Fuel</i> , 2023, 337, 127157.	3.4	4
14124	Computer-aided Screening of High Performance Covalent-Organic Frameworks for Removal of SO ₂ from Flue Gases. <i>Fluid Phase Equilibria</i> , 2023, 567, 113710.	1.4	1
14125	Non-covalently linked donor-acceptor interaction enhancing photocatalytic hydrogen evolution from porphyrin assembly. <i>Applied Catalysis B: Environmental</i> , 2023, 324, 122284.	10.8	21
14126	Porous sulfonyl binuclear carbonate poly(ionic liquid)s for one-pot fixation of diluted CO ₂ into dimethyl carbonate. <i>Applied Catalysis B: Environmental</i> , 2023, 324, 122278.	10.8	9
14127	Crystal structure analysis, magnetic measurement, DFT studies, and adsorption properties of novel 1-(2,5-dimethylphenyl)piperazine tetrachlorocobaltate hydrate. <i>Materials Today Communications</i> , 2023, 34, 104965.	0.9	16
14128	Hydrogen bond interactions between thioethers and amides: A joint rotational spectroscopic and theoretical study of the formamide-dimethyl sulfide adduct. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 288, 122199.	2.0	3
14129	Quantum mechanical modeling of fused rings-based small-donor molecules with enhanced optoelectronic attributes for high performance organic photovoltaic cells. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 174, 111140.	1.9	8

#	ARTICLE	IF	CITATIONS
14130	Fragmentation modeling of gas-phase ionic liquid clusters in high-voltage electric field. <i>Fuel</i> , 2023, 335, 126919.	3.4	2
14131	Molecular modeling, DFT studies and biological evaluation of methyl 2,8-dichloro-1,2-dihydroquinoline-3-carboxylate. <i>Chemical Physics Impact</i> , 2023, 6, 100146.	1.7	11
14132	Electron acceptor, excitation energies, oscillatory strength, spectroscopic and solvent effects on 5-amino-4,6-dichloro-2-(propylthio) pyrimidine - anticancer agent. <i>Chemical Physics Impact</i> , 2023, 6, 100145.	1.7	12
14133	Equilibrium solubility, non-covalent interactions and solvation thermodynamics of thiamphenicol in aqueous cosolvents of n-propanol/acetone/acetonitrile. <i>Journal of Chemical Thermodynamics</i> , 2023, 178, 106972.	1.0	1
14134	Self-assembly of antifungal agent 5-fluorocytosine and nutrient <i>trans-p</i> -coumaric acid furnishes a cocrystal with the potential to reduce toxicity and side effects for the drug: a case study combining theory with experiment. <i>New Journal of Chemistry</i> , 2023, 47, 1328-1341.	1.4	5
14135	Characterization of non-covalent contacts in mono- and di-halo substituted acetaldehydes: Probing the substitution effects of electron donating and withdrawing groups. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
14136	A DFT study of the <i>endo</i> -selectivity mechanism of the Diels-Alder reaction in lindenane dimeric sesquiterpene synthesis promoted by pyridines. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 3772-3779.	1.3	1
14137	Be ₃ B ₁₁ cluster: a dynamically fluxional beryll-borospherene. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 2846-2852.	1.3	3
14138	Computational design of a notable nitrogen-rich energetic compound on the basis of Diels-Alder reactions. <i>New Journal of Chemistry</i> , 2022, 46, 22994-22998.	1.4	3
14139	Remarkable static and dynamic nonlinear optical responses of Al ₁₃ -TCNQ/F4-TCNQ complexes: a quantum chemical study. <i>New Journal of Chemistry</i> , 2022, 46, 22786-22796.	1.4	0
14140	Theoretical Study on Hydrogen Transfer in the Dissociation of Dimethyl Disulfide Radical Cation. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
14141	An over 16% efficiency organic solar cell enabled by a low-cost pyrazine-based polymer donor. <i>Journal of Materials Chemistry A</i> , 2022, 10, 25595-25601.	5.2	7
14142	Revealing incorporation of NH ₂ group into the edge of carbon dots for H ₂ O ₂ sensing via C-N-H hydrogen bond interaction. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	2
14143	A Highly Selective and High-Contrast Colorimetric Off-On-Chemosensor for Cu ²⁺ Based on Boron-Dipyrromethene (BODIPY) Derivatives. <i>Chinese Journal of Organic Chemistry</i> , 2022, 42, 3757.	0.6	1
14144	DFT and COSMO-RS studies on dicationic ionic liquids (DILs) as potential candidates for CO ₂ capture: the effects of alkyl side chain length and symmetry in cations. <i>RSC Advances</i> , 2022, 12, 35418-35435.	1.7	2
14145	B- and Al-Doped Porous 2D Covalent Organic Frameworks as Nanocarriers for Biguanides and Metformin Drugs. <i>ACS Applied Bio Materials</i> , 2022, 5, 5887-5900.	2.3	7
14146	Calixarenes enabling well-adjusted organic-inorganic interface for inverted organic solar cells with 18.25% efficiency and multifold improved photostability under max power point tracking. <i>Science China Chemistry</i> , 2023, 66, 195-201.	4.2	9
14147	Organic Single-Component Enantiomers with High Phase Transition Temperatures and Dielectric Switching Properties. <i>Crystal Growth and Design</i> , 2022, 22, 7501-7507.	1.4	4

#	ARTICLE	IF	CITATIONS
14148	A DFT/TDDFT Investigation on Fluorescence and Electronic Properties of Chromone Derivatives. <i>Journal of Fluorescence</i> , 2023, 33, 453-458.	1.3	2
14149	Poly-L-aspartic acid based nonconventional luminescent biomacromolecules with efficient emission in dilute solutions for Al ³⁺ detection. <i>International Journal of Biological Macromolecules</i> , 2023, 226, 1387-1395.	3.6	9
14150	Density Functional Theory Study on the H ₂ -Acceptorless Dehydrogenative Boration of Alkenes Catalyzed by a Zirconium Complex. <i>Journal of Organic Chemistry</i> , 2022, 87, 16632-16643.	1.7	1
14151	Theoretical designing of non-fullerene derived organic heterocyclic compounds with enhanced nonlinear optical amplitude: a DFT based prediction. <i>Scientific Reports</i> , 2022, 12, .	1.6	9
14152	Pyrazole Derivative Containing Naphthalene Moiety: Cytotoxicity (Breast and Cervical Cancer), Antibacterial and Antifungal Studies Using Experimental and Theoretical Tools. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-18.	1.4	0
14153	Theoretical Analysis of Polynuclear Zinc Complexes Isobally Related to Hydrocarbons. <i>International Journal of Molecular Sciences</i> , 2022, 23, 14858.	1.8	1
14154	Trapping the Transition State in a [2,3]-Sigmatropic Rearrangement by Applying Pressure. <i>ACS Omega</i> , 2022, 7, 45208-45214.	1.6	3
14155	Coordination configurations of cupric tartrate in electronic industry wastewater. <i>Transactions of Nonferrous Metals Society of China</i> , 2022, 32, 3753-3766.	1.7	4
14156	How Water Interacts with the NOH Group: The Rotational Spectrum of the 1:1 N,N-diethylhydroxylamine-Water Complex. <i>Molecules</i> , 2022, 27, 8190.	1.7	6
14157	Unexpectedly efficient ion desorption of graphene-based materials. <i>Nature Communications</i> , 2022, 13, .	5.8	9
14158	Selective coordination behaviors of Uranium(VI) with novel asymmetrical tetra-alkylcarbamides. <i>Journal of Molecular Liquids</i> , 2022, , 120924.	2.3	0
14159	Mechanistic Insights into Oxidation-Induced Size Conversion of [Au ₆ (dppp) ₄] ²⁺ to [Au ₈ (dppp) ₄ Cl ₂] ²⁺ . <i>Inorganic Chemistry</i> , 2022, 61, 19773-19779.	1.9	1
14160	Chloride recovery and simultaneous CO ₂ mineralization from rare earths high salinity wastewater by the Reaction-extraction-crystallization process. <i>Chemical Engineering Journal</i> , 2023, 455, 140620.	6.6	4
14161	Balancing Energy and Stability of Nitroamino-1,2,4-Oxadiazoles through a Planar Bridge. <i>Organic Letters</i> , 2022, 24, 8832-8836.	2.4	8
14162	Regulating the solventized structure to achieve highly reversible zinc plating/stripping for dendrite-free Zn anode by sulfolane additive. <i>Chemical Engineering Journal</i> , 2023, 455, 140538.	6.6	11
14163	Selectivity Mechanism of Hsp90 Isoform Inhibition through Computational Investigation. <i>Journal of Computational Biophysics and Chemistry</i> , 0, , .	1.0	0
14164	Electronic and Steric Control of Rates and Selectivities in Rhodium-Catalyzed [2+2+2] Cycloadditions for Constructing Fused Tricyclic Hydronaphthofurans: A Density Functional Theory Study. <i>Journal of Organic Chemistry</i> , 2022, 87, 16328-16342.	1.7	1
14165	Coupling of Thiazole-2-Amines with Isocyanide Ligands in bis-(Isocyanide) Platinum Complex: A New Type of Reactivity. <i>Inorganics</i> , 2022, 10, 221.	1.2	0

#	ARTICLE	IF	CITATIONS
14166	How Does Spin Play with the Cycloaddition to Paramagnetic Endohedral Metallofullerenes? The Curious Case of TiSc ₂ N@C ₈₀ . <i>Inorganic Chemistry</i> , 2022, 61, 19183-19192.	1.9	0
14167	Influence mechanism of ammonia mixing on NO formation characteristics of pulverized coal combustion and N oxidation in ammonia-N/coal-N. <i>Fuel</i> , 2023, 336, 126813.	3.4	15
14168	Reconfiguration toward Self-Assembled Monolayer Passivation for High-Performance Perovskite Solar Cells. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	13
14169	Generation of reactive oxygen species through dissolved oxygen activation on defected porous carbon for efficient degradation of antibiotics. <i>Chemical Engineering Journal</i> , 2023, 455, 140602.	6.6	12
14170	Diels-Alder Reactivity of Allenylboronic Acid Pinacol Ester and Related Dienophiles: Mechanistic Studies and Distortion/Interaction-Activation Strain Model Analysis. <i>Journal of Organic Chemistry</i> , 2022, 87, 16776-16784.	1.7	1
14171	Rare Earth Complexes of Europium(II) and Substituted Bis(pyrazolyl)borates with High Photoluminescence Efficiency. <i>Molecules</i> , 2022, 27, 8053.	1.7	0
14172	Computational and Experimental Investigation of the Selective Adsorption of Indium/Iron Ions by the Epigallocatechin Gallate Monomer. <i>Materials</i> , 2022, 15, 8251.	1.3	2
14173	Bioactive Small Molecule, Piperazinium Bis(4-Hydroxybenzenesulphonate) upon Spectral Investigation, Hirshfeld Surface Analysis, Molecular Docking and ADMET Prediction: A Complement DFT Calculations. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-23.	1.4	0
14174	A computational study of Mg _m H _n nanoclusters with m:n = 2:1 for efficient hydrogen storage. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	2
14175	Enlarging the Stokes Shift by Weakening the π -Conjugation of Cyanines for High Signal-to-Noise Ratiometric Imaging. <i>Advanced Science</i> , 2023, 10, .	5.6	18
14176	The Origin of Stereoselectivity in the Hydrogenation of Oximes Catalyzed by Iridium Complexes: A DFT Mechanistic Study. <i>Molecules</i> , 2022, 27, 8349.	1.7	2
14177	Amphiphilic Silver Nanoparticles for Inkjet-Printable Conductive Inks. <i>Nanomaterials</i> , 2022, 12, 4252.	1.9	4
14178	Structural, electronic, and nonlinear optical properties of small silver clusters doped graphyne and pyrazine-modified graphyne: A computational and comparative study. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	1
14180	HALOGEN BOND IN POROUS MATERIALS: RATIONAL SELECTION OF BUILDING BLOCKS. <i>Journal of Structural Chemistry</i> , 2022, 63, 1880-1886.	0.3	1
14181	[3 + 2]-Cycloadditions with Porphyrin $\hat{\pi}$, $\hat{\pi}^2$ -Bonds: Theoretical Basis of the Counterintuitive <i>meso</i> -Aryl Group Influence on the Rates of Reaction. <i>Journal of Organic Chemistry</i> , 2022, 87, 16473-16482.	1.7	1
14182	Boosting near-infrared photothermal/photoacoustic conversion performance of anthracene-fused porphyrin via paramagnetic ion coordination strategy. <i>Science China Chemistry</i> , 2023, 66, 164-173.	4.2	4
14183	Correlation of adsorbent cavity structure with adsorption behavior and interaction of long-chain $\hat{\pi}$ -olefin/paraffin on microporous adsorbents. <i>Nano Research</i> , 2023, 16, 5721-5732.	5.8	2
14184	A density fitting scheme for the fast evaluation of molecular electrostatic potential. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	3

#	ARTICLE	IF	CITATIONS
14185	The interaction mechanism of polystyrene microplastics with pharmaceuticals and personal care products. <i>Science of the Total Environment</i> , 2023, 861, 160632.	3.9	16
14187	Novel Carbonyl Cathode for Green and Sustainable Aluminum Organic Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 53702-53710.	4.0	13
14188	Effect of Hydrogen Bond Interaction on the Decomposition Temperature, Aromaticity, and Bond Order of Nonmetallic Pentazolates. <i>Crystal Growth and Design</i> , 2022, 22, 7062-7073.	1.4	6
14189	A Molybdenum Polysulfide <i>In-Situ</i> Generated from Ammonium Tetrathiomolybdate for High-Capacity and High-Power Rechargeable Magnesium Battery Cathodes. <i>ACS Nano</i> , 2022, 16, 20510-20520.	7.3	17
14190	Impact of end-group modifications and planarity on BDP-based non-fullerene acceptors for high-performance organic solar cells by using DFT approach. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	17
14191	Theoretical prediction of two-dimensional WSi ₂ N ₄ materials for photocatalytic water splitting. <i>Journal of Applied Physics</i> , 2022, 132, .	1.1	2
14192	Steering H^+ -triggered radicalization of surface phosphate functionality and its protonated analogues to accelerate mineralization of aqueous organic wastes. <i>Chemical Engineering Journal</i> , 2023, 455, 140537.	6.6	8
14193	Folding Dynamics of 3,4,3-LI(1,2-HOPO) in Its Free and Bound State with U ⁴⁺ Implicated by MD Simulations. <i>Molecules</i> , 2022, 27, 8151.	1.7	1
14194	Efficient Separation of Methyl <i>tert</i> -Butyl Ether Using Ionic Liquids from Computational Thermodynamics to Process Intensification. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 17631-17643.	1.8	10
14195	Fe Single-Atom Catalyst for Cost-Effective yet Highly Efficient Heterogeneous Fenton Catalysis. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 53767-53776.	4.0	15
14196	Ambimodal Bispericyclic [6 + 4]/[4 + 6] Transition State Competes with Diradical Pathways in the Cycloheptatriene Dimerization: Dynamics and Experimental Characterization of Thermal Dimers. <i>Journal of the American Chemical Society</i> , 2022, 144, 22251-22261.	6.6	8
14197	Theoretical Model of Polarization Effects on Third-Order NLO Properties of the Stilbazolium Derivative Crystal. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8901-8909.	1.1	3
14198	A Mechanistic Study of Asymmetric Transfer Hydrogenation of Imines on a Chiral Phosphoric Acid Derived Indium Metal-Organic Framework. <i>Molecules</i> , 2022, 27, 8244.	1.7	2
14199	Interactions of Antibacterial Naphthoquinones with Mesoporous Silica Surfaces: A Physicochemical and Theoretical Approach. <i>Pharmaceutics</i> , 2022, 15, 1464.	1.7	0
14200	Gaseous formaldehyde adsorption by eco-friendly, porous bamboo carbon microfibers obtained by steam explosion, carbonization, and plasma activation. <i>Chemical Engineering Journal</i> , 2023, 455, 140686.	6.6	10
14201	Metalloporphyrin-Based Metal-Organic Framework Nanorods for Peroxidase-Like Catalysis. <i>ACS Applied Nano Materials</i> , 2022, 5, 17909-17918.	2.4	4
14202	Quantum mechanical study on complexation phenomenon of pillar[5]arene towards neutral dicyanobutane. <i>Supramolecular Chemistry</i> , 2021, 33, 634-646.	1.5	0
14203	Iodine-Mediated Furoxan Formation Facilitates the Synthesis of High-Density Tricyclic Fused Energetic Materials. <i>Crystal Growth and Design</i> , 2023, 23, 532-538.	1.4	8

#	ARTICLE	IF	CITATIONS
14204	Substituent-controlled aggregate luminescence: Computational unraveling of S_1/S_0 surface crossing. <i>Aggregate</i> , 2023, 4, .	5.2	3
14205	Structure-“aromaticity”-reactivity relationship of one- and two-dimensional polyaromatic hydrocarbons and polyborazines. <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	0
14206	Reversible adhesive hydrogel with enhanced sampling efficiency boosted by hydrogen bond and van der Waals force for visualized detection. <i>Chemical Engineering Journal</i> , 2023, 455, 140493.	6.6	12
14207	Coupled carbon structure and iron species for multiple periodate-based oxidation reaction. <i>Chemical Engineering Journal</i> , 2023, 455, 140560.	6.6	5
14208	4-(Aryl)-Benzo[4,5]imidazo[1,2-a]pyrimidine-3-Carbonitrile-Based Fluorophores: Povarov Reaction-Based Synthesis, Photophysical Studies, and DFT Calculations. <i>Molecules</i> , 2022, 27, 8029.	1.7	3
14209	Engineering Single-Atom Sites into Pore-Confined Nanospaces of Porphyrinic Metal-Organic Frameworks for the Highly Efficient Photocatalytic Hydrogen Evolution Reaction. <i>Journal of the American Chemical Society</i> , 2022, 144, 22747-22758.	6.6	53
14210	Polymorphism and Mechanochromism in 2-Phenylbenzothiazole Cyclometalated Pt^{II} Complexes with Chelating $N^{\wedge}S^{\wedge}O$ Ligands. <i>Inorganic Chemistry</i> , 2022, 61, 20043-20056.	1.9	7
14211	Gold(I)-Lanthanide(III) Bonds in Discrete Heterobimetallic Compounds: A Combined Computational and Topological Study. <i>Inorganic Chemistry</i> , 2022, 61, 20308-20315.	1.9	0
14212	N-(p-Toluenesulfonyl)-1-(4-acetylphenoxy)acrylimidate: Synthesis, Crystal Structure and Theoretical Studies. <i>MolBank</i> , 2022, 2022, M1509.	0.2	0
14213	Supramolecular Diversity, Theoretical Investigation and Antibacterial Activity of Cu, Co and Cd Complexes Based on the Tridentate N,N,O-Schiff Base Ligand Formed In Situ. <i>Molecules</i> , 2022, 27, 8233.	1.7	2
14214	Effects of Electron-Withdrawing and -Donating Substituents in N -Donor Scorpionate Ligands and the Metal $5d$ / $4f$ Orbitals on $Am(III)/Eu(III)$ Complexation and Separation. <i>ChemistrySelect</i> , 2022, 7, .	0.7	3
14215	Synthesis, characterization and properties of halogen-substituted 1,1-diamino-2-nitro-2-(1-amino-1H-tetrazol-5-yl) ethene derivatives as energetic materials. <i>FirePhysChem</i> , 2023, 3, 135-141.	1.5	1
14216	Isomer effects and diffraction features in electron scattering from C_{20} compounds. <i>European Physical Journal D</i> , 2022, 76, .	0.6	0
14217	Selective Raman Enhancement with Electronic Sensitivity in Tip-Enhanced Raman Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9147-9153.	1.1	1
14218	Ability of Peripheral H Bonds to Strengthen a Halogen Bond. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9691-9698.	1.1	5
14219	Critical dopant concentrations govern integer and fractional charge-transfer phases in doped P3HT. <i>JPhys Materials</i> , 2023, 6, 014004.	1.8	8
14220	Controlled Halogen-Bond-Involving Assembly of Double- π -Hole-Donating Diaryliodonium Cations and Ditopic Arene Sulfonates. <i>Crystal Growth and Design</i> , 2023, 23, 413-423.	1.4	2
14221	Isomerically Pure Oxindole-Terminated Quinoids for n -Type Organic Thin-Film Transistors Enabled by the Chlorination of Quinoidal Core. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	5

#	ARTICLE	IF	CITATIONS
14222	Enantiomeric Resolution of Pidotimod and Its Isomers in Pidotimod Oral Solutions Using Chiral RP-HPLC with Quadrupole Dalton Analyzer Detection. <i>Chromatographia</i> , 2023, 86, 55-62.	0.7	1
14223	Ursolic Acid and Oleanolic Acid Dissolved in Methanol/Acetone + Water Blends: Thermodynamic Solubility, Intermolecular Interactions, and Solvation Behavior. <i>Journal of Chemical & Engineering Data</i> , 2023, 68, 236-250.	1.0	2
14224	Detection of hydrogen fluoride (HF) gas by Mg ₁₂ O ₁₁ -X (X = S, P, N, and B) nanosurfaces. <i>Chemical Physics Impact</i> , 2022, 5, 100129.	1.7	20
14225	Chlorine counterion effect into the supramolecular arrangement of phenylephrine solid state. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 113992.	1.1	1
14226	Energy property and covalency of H ₂ S $\cdot\cdot$ X (X = N ₂ , CO, CS and SiO) hydrogen bond. <i>Physica Scripta</i> , 2023, 98, 015407.	1.2	0
14227	Evaluation of experimental, computational, molecular docking and dynamic simulation of flucytosine. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-20.	2.0	0
14228	Synergistic Adsorption \cdot Photocatalysis based on Magnetic Metal \cdot Organic Framework Nanoplatfoms for Organic Pollutant Removal. <i>ACS Applied Nano Materials</i> , 2022, 5, 18930-18939.	2.4	4
14229	Chemical Bonding Perspective on Low-Lying SiC ₄ H ₂ Isomers: Conceptual Quantum Chemical Views. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9366-9374.	1.1	3
14230	Evolution of Ceftriaxone Resistance of Penicillin-Binding Proteins 2 Revealed by Molecular Modeling. <i>International Journal of Molecular Sciences</i> , 2023, 24, 176.	1.8	0
14231	Synthesis, Photophysics and Optical Limiting Properties of Functionalized Benzofuran Derivatives. <i>Asian Journal of Organic Chemistry</i> , 2023, 12, .	1.3	1
14232	Initial unimolecular decomposition of 3,4-bis(3-fluorodinitromethylfuroxan-4-yl) furoxan from quantum mechanics and ReaxFF molecular dynamics simulation. <i>FirePhysChem</i> , 2023, 3, 149-157.	1.5	2
14233	Synthesis, spectral characterization, and theoretical investigation of the photovoltaic properties of	1.6	19
14234	Fluorination of Terminal Groups Promoting Electron Transfer in Small Molecular Acceptors of Bulk Heterojunction Films. <i>Molecules</i> , 2022, 27, 9037.	1.7	1
14235	Stereoelectronic Effect from B-Site Dopants Stabilizes Black Phase of CsPb ₃ . <i>Chemistry of Materials</i> , 2023, 35, 271-279.	3.2	9
14236	Stability, spectroscopic, electrochemistry and QTAIM analysis of Cu-Znn ¹⁰ n clusters for glucose sensing application: A study on theoretical and experimental insights. <i>Heliyon</i> , 2022, 8, e12387.	1.4	3
14237	Key Factor Managing the Horizontal Emitting Dipole Orientation of a Thermally Activated Delayed Fluorescence Emitter in a Mixed Host. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 54907-54913.	4.0	5
14238	Combined Experimental and Theoretical Investigation into the Photophysical Properties of Halogenated Coelenteramide Analogs. <i>Molecules</i> , 2022, 27, 8875.	1.7	3
14239	Liver Injury Traceability: Spatiotemporally Monitoring Oxidative Stress Processes by Unit-Emitting Carbon Dots. <i>Analytical Chemistry</i> , 2023, 95, 2765-2773.	3.2	8

#	ARTICLE	IF	CITATIONS
14259	Insights into the Structure of Keggin-Type Polyoxometalate-Based Organic-Inorganic Hybrid Materials: The Actual Ratio of Organic Cations to Heteropolyanions. <i>Inorganic Chemistry</i> , 2023, 62, 4054-4065.	1.9	3
14260	Suppressing Deep Oxidation by Detached Nano-sized Boron Oxide in Oxidative Dehydrogenation of Propane Revealed by the Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2022, 126, 21263-21271.	1.5	3
14261	Transition metal-free ketene formation from carbon monoxide through isolable ketenyl anions. <i>Science</i> , 2022, 378, 1331-1336.	6.0	28
14262	A DFT Investigation on Different Graphene Based Substrates on SERS: A Case Study of TiO ₂ Adsorbed Gold/Graphene. , 0, , .		0
14263	Fully Saturated Hydrocarbons as Hosts of Optical Cycling Centers. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9644-9650.	1.1	4
14264	N-Heterocyclic Carbene/Bronsted Acid Cooperatively Catalyzed Conversions of \hat{I}^{\pm} , \hat{I}^2 -Unsaturated Carbonyls: Hydrogen Bond Donor/Acceptor-Electrophile/Nucleophile Combination Models. <i>ACS Catalysis</i> , 2023, 13, 612-623.	5.5	9
14265	Effects of Atypical Hydrogen Bonds and π - π Interactions on Nonlinear Optical Properties: Dimers of Triangular Structures Based on Perylene, Naphthalene, and Pyromellitic Diimides. <i>Langmuir</i> , 2023, 39, 357-366.	1.6	4
14266	Nonflammable Dual-Salt Electrolytes for Graphite/LiNi _{0.8} Co _{0.1} Mn _{0.1} O ₂ Lithium-Ion Batteries: Li ⁺ Solvation Structure and Electrode/Electrolyte Interphase. <i>ACS Applied Energy Materials</i> , 2022, 5, 15491-15501.	2.5	3
14267	Solvent-Type Passivation Strategy Controls Solid-State Self-Quenching-Resistant Behavior in Sulfur Dots. <i>Inorganic Chemistry</i> , 2022, 61, 21157-21168.	1.9	3
14268	Tuning the Charge Transport in Nickel Salicylaldimine Polymers by the Ligand Structure. <i>Molecules</i> , 2022, 27, 8798.	1.7	0
14269	Design of derivatives of FOX-7-based new four-member heterocyclic insensitive high energy density molecules: a theoretical perspectives. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	4
14270	A theoretical study on the effects of intramolecular and intermolecular interactions on excited state properties of two NIR-TADF combined with AIE molecules. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 114000.	1.1	2
14271	Hydrogen adsorption and sensing properties of p-tert-butylcalix[4]arene and its transition metal complexes: A DFT study. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 23348-23361.	3.8	8
14272	Polarity- and Pressure-Induced Emission from a Benzophenone-Based Luminophore. <i>Molecules</i> , 2022, 27, 8748.	1.7	2
14273	Tetrel Bonding in Anion Recognition: A First Principles Investigation. <i>Molecules</i> , 2022, 27, 8449.	1.7	7
14274	Nature and Strength of Weak O...O Interactions in Nitril Halide Dimers. <i>ChemPhysChem</i> , 2023, 24, .	1.0	1
14275	Amide Linkages in Pyrene-Based Covalent Organic Frameworks toward Efficient Photocatalytic Reduction of Uranyl. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 57225-57234.	4.0	7
14277	The Chemistry of Phenylimidotechnetium(V) Complexes with Isocyanides: Steric and Electronic Factors. <i>Molecules</i> , 2022, 27, 8546.	1.7	5

#	ARTICLE	IF	CITATIONS
14278	Efficient adsorption and degradation of dyes from water using magnetic covalent organic frameworks with a pyridinic structure. <i>Environmental Science and Pollution Research</i> , 2023, 30, 34669-34683.	2.7	4
14279	Benzo[1,4]diazocinone/Pyrrrole Ensembles via the Catalytic Free Insertion of Pyrrolylacetylenic Ketones into Benzimidazoles. <i>ChemistrySelect</i> , 2022, 7, .	0.7	3
14280	Probing into complexation and separation of chiral Ce^{IV} uranium complex to chiral sulfur enantiomers R/S -ethioproles. <i>Applied Organometallic Chemistry</i> , 0, , .	1.7	2
14281	Heteroatoms (B, N, and P) doped on nickel-doped graphene for phosgene (COCl_2) adsorption: insight from theoretical calculations. <i>Materials Today Sustainability</i> , 2023, 21, 100294.	1.9	15
14282	Over 19% Efficiency Organic Solar Cells by Regulating Multidimensional Intermolecular Interactions. <i>Advanced Materials</i> , 2023, 35, .	11.1	114
14283	$\text{P} \rightarrow \text{P}$ Orbital Interaction Enables Single-Crystalline Semimetallic $\text{I}^2\text{-MoTe}_2$ Nanosheets as Efficient Electrocatalysts for Lithium-Sulfur Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 55616-55626.	4.0	3
14284	Liesegang Phenomenon of Liquid Metals on Au Film. <i>Advanced Materials</i> , 2023, 35, .	11.1	7
14285	Unveiling the effect of solvent polarity on the excited state intramolecular proton transfer and hydrogen bond mechanisms of DHP. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	1
14286	Unveiling novel reactivity of P/Al frustrated Lewis pair: ring size-dependent activation of cyclic ethers/thioethers and CO_2 insertion therein. <i>Journal of Chemical Sciences</i> , 2022, 134, .	0.7	4
14287	Pore Geometry and Surface Engineering of Covalent Organic Frameworks for Anhydrous Proton Conduction. <i>Angewandte Chemie</i> , 0, , .	1.6	0
14288	High-efficiency emissive dendritic phosphorescent iridium (III) complex with thermally activated delayed fluorescence molecules as functional light-harvesting moieties. <i>Chemical Engineering Journal</i> , 2022, , 140747.	6.6	3
14289	Enhanced Ultrafast Broadband Reverse Saturable Absorption in Twistacenes with Enlarged π -Conjugated Central Bridge. <i>Molecules</i> , 2022, 27, 9059.	1.7	1
14290	Dissecting Bonding Interactions in Cysteine Dimers. <i>Molecules</i> , 2022, 27, 8665.	1.7	1
14291	Triel Bonds with Au Atoms as Electron Donors. <i>ChemPhysChem</i> , 0, , .	1.0	3
14292	Giant Polyoxoniobate-Based Inorganic Molecular Tweezers: Metal Recognitions, Ion-Exchange Interactions and Mechanism Studies. <i>Angewandte Chemie</i> , 0, , .	1.6	0
14293	A first principles study of nonlinear optical properties of a quinoline derivative. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	2
14294	Mechanism study of the conductivity characteristics of cellulose electrical insulation influenced by moisture. <i>Journal of Applied Physics</i> , 2022, 132, 215104.	1.1	0
14295	Chemoselective carbene insertion into the $\text{N} \sim \text{H}$ bonds of $\text{NH}_3 \cdot \text{H}_2\text{O}$. <i>Nature Communications</i> , 2022, 13, .	5.8	10

#	ARTICLE	IF	CITATIONS
14296	Designing of gigantic first-order hyperpolarizability molecules via joining the promising organic fragments: a DFT study. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	7
14297	Intramolecular Proton Transfer Modulation of Magnetic Spin Coupling Interaction in Photochromic Azobenzene Derivatives with an Ortho-Site Hydroxyl as a Modulator. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9165-9177.	1.1	5
14298	Separation of ethyl acetate and ethanol by imidazole ionic liquids based on mechanism analysis and liquid-liquid equilibrium experiment. <i>Journal of Molecular Liquids</i> , 2023, 371, 121108.	2.3	6
14299	Dioxetane and lactone pathways in dioxygenolytic ring cleavage catalyzed by 2,5-dihydroxypyridine dioxygenase. <i>Chem Catalysis</i> , 2023, 3, 100480.	2.9	3
14300	S π -H \cdots O Hydrogen Bond Can Win over O π -H \cdots S Hydrogen Bond: Gas-Phase Spectroscopy of 2-Fluorothiophenol \cdots H ₂ O Complex. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9178-9189.	1.1	2
14301	Clarifying the Active Site Role of meso-Carboxyphenyl Group for Free Base Porphyrins in Photocatalytic H ₂ Evolution Reaction. <i>ChemCatChem</i> , 2023, 15, .	1.8	1
14302	Photoliquefiable Azobenzene Surfactants toward Solar Thermal Fuels that Upgrade Photon Energy Storage via Molecular Design. <i>Small</i> , 2023, 19, .	5.2	4
14303	A PEGylated Viologen for Crossover-Free and High-Capacity pH-Neutral Aqueous Organic Redox Flow Batteries. <i>Batteries and Supercaps</i> , 0, .	2.4	4
14304	Spectroscopic, DFT study, and molecular docking investigation of N-(3-methylcyclohexyl)-2-phenylcyclopropane-1-carbohydrazide as a potential antimicrobial drug. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100806.	1.3	14
14305	Synthesis of Carrier-Free Paclitaxel-Curcumin Nanoparticles: The Role of Curcuminoids. <i>Bioengineering</i> , 2022, 9, 815.	1.6	1
14306	Dramatic Size-Dependence of Rh _n ⁺ Clusters in Reacting with Small Hydrocarbons: Rh ₃ ⁺ Cluster Catalysis for Dehydrogenation. <i>ChemistrySelect</i> , 2022, 7, .	0.7	1
14307	Highly efficient charge transport across carbon nanobelts. <i>Science Advances</i> , 2022, 8, .	4.7	8
14308	Computational Quantification of the Zwitterionic/Quinoid Ratio of Phenolate Dyes for Their Solvatochromic Prediction. <i>Molecules</i> , 2022, 27, 9023.	1.7	5
14309	As(V) removal from aqueous environments using quaternary ammonium modified ZIF-8/chitosan composite adsorbent. <i>Applied Surface Science</i> , 2023, 614, 156179.	3.1	10
14310	A new α -off-on-off-Schiff base from quinoline and thiophene as a fluorescent sensor for sequential monitoring Ga ³⁺ and Pd ²⁺ . <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 438, 114510.	2.0	3
14311	Comparative antibacterial analysis of the anthraquinone compounds based on the AIM theory, molecular docking, and dynamics simulation analysis. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	2
14312	AIEE active J-aggregates of naphthalimide based fluorescent probe for detection of Nitrobenzene: Combined experimental and theoretical approaches for Non-covalent interaction analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 290, 122273.	2.0	15
14313	Regulating the charge densities of s-Block calcium single-atom site catalysts for efficient N ₂ activation and reduction. <i>Chemical Engineering Journal</i> , 2023, 457, 141187.	6.6	6

#	ARTICLE	IF	CITATIONS
14314	Construction of an MLR-QSAR Model Based on Dietary Flavonoids and Screening of Natural β -Glucosidase Inhibitors. <i>Foods</i> , 2022, 11, 4046.	1.9	4
14315	Reversible H ₂ Storage Capacity of Ni Functionalized Carbyne (C ₁₀) Complex. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2023, 33, 515-528.	1.9	2
14316	To cleave or not a disulfide bond of cystine on nanocopper: a computational approach. <i>Journal of Nanoparticle Research</i> , 2023, 25, .	0.8	0
14317	Structurally defined anti- π -allyliridium complexes catalyze Z-retentive asymmetric allylic alkylation of oxindoles. <i>Nature Catalysis</i> , 2022, 5, 1089-1097.	16.1	14
14318	Tumor Targeting and pH-Sensitive Inclusion Complex Based on HP- β -CD as a Potential Carrier for Paclitaxel: Fabrication, Molecular Docking, and Characterization. <i>Biomacromolecules</i> , 0, , .	2.6	1
14319	Improving Electroluminescence Efficiency by Linear Polar Host Capable of Promoting Horizontal Dipole Orientation for Dopant. <i>Advanced Science</i> , 2023, 10, .	5.6	6
14320	Steric and Electronic Analyses of Ligand Effects on the Stability of η^5 -Methane Coordination Complexes: A DFT Study. <i>Organometallics</i> , 2022, 41, 3834-3844.	1.1	1
14321	Effects of Cocrystallization on the Structure and Properties of Melt-Cast Explosive 2,4-Dinitroanisole: A Computational Study. <i>Molecules</i> , 2022, 27, 9010.	1.7	2
14322	How a Chromium Tricarbonyl Complex Catalyzes the [3 + 2] Cycloaddition Reaction of <i>N</i> -Substituted Phenylnitrones with Styrene: A Molecular Electron Density Theory Analysis. <i>Organometallics</i> , 2022, 41, 3809-3822.	1.1	3
14323	One-dimensional stacking array of 10,20-diphenyl-5,15-diazaporphyrin metal complexes. <i>Journal of Porphyrins and Phthalocyanines</i> , 0, , .	0.4	1
14324	A Twisted Chiral Cavitand with 5-Fold Symmetry and Its Length-Selective Binding Properties. <i>Journal of the American Chemical Society</i> , 2022, 144, 23677-23684.	6.6	10
14325	The development of nucleic acids force fields: From an unchallenged past to a competitive future. <i>Biophysical Journal</i> , 2023, 122, 2841-2851.	0.2	9
14326	Binding mechanism and SERS spectra of 5-fluorouracil on gold clusters. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	3
14327	Sensitivity and Weak Interaction of Energetic Ionic Salts: An Example Case of C ₄ N ₁₈ H ₂ . <i>Crystal Growth and Design</i> , 2023, 23, 104-111.	1.4	4
14328	Amide group enhanced self-assembly and adsorption of dicarboxylic amino acid surfactants on a rhodochrosite surface through intermolecular weak interaction. <i>Separation and Purification Technology</i> , 2023, 309, 122905.	3.9	9
14329	Probing Diversity in Binding Affinities of Polymorphs of an Anticancer Agent against Human β -Enolase: A Quantum Crystallographic Perspective. <i>Crystal Growth and Design</i> , 2023, 23, 580-591.	1.4	1
14330	First Insight into the Formation of <i>In Vivo</i> Transformation Products of 2-Ethylhexyl diphenyl phosphate in Zebrafish and Prediction of Their Potential Toxicities. <i>Environmental Science & Technology</i> , 2023, 57, 451-462.	4.6	11
14331	Intracellular pH Sensor Based on Heteroleptic Bis-Cyclometalated Iridium(III) Complex Embedded into Block-Copolymer Nanospecies: Application in Phosphorescence Lifetime Imaging Microscopy. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	3

#	ARTICLE	IF	CITATIONS
14332	Density functional theory simulation of heterogeneous polymerization reactions during biomass hydrothermal carbonization. <i>Canadian Journal of Chemical Engineering</i> , 2023, 101, 5519-5529.	0.9	1
14333	Three-Component Synthesis of Dioxaphosphorane-Fused Diphosphacycles Exhibiting Unique Dynamic Fluorescence On/Off-Properties. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	0
14334	Theoretical study on the mechanism of sulfur migration to gas in the pyrolysis of benzothiophene. <i>Frontiers of Chemical Science and Engineering</i> , 2023, 17, 334-346.	2.3	2
14335	An efficient pathway to the elaboration of glassy amphiphilic ester based hydroxyethyl cellulose and ionic liquids. <i>Cellulose</i> , 2023, 30, 1483-1502.	2.4	1
14336	Blue Emission of Tetrafluorobenzocarbazole Under the Interactions of Nitrogen-oxygen Saturated hydrogen Bonds with Aggregated Proton Acid. <i>Journal of Fluorescence</i> , 0, , .	1.3	0
14337	Three-Component Synthesis of Dioxaphosphorane-Fused Diphosphacycles Exhibiting Unique Dynamic Fluorescence On/Off-Properties. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	2
14338	Solid-State Self-Assembly of Heteroditopic Copillar[5]arenes. <i>Crystal Growth and Design</i> , 2023, 23, 68-76.	1.4	3
14339	Synthesis, Structural Characterization, Hirshfeld Analysis and AIM Analysis of 2,4,8,10-tetra-tert-butyl-6-phenyldibenzo[d,g][1,3,6,2]-dioxaselenaphosphocine and its Oxide and Selenide Derivatives. <i>Journal of Chemical Crystallography</i> , 0, , .	0.5	1
14340	Liquid-liquid equilibrium and mechanism study on separation of short carbon chain hydrocarbon mixtures by Cyrene. <i>Canadian Journal of Chemical Engineering</i> , 2023, 101, 4731-4745.	0.9	1
14341	Pore Geometry and Surface Engineering of Covalent Organic Frameworks for Anhydrous Proton Conduction. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	16
14342	Catalytic asymmetric C-H insertion reactions of vinyl carbocations. <i>Science</i> , 2022, 378, 1085-1091.	6.0	19
14343	Diantimony Complexes [Cp ^R ₂ Mo ₂ (CO) ₄ (η^4, η^2 -Sb ₂)] (Cp ^R =C ₅ H ₅ , C ₅ H ₄ t ^{Bu}) as Unexpected Ligands Stabilizing Silver(I) π -Alkyne Monomers, Dimers and Chains. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	3
14344	The (E, Z) Isomerization of C-methoxycarbonyl-N-aryl Chlorohydrazones. <i>Chemistry</i> , 2022, 4, 1624-1653.	0.9	0
14345	Design and application of molecularly imprinted electrochemical sensor for the new generation antidiabetic drug saxagliptin. <i>Electroanalysis</i> , 2023, 35, .	1.5	2
14346	Accurate Geometry and Non-Covalent Interactions in 1-Phenylethanol and its Monohydrate: A Rotational Study. <i>ChemPhysChem</i> , 2023, 24, .	1.0	1
14347	Coordination and Stabilization of a Lithium Ion with a Silylene. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	3
14348	Prediction model on hydrolysis kinetics of phthalate monoester: A density functional theory study. <i>Journal of Environmental Sciences</i> , 2024, 135, 51-58.	3.2	1
14349	Highly Efficient and Stable Blue π -OLEDs Based on B-N Bonds Embedded 6,12-Diphenyl-1,11-dihydroindolo[3,2-b]carbazole with Narrowband Emission and Extended Lifetime. <i>Chinese Journal of Chemistry</i> , 2023, 41, 657-664.	2.6	6

#	ARTICLE	IF	CITATIONS
14350	The intermolecular interactions of ammonia with chlorine and bromine oxides: a theoretical study. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	0
14351	Metal chelation ability of Protocatechuic acid anion with $^{210}\text{Po}84$; a theoretical insight. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 113996.	1.1	9
14352	Exploring the Dynamical Nature of Intermolecular Hydrogen Bonds in Benzamide, Quinoline and Benzoic Acid Derivatives. <i>Molecules</i> , 2022, 27, 8847.	1.7	3
14353	In Situ Formation of <i>o</i> -Phenylenediamine Cascade Polymers Mediated by Metal-Organic Framework Nanozymes for Fluorescent and Photothermal Dual-Mode Assay of Acetylcholinesterase Activity. <i>Analytical Chemistry</i> , 2022, 94, 17263-17271.	3.2	20
14354	Supramolecular Self-Assembly Process during Gelation and Crystallization of Cefradine. <i>Industrial & Engineering Chemistry Research</i> , 2023, 62, 405-415.	1.8	2
14355	DFT, Hirshfeld Surface, Molecular Docking and Drug Likeness Studies of Medicinally Important Coumarin Molecule. <i>Arabian Journal for Science and Engineering</i> , 2023, 48, 7445-7462.	1.7	5
14356	Neutral Homoaromatic Diboradisilacyclobutene: Synthesis, Structure, and Reactivity. <i>Journal of the American Chemical Society</i> , 2022, 144, 22446-22450.	6.6	7
14357	Biocompatible ratiometric fluorescent chemosensor for ultrasensitive detection of endogenous aminopeptidase N In Vitro and In Vivo. <i>Sensors and Actuators B: Chemical</i> , 2023, 379, 133228.	4.0	5
14358	Theoretical study of $[\text{3}^6\text{Adamanzane}(\text{3}^6\text{Adz})]$ based alkalides with remarkable non-linear optical properties. <i>Physica Scripta</i> , 2023, 98, 025504.	1.2	2
14359	Substituent effect on the photo-induced geometrical changes of Cu^{I}	0.9	1
14360	Study of the hydrogen evolution properties of cluster ConMoS ($n=1-5$) using density functional theory. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	0
14361	Synthesis, Characterization and Theoretical Investigations on the Molecular Structure, Electronic Property and anti-Trypanosomal Activity of Benzenesulphonamide-Based Carboxamide and Its Derivatives. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 8690-8709.	1.4	20
14362	Theoretical and experimental exploration for efficient separation of carbazole from anthracene oil with quaternary ammonium salts via forming deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2022, 368, 120831.	2.3	2
14363	Behavior of HF and $(\text{HF})_2$ inside a fullerene cage: An in silico study using different density functionals. <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	1
14364	Are benzoilium and nitrilium ions produced from substituted 2-oxazolines during mass spectrometry? A study based on DFT calculations, QTAIM, and ESI-MS/MS. <i>Rapid Communications in Mass Spectrometry</i> , 0, , .	0.7	0
14365	Synthesis, Electronic Structure, UV-Vis, Wave Function, and Molecular Docking Studies of Schiff Base (Z)-N-(Thiazol-2-yl)-4-((Thiophene-2-ylmethylene)Amino)Benzenesulfonamide. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-19.	1.4	11
14366	Amino acids modified nanoscale zero-valent iron: Density functional theory calculations, experimental synthesis and application in the Fenton-like degradation of organic solvents. <i>Journal of Environmental Sciences</i> , 2024, 135, 296-309.	3.2	2
14367	Some Theoretical and Experimental Evidence for Particularities of the Siloxane Bond. <i>Molecules</i> , 2022, 27, 8563.	1.7	0

#	ARTICLE	IF	CITATIONS
14368	Optoelectrical, electronic, and thermodynamic DFT study of a carbon nanoring and its derivative: application as active layer material in organic solar cell performance improvement and nonlinear optics. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	2
14369	Interwoven Poly(Anthraquinonyl Sulfide) Nanosheetsâ€Decorated Carbon Nanotubes as Coreâ€Sheath Heteroarchitected Cathodes for Polymerâ€Based Asymmetrical Full Batteries. <i>Energy and Environmental Materials</i> , 2023, 6, .	7.3	0
14370	Computational Studies on the Reactivity of Polycyclic Aromatic Hydrocarbons. <i>ChemPhysChem</i> , 0, , .	1.0	1
14371	Giant Polyoxoniobateâ€Based Inorganic Molecular Tweezers: Metal Recognitions, Ionâ€Exchange Interactions and Mechanism Studies. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	3
14372	Synthesis, Spectroscopic, DFT Study, and Molecular Modeling of Thiophene-Carbonitrile Against Enoyl-ACP Reductase Receptor. <i>Chemistry Africa</i> , 2023, 6, 945-966.	1.2	11
14373	Efficient hydrogen storage capacity of La3B18: A DFT study. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 7807-7813.	3.8	3
14374	Identification of potential inhibitors of omicron variant of SARS-Cov-2 RBD based virtual screening, MD simulation, and DFT. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	1
14375	Constructing high-efficiency orange-red thermally activated delayed fluorescence emitters by three-dimension molecular engineering. <i>Nature Communications</i> , 2022, 13, .	5.8	20
14376	Two Luminescent Materials of CuI Clusters Based on Mono-phosphine Ligands and Their Fluorescence Sensing Properties. <i>Journal of Cluster Science</i> , 0, , .	1.7	3
14377	Unsymmetric N-Aryl Substituent Effects on Chiral NHC-Cu: Enantioselectivity and Reactivity Enhancement by Ortho-H and Syn-Configuration. <i>ACS Catalysis</i> , 2023, 13, 407-421.	5.5	1
14378	Facile and Efficient Synthesis of Fluorene and Indenoarene Carboxylates from Biaryldiazoacetates via BlueLightâ€Promoted Intramolecular CarbeneCâˆH Insertion. <i>Asian Journal of Organic Chemistry</i> , 2023, 12, .	1.3	1
14379	Selectivity Rule of Cryptands for Anions: Molecular Rigidity and Bonding Site. <i>Chemistry - A European Journal</i> , 0, , .	1.7	0
14380	Synthesis, characterization and biological evaluation of novel 2-aminopridinium nicotinate invitro antifungal, insilico ADME and molecular docking studies. <i>Journal of Molecular Structure</i> , 2023, 1277, 134794.	1.8	6
14381	Prediction models of the ionization coefficient and ionization cross-section based on multi-layer molecular parameters. <i>Plasma Science and Technology</i> , 0, , .	0.7	0
14382	Water activation and splitting by single anionic iridium atoms. <i>Journal of Chemical Physics</i> , 2022, 157, 234304.	1.2	2
14383	Phase Equilibria and Mechanism Insights into the Separation of Isopropyl Acetate and Methanol by Deep Eutectic Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 18881-18893.	1.8	6
14384	New Schiff bases based on isatin and (thio)/carbohydrazone: preparation, experimentalâ€theoretical spectroscopic characterization, and DFT approach to antioxidant characteristics. <i>Research on Chemical Intermediates</i> , 2023, 49, 1463-1484.	1.3	4
14385	Structure-Based Design, Synthesis, and Biological Evaluation of the Cageâ€Amide Derived Orthopox Virus Replication Inhibitors. <i>Viruses</i> , 2023, 15, 29.	1.5	3

#	ARTICLE	IF	CITATIONS
14386	Interchangeability and Disorder in the Solid-State Structures of "Two Wall-Calix[4]pyrroles Equipped with Iodine and Ethynyl" Substituents. <i>Chemistry - an Asian Journal</i> , 0, , .	1.7	0
14387	Tricyclic compounds with 1,4,2,5-dioxadiazine bridged triazoles and pyrazoles as potential energetic materials. <i>Energetic Materials Frontiers</i> , 2023, 4, 10-15.	1.3	4
14388	Catalytic activation of formic acid using Pd nanocluster decorated graphitic carbon nitride for diclofenac reductive hydrodechlorination. <i>Journal of Hazardous Materials</i> , 2023, 446, 130677.	6.5	8
14389	C=O Bond Activation in Mononuclear Lanthanide Oxocarbonyl Complexes $OLn(\text{I}^{2+}-CO)$ ($Ln = \text{Tj, Er, Yb, Lu, Sm, Gd, Tb, Dy, Ho, Er, Yb, Lu}$)	1.9	0
14390	Assessing the Performance of $Al_{12}N_{12}$ and $Al_{12}P_{12}$ Nanostructured Materials for Alkali Metal Ion (Li, Na, K) Batteries. <i>ACS Omega</i> , 2022, 7, 46183-46202.	1.6	14
14391	One-step fabrication of robust polyvinyl chloride loose nanofiltration membranes by synthesizing a novel polyether amine grafted styrene-maleic anhydride copolymer. <i>Separation and Purification Technology</i> , 2023, 309, 123033.	3.9	9
14392	Understanding Ramachandran plot for dipeptide: A density functional theory and information theoretic approach study. <i>Journal of the Chinese Chemical Society</i> , 0, , .	0.8	2
14393	Anticancer Agents as Design Archetypes: Insights into the Structure-Property Relationships of Ionic Liquids with a Triarylmethyl Moiety. <i>ACS Physical Chemistry Au</i> , 2023, 3, 94-106.	1.9	3
14394	Moderate and Universal Synthesis of Undoped Covalent Organic Framework Aerogels for Enhanced Iodine Uptake. <i>Chemistry of Materials</i> , 2022, 34, 11062-11071.	3.2	25
14395	Vibrational spectroscopic, quantum computational (DFT), reactivity (ELF, LOL and Fukui), molecular docking studies and molecular dynamic simulation on (6-methoxy-2-oxo-2H-chromen-4-yl) methyl morpholine-4-carbodithioate. <i>Journal of Molecular Liquids</i> , 2023, 371, 121147.	2.3	18
14396	Mechanistic Study of Diketopiperazine Formation during Solid-Phase Peptide Synthesis of Tirzepatide. <i>ACS Omega</i> , 2022, 7, 46809-46824.	1.6	7
14397	Detection of hydroxymethanesulfonate (HMS) by transition metal-anchored fullerene nanoclusters. <i>Journal of the Iranian Chemical Society</i> , 2023, 20, 713-729.	1.2	18
14398	Anti-inflammatory biomolecular activity of chlorinated-phenyldiazenyl-naphthalene-2-sulfonic acid derivatives: perception from DFT, molecular docking, and molecular dynamic simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 10136-10160.	2.0	17
14399	Fluorine Added to Lead the Way to Future Energetic Materials: 3,5-difluoro-2,4,6-trinitroaniline. <i>Journal of Energetic Materials</i> , 0, , 1-10.	1.0	1
14401	Elucidating the Mechanism of Simultaneous Activation of CH_4 and CO_2 Mediated by Single Group 10 Metal Anions in Gas Phase. <i>ChemPhysChem</i> , 2023, 24, .	1.0	1
14402	Cavity Size Effect on Host-Guest Property of Tiara-like Structural $Mn(SR)_2n$ Nanoclusters Probed by NMR Spectroscopy. <i>Processes</i> , 2022, 10, 2683.	1.3	0
14403	aRDG Analysis of Asphaltene Molecular Viscosity and Molecular Interaction Based on Non-Equilibrium Molecular Dynamics Simulation. <i>Materials</i> , 2022, 15, 8771.	1.3	1
14404	3D-QSAR Directed Discovery of Novel Halogenated Phenyl 3-Trifluoroethoxypyrazole Containing Ultrahigh Active Insecticidal Anthranilic Diamides. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 15665-15681.	2.4	6

#	ARTICLE	IF	CITATIONS
14405	An Isolable Bis(Germylene)-Stabilized Plumblylone. <i>Angewandte Chemie</i> , 0, , .	1.6	0
14406	Sodium humate based double network hydrogel for Cu and Pb removal. <i>Chemosphere</i> , 2023, 313, 137558.	4.2	2
14407	Design, Synthesis, Calculation and Biological Activity Studies Based on Privileged Coumarin Derivatives as Multifunctional Anti-AD Lead Compound. <i>Chemistry and Biodiversity</i> , 0, , .	1.0	1
14408	An Isolable Bis(Germylene)-Stabilized Plumblylone. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	8
14409	Ultralong room temperature phosphorescence via the charge transfer-separation-recombination mechanism based on organic small molecule doping strategy. <i>Chinese Chemical Letters</i> , 2023, 34, 108062.	4.8	3
14410	N-Functionalization of 5-Aminotetrazoles: Balancing Energetic Performance and Molecular Stability by Introducing ADNP. <i>International Journal of Molecular Sciences</i> , 2022, 23, 15841.	1.8	3
14412	Designing metal-free organic superalkalis by modifying benzene: a theoretical perspective. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	1
14413	End-group engineering of non-fused benzothiadiazol derivatives with thiophene rings based small donor molecules for tuning the photovoltaic properties via DFT approach. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 114001.	1.1	3
14414	Effects of Encapsulating Tube and Encapsulated Molecular Chain Length on the Second-Order Nonlinear Optical Responses of Carbon Nanotubes Filled with Head-To-Tail Polar Molecules. <i>Journal of Physical Chemistry C</i> , 2022, 126, 21328-21337.	1.5	1
14415	CO ₂ capture using dicationic ionic liquids (DILs): Molecular dynamics and DFT-IR studies on the role of cations. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	1
14416	Cooperativity and reactivity properties of medium-sized boron clusters: a combined density functional theory and information-theoretic approach study. <i>Molecular Physics</i> , 0, , .	0.8	2
14417	N,N'-Diaryldihydrophenazines as a Sustainable and Cost-Effective Alternative to Precious Metal Complexes in the Photoredox-Catalyzed Alkylation of Aryl Alkyl Ketones. <i>Molecules</i> , 2023, 28, 221.	1.7	1
14418	Degradation of bisphenol A in an oxidation system constructed from Mo ₂ C MXene and peroxymonosulfate. <i>Npj Clean Water</i> , 2022, 5, .	3.1	9
14419	Electron-deficient moiety regulated structure: an efficient strategy for the design of a highly sensitive cyanide -on-fluorescent probe. <i>Sensors and Actuators B: Chemical</i> , 2023, 379, 133218.	4.0	5
14420	The Reaction Mechanism of the Cu(I) Catalyzed Alkylation of Heterosubstituted Alkynes. <i>Catalysts</i> , 2023, 13, 17.	1.6	0
14421	Experimental Spectroscopic, DFT, Molecular Docking, and Molecular Dynamics Simulation Investigations on m-Phenylenediamine (Monomer and Trimer). <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 8599-8631.	1.4	4
14422	Die Diantimonkomplexe [Cp ^R ₂ Mo ₂ (CO) ₄ ($\frac{1}{4}$, $\frac{1}{4}$) ₂] ₂ (Cp ^R ₂ Mo ₂ (CO) ₄ ($\frac{1}{4}$, $\frac{1}{4}$) ₂) ₂ als unerwartete stabilisierende Liganden von Silber(I) (Ag^+) Monomeren, -Dimeren und -Ketten. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	2
14423	Multifunctional polyimides for resistive switching memory devices based on flexible transparent polyimide-silver nanowires hybrid electrodes. <i>Engineering Reports</i> , 2023, 5, .	0.9	0

#	ARTICLE	IF	CITATIONS
14424	Hydrothermal Synthesis, crystal structure, DFT studies, and molecular docking of Zn-BTC MOF as potential antiprotozoal agents. <i>Journal of Molecular Structure</i> , 2023, 1277, 134825.	1.8	13
14425	C [~] C linked fused triazolo-triazine with vicinal C [~] NH ₂ /C [~] NO ₂ groups: A new heat-resistant explosive. <i>Energetic Materials Frontiers</i> , 2022, , .	1.3	0
14426	Intrinsic kinetics mechanisms for the catalytic reduction of NO by Na-loaded char. <i>Proceedings of the Combustion Institute</i> , 2022, , .	2.4	1
14427	Hollow and oval-configured ultrafine Co ₃ O ₄ as a highly-efficient activator of monopersulfate for catalytic elimination of Azorubin S. <i>Sustainable Environment Research</i> , 2022, 32, .	2.1	4
14428	Regulating the melting point by non-covalent interaction toward a promising insensitive melt-castable energetic material: 1,2-difluoro-4,5-dinitrobenzene. , 2022, , 100002.		1
14429	Uncovering the Mechanism of Thermally Activated Delayed Fluorescence in Coplanar Emitters Using Potential Energy Surface Analysis. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 310-317.	2.1	3
14431	Unraveling the Nature of Hydrogen Bonds of "Proton Sponges" Based on Car-Parrinello and Metadynamics Approaches. <i>International Journal of Molecular Sciences</i> , 2023, 24, 1542.	1.8	0
14432	Thermal Degradation and Carbonization Mechanism of Fe-Based Metal-Organic Frameworks onto Flame-Retardant Polyethylene Terephthalate. <i>Polymers</i> , 2023, 15, 224.	2.0	0
14433	Overall structure of Au ₁₂ Ag ₆₀ (S ₆ H ₁₁) ₃₁ Br ₉ (D _{3h}) ₆ achieving a stronger assembly of icosahedral M ₁₃ units. <i>Nanoscale</i> , 2023, 15, 2633-2641.		
14434	Novel supported low-temperature solid molten salt (SMS) anode materials for Li-ion batteries. <i>Chemical Engineering Journal</i> , 2023, 458, 141451.	6.6	6
14435	Molecular Engineering Design for High-Performance Aqueous Zinc-Organic Battery. <i>Nano-Micro Letters</i> , 2023, 15, .	14.4	29
14436	Effect of regio-specific arylamine substitution on novel "extended zinc salophen complexes: density functional and time-dependent density functional study on DSSC applications. <i>RSC Advances</i> , 2023, 13, 2501-2513.	1.7	2
14437	Hyperbranched Conjugated Polymer with Multiple Charge Transfer Enables High-Efficiency Nondoped Red Electroluminescence with Low Driving Voltage. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 4257-4266.	4.0	7
14438	Assisted Tandem Pd Catalysis Enables Regiodivergent Heck Arylation of Transiently Generated Substituted Enol Ethers. <i>Jacs Au</i> , 2023, 3, 261-274.	3.6	4
14439	Role of Chiral Skeleton in Chiral Phosphoric Acids Catalyzed Asymmetric Transfer Hydrogenation: A DFT Study. <i>Catalysts</i> , 2023, 13, 98.	1.6	1
14440	Nonlinear properties of benzothiadiazole-based intramolecular charge-transfer compounds. <i>New Journal of Chemistry</i> , 2023, 47, 4299-4305.	1.4	2
14441	Hydrogen storage capacity of Al, Ca, Mg, Ni, and Zn decorated phosphorus-doped graphene: Insight from theoretical calculations. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 13362-13376.	3.8	16
14442	Microwave assisted synthesis, vibrational spectra, Hirshfeld surface and interaction energy, DFT, topology, in silico ADMET and molecular docking studies of 1,2-bis(4-methoxybenzylidene)hydrazine. <i>Journal of Molecular Structure</i> , 2023, 1278, 134946.	1.8	12

#	ARTICLE	IF	CITATIONS
14443	Synthesis, Crystal Structure, DFT Studies on Tetramethyl-(p-Tolyl)-Hexahydro-1H-Xanthene-1,8(2H)-Dione. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-23.	1.4	1
14444	Branched Fluorine/Adamantane Interfacial Compatibilizer for <i>PBO</i> Fibers/Cyanate Ester <i>Wave-transparent</i> Laminated Composites. <i>Chinese Journal of Chemistry</i> , 2023, 41, 939-950.	2.6	34
14445	A Tb ³⁺ -anchored Zr(IV)-bipyridine MOF to promote photo-induced electron transfer and simultaneously enhance photoluminescence ability and photocatalytic reduction efficiency towards Cr ₂ O ₇ ²⁻ . <i>Journal of Materials Chemistry A</i> , 2023, 11, 2957-2968.	5.2	19
14446	Transport Coefficients of H ₂ –Cu/Al ₂ O ₃ Plasma Mixtures Considering Solid and Liquid Status. <i>IEEE Transactions on Plasma Science</i> , 2023, 51, 2-14.	0.6	0
14447	High-capacity proton battery based on ĩ-conjugated N-containing organic compound. <i>Electrochimica Acta</i> , 2023, 442, 141870.	2.6	4
14448	TDDFT calculations of the PETN’s ultraviolet absorption spectrum under the electric field loading. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	0
14449	Computer-aided structure-based optimization of 4,5,6,7-tetrahydrobenzo[<i>d</i>]thiazole-2,6-diamine derivatives as DNA gyrase B inhibitors. <i>New Journal of Chemistry</i> , 0, , .	1.4	1
14450	Electronic Transmutation Concept: Is the Inverse Process Possible? An Evaluation of Main Group Compounds. <i>ACS Omega</i> , 0, , .	1.6	0
14451	The El-Sayed’s rule analogy enables long-lived room temperature phosphorescence in twisted biphenyls. <i>Cell Reports Physical Science</i> , 2023, 4, 101245.	2.8	10
14452	A Computational Study of the Immobilization of New 5-Nitroisatine Derivatives with the Use of C60-Based Functionalized Nanocarriers. <i>Symmetry</i> , 2023, 15, 226.	1.1	0
14454	Non-covalent interactions in the monohydrated complexes of 1,2,3,4-tetrahydroisoquinoline. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	0
14455	[ReH ₃ (PPh ₃) ₄] – A Key Compound in the Rhenium Hydride Chemistry. <i>Chemistry - A European Journal</i> , 0, , .	1.7	0
14456	<i>In silico</i> screening of ethyl 4-[(E)-(2-hydroxy-4-methoxyphenyl)methyleneamino]benzoate and some of its derivatives for their NLO activities using DFT. <i>Royal Society Open Science</i> , 2023, 10, .	1.1	4
14457	The oxidation dissolution of uranium oxides in carbonate-peroxide aqueous solution. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2023, 332, 917-923.	0.7	1
14458	Quasi-intrinsic fluorescent probes for detecting the DNA adduct (ABP-dG) based on an excited-state intermolecular charge transfer mechanism. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
14459	Novel A–D–A type non-fullerene acceptors of dithienyl diketopyrropopyrrole derivatives to enhance organic photovoltaic applications: a DFT study. <i>RSC Advances</i> , 2023, 13, 1640-1658.	1.7	17
14460	Unveiling the influence of the various-membered ring structures on the performance of Ir(III) complexes: phosphorescent quantum yields and stabilities. <i>New Journal of Chemistry</i> , 2023, 47, 3793-3801.	1.4	2
14461	Investigating the factors that influence sacrificial hydrogen evolution activity for three structurally-related molecular photocatalysts: thermodynamic driving force, excited-state dynamics, and surface interaction with cocatalysts. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1

#	ARTICLE	IF	CITATIONS
14462	The location of benzothiazole on the skeleton of rofecoxib defines an AI Egen and its potential application as multifunctional materials. <i>Journal of Molecular Structure</i> , 2023, 1279, 134983.	1.8	1
14463	On the Catalytic Performance of (ZrO) _n (n=1-4) Clusters for CO Oxidation: A DFT Study. <i>ChemPhysChem</i> , 2023, 24, .	1.0	1
14464	Manipulation of π -aromatic conjugation in two-dimensional Sn-organic materials for efficient lithium storage. <i>EScience</i> , 2023, 3, 100094.	25.0	16
14465	Physicochemical properties and intermolecular interactions of a novel diacylglycerol oil oleogel made with ethyl cellulose as affected by β -oryzanol. <i>Food Hydrocolloids</i> , 2023, 138, 108484.	5.6	4
14466	Spontaneous Fe ^{III} /Fe ^{II} redox cycling in single-atom catalysts: Conjugation effect and electron delocalization. <i>IScience</i> , 2023, 26, 105902.	1.9	1
14467	Modeling coarse-grained van der Waals interactions using dipole-coupled anisotropic quantum Drude oscillators. <i>Journal of Computational Chemistry</i> , 2023, 44, 1164-1173.	1.5	1
14468	Virtual Screening of Soybean Protein Isolate-Binding Phytochemicals and Interaction Characterization. <i>Foods</i> , 2023, 12, 272.	1.9	0
14469	A DFT study on the transition metal doped BN and AlN nanocages as a drug delivery vehicle for the cladribine drug. <i>Journal of Molecular Liquids</i> , 2023, 374, 121262.	2.3	13
14470	Micro/macroscopic and density functional studies of the interactions between Molybdenum Trioxide and C ₆₀ molecule. <i>Journal of Chemical Physics</i> , 0, , .	1.2	0
14471	Spectroscopic, structural, and intermolecular interactions of 4-(2-hydroxy-3-methoxybenzylideneamino)-N-(5-methylisoxazol-3-yl)benzenesulfonamide enol-imine and keto-amine isomers. <i>Journal of Molecular Structure</i> , 2023, 1279, 134978.	1.8	9
14472	Approaching the Dimerization Mechanism of Small Molecule Inhibitors Targeting PD-L1 with Molecular Simulation. <i>International Journal of Molecular Sciences</i> , 2023, 24, 1280.	1.8	5
14473	Electrochemical methods, quantum chemical, and molecular dynamics methods to analyze the corrosion inhibition mechanism of phytic acid/praseodymium composite conversion coating on the AZ31B magnesium alloy. <i>Molecular Crystals and Liquid Crystals</i> , 0, , 1-24.	0.4	0
14474	F2BMF (M = B and Al) Molecules: A Matrix Infrared Spectra and Theoretical Calculations Investigation. <i>Molecules</i> , 2023, 28, 554.	1.7	0
14475	Synthesis, Crystal Structure, and Characterization of Energetic Salts Based on 3,5-Diamino-4H-Pyrazol-4-One Oxime. <i>Molecules</i> , 2023, 28, 457.	1.7	2
14476	Energy transfer between Si nanocrystals and protoporphyrin molecules as a function of distance, orientation and size. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	0
14477	Pyridinium-Inspired Organocatalysts for Carbon Dioxide Fixation: A Density Functional Theory Inspection. <i>Journal of Physical Chemistry A</i> , 2023, 127, 29-37.	1.1	0
14478	A DFT study of plasma-catalytic ammonia synthesis: the effect of electric fields, excess electrons and catalyst surfaces on N ₂ dissociation. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 3920-3929.	1.3	3
14479	Dual-strategy modification on g-C ₃ N ₄ for highly efficient inactivation of <i>Microcystis aeruginosa</i> under visible light. , 2022, 1, 316-324.		1

#	ARTICLE	IF	CITATIONS
14480	Density functional studies of probucol excited states and spectral properties. <i>European Physical Journal D</i> , 2023, 77, .	0.6	0
14481	The Prominence of Facilitator-â€Holes: The Classic Nâ†N Pnictogen Bonding in Nitrobenzeneâ€Ammonia Dimer with its Structural Elucidation and Experimental Characterization at Low Temperatures. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	0
14482	The investigation of modification in structural flexibility and coordination modes in a solvent free Î²-diketone Cu(II) complex by crystal structure and DFT studies. <i>Polyhedron</i> , 2023, , 116293.	1.0	0
14483	Toward Site-Specific Interactions of <i>n</i>H₂ (<i>n</i> = 1â€4) with Ga₁₂As₁₂ Nanostructured for Hydrogen Storage Applications. <i>Energy & Fuels</i> , 2023, 37, 1353-1369.	2.5	12
14484	Conjugation-Modulated Excitonic Coupling Brightens Multiple Triplet Excited States. <i>Journal of the American Chemical Society</i> , 2023, 145, 1945-1954.	6.6	27
14485	Heptacoordinate transition-metal-decorated metallo-borosphenes and multiple-helix metallo-boronanotubes. <i>Nanoscale</i> , 0, , .	2.8	1
14486	Bonding in PdCl(NO) and Related Nitrosylmetal Species of the Enemarkâ€Feltham {MNO}¹⁰Type. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2023, 649, .	0.6	3
14487	Donor Extension on Spiroâ€Acridine Enables Highly Efficient TADFâ€OLEDs with Relieved Efficiency Rollâ€Off. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	10
14488	Structure-activity relationship and experimental study of organic solvents and deep eutectic solvents in separation of cyclohexane-ethyl acetate. <i>Journal of Molecular Liquids</i> , 2023, 373, 121263.	2.3	2
14489	Theoretical Insight on the High Reactivity of Reductive Elimination of Ni^{III} Based on Energy- and Electron-Transfer Mechanisms. <i>Inorganic Chemistry</i> , 2023, 62, 1156-1164.	1.9	3
14490	Syntheses and Structures of Facial and Meridional Stereoisomers of Î²²â€i>N,S</i>â€Chelated Ruthenium Borate Complexes. <i>European Journal of Organic Chemistry</i> , 2023, 26, .	1.2	1
14491	Mechanistic study of nickel-catalyzed intramolecular [4 + 2] cycloaddition of cyclobutanone with allene: origin of selectivity and ligand effect. <i>Organic Chemistry Frontiers</i> , 2023, 10, 1134-1146.	2.3	3
14492	Investigation of enhanced Am selectivity for Eu in solvent extraction using a BTPPhen ligand substituted with halogen. <i>RSC Advances</i> , 2023, 13, 2476-2482.	1.7	0
14493	Non-negligible roles of charge transfer excitons in ultrafast excitation energy transfer dynamics of a double-walled carbon nanotube. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	2
14494	Visible light enhanced persulfate activation for degradation of tetracycline via boosting adsorption of persulfate by ligand-deficient MIL-101(Fe) icosahedron. <i>Chemosphere</i> , 2023, 317, 137857.	4.2	7
14495	Regulating the Solvation Shell Structure of Lithium Ions for Smooth Li Metal Deposition in Quasiâ€Solidâ€State Batteries. <i>ChemSusChem</i> , 2023, 16, .	3.6	0
14496	Factors contributing to halogen bond strength and stretch or contraction of internal covalent bond. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 2907-2915.	1.3	7
14497	Isolation and Identification of Novel Antioxidant Polyketides from an Endophytic Fungus <i>Ophiobolus cirsi</i> LZU-1509. <i>Journal of Agricultural and Food Chemistry</i> , 2023, 71, 1593-1606.	2.4	0

#	ARTICLE	IF	CITATIONS
14498	Isomeric thermally activated delayed fluorescence emitters for highly efficient organic light-emitting diodes. <i>Chemical Science</i> , 2023, 14, 1551-1556.	3.7	12
14499	Direct detection of a single [4Fe μ S] cluster in a tungsten-containing enzyme: Electrochemical conversion of CO ₂ into formate by formate dehydrogenase. , 2023, 5, .		3
14500	Restriction of photoinduced electron transfer as a mechanism for the aggregation-induced emission of a trityl-functionalised maleimide fluorophore. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 4193-4200.	1.3	1
14501	Combining <i>ab initio</i> and <i>ab initio</i> molecular dynamics simulations to predict the complex refractive indices of organic polymers. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 4950-4958.	1.3	2
14502	Porous organic polycarbene nanotrap for efficient and selective gold stripping from electronic waste. <i>Nature Communications</i> , 2023, 14, .	5.8	18
14503	Experiment and Molecular Mechanism of Two Chlorinated Volatile Organic Compounds in Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2023, 62, 1160-1171.	1.8	10
14504	The additional Nitrogen atom breaks the uranyl structure:A combined photoelectron spectroscopy and theoretical study of NUO ₂ ⁺ . <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
14505	Halogen bonding between metal-bound I ₃ ⁺ and unbound I ₂ : the trapped I ₂ ⁻ I ₃ ⁺ intermediate in the controlled assembly of copper(<i>scp</i>)-based polyiodides. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 1522-1533.	3.0	4
14506	Amide group enhanced self-assembly and adsorption of thioether-containing hydroxamic acid on cassiterite surface. <i>AIChE Journal</i> , 2023, 69, .	1.8	3
14507	Color-tunable, time-dependent, temperature and humidity-responsive afterglow from hyaluronic acid-based films. <i>Dyes and Pigments</i> , 2023, 212, 111113.	2.0	1
14508	How Does Molecular Diameter Correlate with the Penetration Barrier of Small Gas Molecules on Porous Carbon-Based Monolayer Membranes?. <i>Journal of Physical Chemistry A</i> , 2023, 127, 517-526.	1.1	1
14509	The effect of water content on lignin solubilization in deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2023, 374, 121271.	2.3	10
14510	Transport properties of GNR-C ₆₀ single-molecule devices. <i>Journal of Materials Chemistry C</i> , 2023, 11, 2251-2266.	2.7	3
14511	A confinement strategy for constructing C _x Mn _{1-x} O ₂ solid solutions with oxygen vacancies confined in interwoven titania nanotubes toward catalytic ozonation of 1,2-dichloroethane. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109299.	3.3	3
14512	Cooperative hydrogen- and halogen-bonding interaction promoted deep eutectic solvent-functionalized magnetic metal-organic framework for perfluoroalkyl iodides detection in edible oils. <i>Food Control</i> , 2023, 148, 109625.	2.8	8
14513	Yttrium separation by phosphorylcarboxylic acid and the underlying tetrad effect along lanthanide unveiled from different microscopic interactions. <i>Fundamental Research</i> , 2023, , .	1.6	1
14514	Functionality-Induced Locking of Zeolitic Imidazolate Frameworks. <i>Chemistry of Materials</i> , 2023, 35, 490-498.	3.2	5
14515	Unusual Turn-on Ratiometric Response of Fluorescent Porphyrin-Pyrene Dyads to the Nitroaromatic Compounds. <i>Chemosensors</i> , 2023, 11, 43.	1.8	1

#	ARTICLE	IF	CITATIONS
14516	Revealing the Generation of High-Valent Cobalt Species and Chlorine Dioxide in the Co ₃ O ₄ -Activated Chlorite Process: Insight into the Proton Enhancement Effect. <i>Environmental Science & Technology</i> , 2023, 57, 1882-1893.	4.6	23
14517	Insights into the interactions between cellulose and biological molecules. <i>Carbohydrate Research</i> , 2023, 523, 108738.	1.1	1
14518	Decontamination of enoxacin containing aqueous phase through hydrophobic deep eutectic solvents: Solvent regeneration and quantum chemical insights. <i>Journal of Molecular Liquids</i> , 2023, 374, 121254.	2.3	4
14519	Quantum computational, spectroscopic and molecular docking studies on 6-amino-3-bromo-2-methylpyridine. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100868.	1.3	0
14520	Atmospheric fate of typical liquid crystal monomers in the tropospheric gas, liquid, and granular phases. <i>Journal of Environmental Sciences</i> , 2024, 136, 348-360.	3.2	4
14521	Rational Design of Biological Crystals with Enhanced Physical Properties by Hydrogen Bonding Interactions. <i>Research</i> , 2023, 6, .	2.8	2
14522	18-valence-electron rule lighted planar tetracoordinate carbon and nitrogen: the global energy minima of CAI ₄ Zn and NAI ₄ Zn ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 4211-4215.	1.3	5
14523	Is the Triggering of PD-L1 Dimerization a Potential Mechanism for Food-Derived Small Molecules in Cancer Immunotherapy? A Study by Molecular Dynamics. <i>International Journal of Molecular Sciences</i> , 2023, 24, 1413.	1.8	2
14524	Decomposition mechanism of 1,3,5-trinitro-2,4,6-trinitroaminobenzene under thermal and shock stimuli using ReaxFF molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 3799-3805.	1.3	5
14525	Incorporation of a Boron-Nitrogen Covalent Bond Improves the Charge-Transport and Charge-Transfer Characteristics of Organoboron Small-Molecule Acceptors for Organic Solar Cells. <i>Molecules</i> , 2023, 28, 811.	1.7	6
14526	Rational Design of Polymethine Dyes with NIR Emission and High Photothermal Conversion Efficiency for Multimodal Imaging-Guided Photoimmunotherapy. <i>Advanced Materials</i> , 2023, 35, .	11.1	23
14527	Construction of Z-Scheme Ag ₂ MoO ₄ /ZnWO ₄ Heterojunctions for Photocatalytically Removing Pollutants. <i>Langmuir</i> , 2023, 39, 1159-1172.	1.6	22
14528	Copper coordination compounds based on bis-quinolylhydrazone of 2,6-diacetylpyridine: Synthesis, structure and cytotoxic activity. <i>Polyhedron</i> , 2023, 233, 116292.	1.0	5
14529	High-stable nonflammable electrolyte regulated by coordination-number rule for all-temperature and safer lithium-ion batteries. <i>Energy Storage Materials</i> , 2023, 55, 836-846.	9.5	14
14530	An <i>in silico</i> study of the selective adsorption and separation of CO ₂ from a flue gas mixture (CH ₄ , CO ₂ , N ₂) by ZnLi ₅ clusters. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 5174-5182.	1.3	1
14531	Janus behavior of Au atoms interacting with fluorine. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	1
14532	A New Insight of Anti-Solvent Electrolytes for Aqueous Zinc-Ion Batteries by Molecular Modeling. <i>Small Structures</i> , 2023, 4, .	6.9	9
14533	Organocatalytic Enantioselective Thermal [4 + 4] Cycloadditions. <i>Journal of the American Chemical Society</i> , 2023, 145, 1448-1459.	6.6	13

#	ARTICLE	IF	CITATIONS
14534	Hydroxy-Containing Covalent Organic Framework Combined with Nickel Ferrite as a Platform for the Recognition and Capture of Bisphenols. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 1827-1842.	4.0	8
14535	Fused ring pyrrolo[3,2-b]pyrrole-based tilde-shaped acceptor molecules for highly efficient organic solar cells. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 176, 111228.	1.9	20
14536	A red thermally activated delayed fluorescence emitter based on benzo[c][1,2,5]thiadiazole. <i>Dyes and Pigments</i> , 2023, , 111084.	2.0	1
14537	Regulating the Reaction Pathway of nZVI to Improve the Decontamination Performance Through Magnetic Spatial Confinement Effect. <i>Journal of Hazardous Materials</i> , 2023, , 130799.	6.5	1
14538	Doping of charge-transfer molecules in cocrystals for the design of materials with novel piezo-activated luminescence. <i>Chemical Science</i> , 2023, 14, 1479-1484.	3.7	5
14539	Mechanistic study to reveal steric and electronic aspects involved in the formation of microstructures during Pd-catalyzed olefin/divinyl formal copolymerization: reactivity to catalyst choice. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 2439-2450.	1.3	1
14540	Computational Studies of CuAAC Reaction Mechanism with Diimine and Phosphorus Ligands for Synthesis of 1,4-Disubstituted 1,2,3-Triazoles. <i>New Journal of Chemistry</i> , 0, , .	1.4	3
14541	Structural Evolution and Electronic Properties of Selenium-Doped Boron Clusters SeB_nO_n ($n = 3 \sim 16$). <i>Molecules</i> , 2023, 28, 357.	1.7	4
14542	Catalytic Oxidation of Benzoin by Hydrogen Peroxide on Nanosized HKUST-1: Influence of Substituents on the Reaction Rates and DFT Modeling of the Reaction Path. <i>Molecules</i> , 2023, 28, 747.	1.7	2
14543	Computational study of linear carbon chain based organic dyes for dye sensitized solar cells. <i>RSC Advances</i> , 2023, 13, 1019-1030.	1.7	4
14544	The trianionic hydrazido radical (N_2^{3-}): a promising platform for transforming N_2 . <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 1952-1957.	3.0	2
14545	Thyroid hormone transporters binding affinity of methoxypoly chlorinated biphenyls: Insights from molecular simulations and fluorescence competitive binding experiment. <i>International Journal of Biological Macromolecules</i> , 2023, 231, 123224.	3.6	0
14546	Crystallographic and Computational Analysis of the Solid-Form Landscape of Three Structurally Related Imidazolidine-2,4-dione Active Pharmaceutical Ingredients: Nitrofurantoin, Furazidin, and Dantrolene. <i>Crystal Growth and Design</i> , 2023, 23, 930-945.	1.4	0
14547	The theoretical study of the oxidation reaction of hydroxyl radical for the removal of volatile organic aliphatic and aromatic aldehydes from the atmosphere. <i>Structural Chemistry</i> , 0, , .	1.0	0
14548	Thiophene and diaminobenzo-(1,2,5-thiadiazol)-based DAD-type near-infrared fluorescent probe for nitric oxide: A theoretical research. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	4
14549	Bicyclic High-Energy and Low-Sensitivity Regioisomeric Energetic Compounds Based on Polynitrobenzene and Pyrazoles. <i>Crystal Growth and Design</i> , 2023, 23, 1127-1132.	1.4	6
14550	Characterization of porosity in lack of fusion pores in selective laser melting using the wavefunction. <i>Materials Research Express</i> , 2023, 10, 016501.	0.8	2
14551	Pristine fullerene (C ₂₄) metals (Mo, Fe, Au) engineered nanostructured materials as an efficient electro-catalyst for hydrogen evolution reaction (HER): A density functional theory (DFT) study. <i>Materials Chemistry and Physics</i> , 2023, 297, 127374.	2.0	13

#	ARTICLE	IF	CITATIONS
14552	Poly(ionic liquid)s for Photo-Driven CO ₂ Cycloaddition: Electron Donor-Acceptor Segments Matter. <i>Advanced Science</i> , 2023, 10, .	5.6	10
14553	Computational insight into a mechanistic overview of water exchange kinetics and thermodynamic stabilities of bis and tris-aquated complexes of lanthanides. <i>RSC Advances</i> , 2023, 13, 1516-1529.	1.7	3
14554	Synthesis and thermal stability of a novel polyfunctional pyridine-based derivative featuring amino, nitro, and guanidine groups. <i>Canadian Journal of Chemistry</i> , 2023, 101, 81-88.	0.6	1
14555	Modification of a SOCT-ISC type triphenylamine-BODIPY photosensitizer by a multipolar dendrimer design for photodynamic therapy and two-photon fluorescence imaging. <i>Biomaterials Science</i> , 2023, 11, 1459-1469.	2.6	6
14556	Screening out the Transition Metal Single Atom Supported on Onion-like Carbon (OLC) for the Hydrogen Evolution Reaction. <i>Inorganic Chemistry</i> , 2023, 62, 1001-1006.	1.9	4
14557	Spin-crossover complexes: Self-interaction correction vs density correction. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	4
14558	Exploration of Ligand-Centered Hydride Transfer in La/Y-Catalyzed Deoxygenative Reduction of Tertiary Amides with Pinacolborane. <i>Inorganic Chemistry</i> , 2023, 62, 1580-1590.	1.9	2
14559	Crystal Engineering of Cation-Radical Salts with Weakly Coordinating Carbadodecaborate Anions. <i>Crystals</i> , 2023, 13, 99.	1.0	3
14560	Oxygen vacancies-mediated CuO@N-doped carbon nanocomposites for non-radical-dominated photothermal catalytic degradation of contaminants. <i>Journal of Cleaner Production</i> , 2023, 389, 136054.	4.6	5
14561	An insight into the non-covalent interactions in the solid state structures of dinuclear cobalt(II) complexes with N,O-donor ligands: application of the complexes in the fabrication of Schottky devices. <i>CrystEngComm</i> , 2023, 25, 1006-1017.	1.3	3
14562	Designing and Theoretical Study of Dibenzocarbazole Derivatives Based Hole Transport Materials: Application for Perovskite Solar Cells. <i>Journal of Fluorescence</i> , 2023, 33, 1201-1216.	1.3	3
14563	Deciphering electronic and structural effects in Copper Corrole/Graphene Hybrids. <i>Chemistry - A European Journal</i> , 0, .	1.7	0
14564	Unraveling the electronic influence and nature of covalent bonding of aryl and alkyl radicals on the B12N12 nanocage cluster. <i>Scientific Reports</i> , 2023, 13, .	1.6	6
14565	Unveiling the Mg-promoted [3+2] cycloaddition reaction of mesitronitrile oxide to Baylis-Hillman adduct from the molecular electron density theory perspective. <i>New Journal of Chemistry</i> , 2023, 47, 2495-2506.	1.4	1
14566	Chemical bonding and dynamic structural fluxionality of a boron-based Al ₂ B ₈ binary cluster: the robustness of a doubly 6 π /6 σ aromatic [B ₈] ²⁺ molecular wheel. <i>RSC Advances</i> , 2023, 13, 1964-1973.	1.7	1
14567	Additive-controlled asymmetric iodocyclization enables enantioselective access to both $\hat{1}\pm$ - and $\hat{1}^2$ -nucleosides. <i>Nature Communications</i> , 2023, 14, .	5.8	4
14568	Enhanced hydrogen storage performance of Li and Co functionalized h-GaN nanosheets: DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 120, 108415.	1.3	0
14569	1,3 Dipolar Cycloaddition of M $\frac{1}{4}$ nchnones: Factors behind the Regioselectivity. <i>Journal of Physical Chemistry A</i> , 2023, 127, 645-660.	1.1	0

#	ARTICLE	IF	CITATIONS
14570	Halogen Bonding Channels for Magnetic Exchange in Cu(II) Complexes with 2,5-di(methylthio)-1,3,4-thiadiazole. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	4
14571	Axial vs equatorial: Capturing the intramolecular charge transfer state geometry in conformational polymorphic crystals of a donor-bridge-acceptor dyad in nanosecond-time-scale. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	4
14572	Metal-Free Catalytic Functionalization of Second C_{sp^2} $C-H$ Bond of 1-Methyl Pyrrole Using Bishomocubane-Derived Aminoborane Frustrated Lewis Pairs: A Computational Study. <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
14573	The complexation of lanthanides by glycolamide extractants: Evidences from electronic spectroscopy and DFT calculations. <i>Inorganica Chimica Acta</i> , 2023, 548, 121396.	1.2	3
14574	Revealing and predicting the relationship between the molecular structure and antioxidant activity of flavonoids. <i>LWT - Food Science and Technology</i> , 2023, 174, 114433.	2.5	4
14575	Vacancy Engineering for High-Efficiency Nanofluidic Osmotic Energy Generation. <i>Journal of the American Chemical Society</i> , 2023, 145, 2669-2678.	6.6	18
14576	Oxidation of simulated wastewater by Fe ²⁺ -catalyzed system: The selective reactivity of chlorine radicals and the oxidation pathway of aromatic amines. <i>Chemosphere</i> , 2023, 317, 137816.	4.2	4
14577	Reductive dehalogenation pathways and inhibition mechanisms of 2,5-dichloronitrobenzene in UV/sulfite advanced reduction process. <i>Chemical Engineering Journal</i> , 2023, 459, 141497.	6.6	3
14578	Molecular insights into the functionalization of Au ₁₃ nanocluster with mercaptopurine anti-cancer drug. <i>Physica B: Condensed Matter</i> , 2023, , 414547.	1.3	0
14579	σ -C-H Bond Activation and Dehydrogenative Coupling of Silanes across the Iron-Amide Bond of a Bis(amido)bis(phosphine) Iron(II) Complex. <i>Journal of the American Chemical Society</i> , 2023, 145, 794-799.	6.6	3
14580	Full-color-tunable AIE luminogens for 4D code, security patterns, and multicolor LEDs. <i>Cell Reports Physical Science</i> , 2023, 4, 101202.	2.8	6
14581	New insight into pyrrolic-N site effect towards the first NIR window absorption of pyrrolic-N-rich carbon dots. <i>Nano Research</i> , 2023, 16, 6001-6009.	5.8	8
14582	Desalination behavior of composite membrane with petal shaped pore ^{2D} formed by superimposition of covalent organic framework with large aperture difference. <i>Applied Surface Science</i> , 2023, 616, 156441.	3.1	6
14583	Synthesis and characterization of potential polycyclic energetic materials using bicyclic triazole and azetidine structures as building blocks. <i>RSC Advances</i> , 2023, 13, 2600-2610.	1.7	1
14584	Collective stabilization through $\pi^*-\pi$ and $\pi-\pi$ phosphorous bonding with cooperative halogen and hydrogen bonding in POCl ₃ -Nitrile dimers: Matrix isolation infrared spectroscopic and ab initio computational studies. <i>Journal of Molecular Structure</i> , 2023, 1278, 134916.	1.8	0
14585	Sequence-specific binding behavior of coralyne toward triplex DNA: an ultrafast time-resolved fluorescence spectroscopy study. <i>Journal of Chemical Physics</i> , 0, , .	1.2	2
14586	Computational investigation of interaction of a cycloplatinated thiosemicarbazone as antitumor and antiparasitic agents with B12N12 nano-cage. <i>Results in Chemistry</i> , 2023, 5, 100768.	0.9	8
14587	Cocrystals assembled from iodoperfluorobenzene and flexible NTPO via halogen and π -hole bonds. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2023, 79, 36-42.	0.2	1

#	ARTICLE	IF	CITATIONS
14588	Structural evolution and electronic properties of doped boron clusters Ta ₂ B (n=10, 14, 20): Ta ₂ B ₁₆ and Ta ₂ B ₁₈ with strong aromaticity. <i>Results in Physics</i> , 2023, 45, 106223.	2.0	3
14589	Tourmaline guiding the electric field and dechlorination pathway of 2,3-dichlorophenol by <i>Desulfitobacterium hafniense</i> . <i>Journal of Environmental Sciences</i> , 2024, 135, 262-273.	3.2	1
14590	Role of donors in triggering second order non-linear optical properties of non-fullerene FCO-2FR1 based derivatives: A theoretical perspective. <i>Heliyon</i> , 2023, 9, e13033.	1.4	16
14591	Synthesis and topology analysis of chloridotriphenyl(triphenyl phosphate- <i>o</i>)tin(IV). <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2023, 79, 99-102.	0.2	0
14592	Molecular Modeling of Cu(II), Zn(II), and Hg(II) Metal Complexes of <i>Chemistry Africa</i> , 0, .	1.2	0
14593	Multiple Pathways for Dissociative Adsorption of SiCl ₄ on the Si(100)-c(4×2) Surface. <i>Symmetry</i> , 2023, 15, 213.	1.1	0
14594	Tuning functionalized hexagonal boron nitride quantum dots for full visible-light fluorescence emission. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 3912-3919.	1.3	2
14595	Comprehensive Study of the Ammonium Sulfamate-Urea Binary System. <i>Molecules</i> , 2023, 28, 470.	1.7	2
14596	Theoretical investigation of mechanism on nickel-catalyzed electrochemical cross-coupling of aryl bromides and arylamines. <i>Catalysis Science and Technology</i> , 0, .	2.1	0
14597	Organochlorine detection on transition metals (X=Zn, Ti, Ni, Fe, and Cr) anchored fullerenes (C ₂₃ X). <i>ChemistrySelect</i> , 2023, 8, .	0.7	15
14598	Modelling of Tungsten (C ₅₉ W), Osmium (C ₅₉ O _s), and Platinum (C ₅₉ Pt) Doped Fullerenes for Drug Delivery of Biguanides (BNG) and Metformin (MET): DFT Perspective. <i>ChemistrySelect</i> , 2023, 8, .	0.7	9
14599	Size- and Shape-Dependent Photoexcitation Electron Transfer in Metal Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2023, 127, 816-823.	1.5	7
14600	Conformational Landscape and Hydrogen Bonding Pattern of Psilocin: Computational Insights. <i>ChemistrySelect</i> , 2023, 8, .	0.7	2
14601	Strong Convection-Dependent Adsorption of Phenothiazine Skeleton Levelers and Their Application in Copper Electroplating. <i>Journal of Physical Chemistry C</i> , 0, .	1.5	2
14602	High-performance non-fullerene acceptor-analogues designed from dithienothiophen [3,2-b]-pyrrolobenzothiadiazole (TPBT) donor materials. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	8
14603	Mechanism and Selectivity of Electrochemical Reduction of CO ₂ on Metalloporphyrin Catalysts from DFT Studies. <i>Molecules</i> , 2023, 28, 375.	1.7	1
14604	In silico package models for deriving values of solute parameters in linear solvation energy relationships. <i>SAR and QSAR in Environmental Research</i> , 2023, 34, 21-37.	1.0	2
14605	Understanding the interaction of nucleotides with UVC light: an insight from quantum chemical calculation-based findings. <i>Physical Chemistry Chemical Physics</i> , 0, .	1.3	0

#	ARTICLE	IF	CITATIONS
14606	Substantial second-order nonlinear optical properties of novel hexamolybdate-piperidine hybrids: A density functional theory (DFT) study. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	1
14608	Tuning Intermolecular Singlet Fission Efficiencies of Peryleneimide Derivatives through Bay Aromatic Substitution. <i>Chinese Journal of Chemistry</i> , 2023, 41, 1170-1176.	2.6	1
14609	Structural, Spectroscopic, Quantum Chemical, RDG, AIM, ELF, Fukui, O _H ⋯N Hydrogen Bonding and NLO Activity of 2-Hydroxy-2-Phenyl Acetophenone Oxime: Experimental and Theoretical Approach. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-30.	1.4	0
14610	Synthesis, Spectroscopic (FTIR, FT-Raman and UV-Vis), Structural Investigation, Chemical Reactivity, AIM, NBO, NLO, Hirshfeld Analysis of 4-Aminobenzoic Acid Pyrazinoic Acid. <i>Polycyclic Aromatic Compounds</i> , 2024, 44, 25-50.	1.4	1
14611	Post-synthetic thiol modification of covalent organic frameworks for mercury(II) removal from water. <i>Environmental Science and Ecotechnology</i> , 2023, 14, 100236.	6.7	12
14612	Color-Tunable Upconversion-Emission Switch Based on Cocrystal-to-Cocrystal Transformation. <i>Journal of the American Chemical Society</i> , 2023, 145, 1855-1865.	6.6	23
14613	Stepwise Hydrations of Anhydride Tuned by Hydrogen Bonds: Rotational Study on Maleic Anhydride-(H ₂ O) ₁₋₃ . <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1
14614	Phenanthroimidazole-Based Covalent Organic Frameworks with Enhanced Activity for the Photocatalytic Hydrogen Evolution Reaction. <i>ACS Applied Energy Materials</i> , 2023, 6, 1126-1133.	2.5	5
14615	Reversible multi-electron redox chemistry of organic salt as anode for high-performance Li-ion/dual-ion batteries. <i>Chemical Engineering Journal</i> , 2023, 457, 141335.	6.6	7
14616	Hydrogen-bonding interactions involving the Imidazol-2-ylidene and its Heavy-atom analogues. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 114020.	1.1	4
14617	Chromate ions chemisorption over the exterior surface of pristine boron nitride (B ₁₂ N ₁₂) nanocage: A computational study. <i>Inorganic Chemistry Communication</i> , 2023, 148, 110370.	1.8	1
14618	The role of nature of aromatic ring on cooperativity between π - π stacking and ion- π interactions: A computational study. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 114022.	1.1	2
14619	Investigating the H-bond network of ternary (xylitol-water-acetic acid) aqueous solutions by Raman spectroscopy and DFT. <i>Journal of Molecular Liquids</i> , 2023, 371, 121159.	2.3	3
14620	Insight into the role of [C ₂ C ₁ mim][OAc] and AgNO ₃ in the reaction of propargylic alcohols, CO ₂ , and 2-aminoethanols. <i>Molecular Catalysis</i> , 2023, 537, 112909.	1.0	0
14621	Spiral donor-based host materials for highly efficient blue thermally activated delayed fluorescence OLEDs. <i>Chemical Engineering Journal</i> , 2023, 458, 141416.	6.6	2
14622	Rational design of aza-BODIPY derived near-infrared fluorescent probe for CN ^{•-} in aqueous solutions. <i>Dyes and Pigments</i> , 2023, 210, 111044.	2.0	2
14623	New insights into contribution of aromatic ring versus aliphatic ring to thermal transition temperatures of heat resistant polyamides: A comparison study of PA 10T and t-PA 10C. <i>Polymer</i> , 2023, 267, 125701.	1.8	3
14624	Mechanism for the adsorption of Per- and polyfluoroalkyl substances on kaolinite: Molecular dynamics modeling. <i>Applied Clay Science</i> , 2023, 232, 106804.	2.6	10

#	ARTICLE	IF	CITATIONS
14625	The change of hydrogen position on π -conjugated bridge to affect NLO property of D(NH_2)- π (DHTPs)-A(NO_2) system. Computational and Theoretical Chemistry, 2023, 1220, 114004.	1.1	2
14626	Quantum mechanics/molecular mechanics studies on the photoprotection mechanisms of three chalcones. Journal of Molecular Liquids, 2023, 372, 121165.	2.3	8
14627	Non-concentrated electrolyte with weak anion coordination enables low Li-ion desolvation energy for low-temperature lithium batteries. Chemical Engineering Journal, 2023, 457, 141273.	6.6	5
14628	Exploring the adsorption behavior of pyrazinamide on the surface of X12Y12(X \hat{A} = \hat{A} B, Al; Y \hat{A} = \hat{A} N, P) nanocages: A in-silico study. Journal of Molecular Liquids, 2023, 372, 121211.	2.3	4
14629	Mechanistic insights into the adsorption of endocrine disruptors onto polystyrene microplastics in water. Environmental Pollution, 2023, 319, 121017.	3.7	4
14630	Structural vibrational analysis (FT-IR, FT-Raman), electronic studies based on solvents (UV-Vis), Tj ETQq1 1 0.784314 rgBT /Overlock Indian Chemical Society, 2023, 100, 100871.	1.3	2
14631	New form of high energy primary explosive: Dual structure composed of ionic salt-based coordination polymers. Chemical Engineering Journal, 2023, 457, 141267.	6.6	15
14632	Degradation of 1,3,6,8-tetrabromocarbazole by sulfidated zero-valent iron activated peroxydisulfate: Mechanistic insight and transformation pathways. Chemical Engineering Journal, 2023, 458, 141439.	6.6	3
14633	Investigation of aluminum nitride nanocarrier for drug delivery process of Favipiravir: A DFT study. Journal of Molecular Liquids, 2023, 372, 121209.	2.3	7
14634	A highly selective red-emitting fluorescent probe and its micro-nano-assembly for imaging endogenous peroxynitrite (ONOO^-) in living cells. Analytica Chimica Acta, 2023, 1241, 340778.	2.6	9
14635	Effect of green solvents physical, chemical, biological and bonding nature on 5-acetyl-thiophene-2-carboxylic acid by DFT and TD-DFT approach \hat{A} An antiviral agent. Journal of the Indian Chemical Society, 2023, 100, 100867.	1.3	15
14636	Synthesis, structural and theoretical investigations on 3-diethyl 2-({4-[3-ethoxy-2-(ethoxycarbonyl)-3-oxo-2-phenylpropyl]-2,5-dimethylphenyl}methyl)-2-phenylpropanedioate. Journal of the Indian Chemical Society, 2023, 100, 100869.	1.3	0
14637	NHC-catalyzed N H functionalization/cycloaddition reaction of indole aldehyde and ketone: A DFT perspective. Computational and Theoretical Chemistry, 2023, 1220, 114007.	1.1	5
14638	A novel ZnO/CQDs/PVDF piezoelectric system for efficiently degradation of antibiotics by using water flow energy in pipeline: Performance and mechanism. Nano Energy, 2023, 107, 108162.	8.2	20
14639	Probing the structural evolution and stabilities of CsB \hat{O} / \hat{A} '' (n = 2 \hat{A} ''12) clusters. Physica B: Condensed Matter, 2023, 652, 414628.	1.3	1
14640	Synergistic effect of hydrogen bonding and π - π interaction for enhanced adsorption of rhodamine B from water using corn straw biochar. Environmental Pollution, 2023, 320, 121060.	3.7	19
14641	Film-forming mechanism of 1,3-propanediolcyclic sulfate as a bifunctional additive for 4.45 \hat{A} V graphite/LiCoO $\hat{2}$ batteries. Journal of Power Sources, 2023, 559, 232656.	4.0	2
14642	Enhanced cadmium removal by biochar and iron oxides composite: Material interactions and pore structure. Journal of Environmental Management, 2023, 330, 117136.	3.8	3

#	ARTICLE	IF	CITATIONS
14643	Insights into Lewis/Brønsted acidity of metal chlorides and solvent effect of alcohols for synthesis of β -valerolactone by combining molecular dynamics simulations and experiments. <i>Fuel</i> , 2023, 335, 126749.	3.4	6
14644	Experimental and density functional theory study of benzohydroxamic acid as a corrosion inhibitor in chemical mechanical polishing of Co interconnects. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 660, 130848.	2.3	7
14645	Remarkable improvement of MOF-based triboelectric nanogenerators with strong electron-withdrawing groups. <i>Nano Energy</i> , 2023, 107, 108149.	8.2	16
14646	Synthesis, Hirshfeld surface analysis, computational, wave function properties, anticancer and cytotoxicity activity of di[(p-chlorobenzyl) (dibromo)] (4,7-dimethyl-1,10-phenanthroline)tin (IV) complex. <i>Inorganica Chimica Acta</i> , 2023, 547, 121361.	1.2	16
14647	Eu ³⁺ -activated SrY ₂ O ₄ :Ce ⁴⁺ /3+ red-phosphor for WLEDs: Structural and luminescent insights from experimental and theoretical approaches. <i>Journal of Alloys and Compounds</i> , 2023, 938, 168595.	2.8	5
14648	Structurally various p-terphenyls with neuraminidase inhibitory from a sponge derived fungus <i>Aspergillus</i> sp. SCSIO41315. <i>Bioorganic Chemistry</i> , 2023, 132, 106357.	2.0	2
14649	Theoretical study on the free radical scavenging potency and mechanism of natural coumestans: Roles of substituent, noncovalent interaction and solvent. <i>Phytochemistry</i> , 2023, 207, 113580.	1.4	7
14650	High-performance fluorescent and colorimetric dual-mode nitrite sensor boosted by a versatile coumarin probe equipped with diazotization-coupling reaction-sites. <i>Sensors and Actuators B: Chemical</i> , 2023, 379, 133261.	4.0	9
14651	A new cyano ($\delta^{13}\text{C}$ N) free molecular design perspective for constructing carbazole-thiophene based environmental friendly organic solar cells. <i>Physica B: Condensed Matter</i> , 2023, 652, 414630.	1.3	1
14652	Imidazolium-based AEMs with high dimensional and alkaline-resistance stabilities for extended temperature range of alkaline fuel cells. <i>Journal of Membrane Science</i> , 2023, 670, 121352.	4.1	10
14653	Synthesis, crystal structure, Hirshfeld surface, energy framework, NCI-RDG, theoretical calculations and molecular docking of (Z)-4,4'-bis[3-N-ethyl-2-N'-(phenylimino) thiazolidin-4-one] methane. <i>Journal of Molecular Structure</i> , 2023, 1277, 134781.	1.8	5
14654	Promoting intense mechanoluminescence by strengthening C-H \cdots N interactions in thioxanthene derivatives. <i>Dyes and Pigments</i> , 2023, 211, 111054.	2.0	3
14655	Experimental and theoretical study on photochromism of triphenylvinyl-naphthopyrans. <i>Dyes and Pigments</i> , 2023, 211, 111070.	2.0	2
14656	Enhancing the compatibility of the amyloid-dye hybrid nanostructure for improved photo-biocatalysis. <i>Journal of Energy Chemistry</i> , 2023, 78, 430-437.	7.1	3
14657	Performance enhancement in thermally activated delayed fluorescence emitters by multi-fold layout. <i>Dyes and Pigments</i> , 2023, 212, 111104.	2.0	0
14658	Machine learning-driven assessment of relationship between activator properties in phase change solvent and its absorption performance for CO ₂ capture. <i>Separation and Purification Technology</i> , 2023, 309, 123092.	3.9	21
14659	A DMRG-CASPT2 investigation on the electronic states of NiSi ⁿ⁺ /O ⁿ⁻ (n=1-3) clusters. <i>Computational and Theoretical Chemistry</i> , 2023, 1221, 114031.	1.1	0
14660	Demulsification of water-in-heavy oil emulsions by oxygen-enriched non-ionic demulsifier: Synthesis, characterization and mechanisms. <i>Fuel</i> , 2023, 338, 127274.	3.4	10

#	ARTICLE	IF	CITATIONS
14661	The two-pronged approach of heteroatoms and substituents to achieve a synergistic regulation of the ES IPT process in amino 2-(2-hydroxyphenyl)benzoxazole derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 291, 122318.	2.0	4
14662	The regulation of electron distribution on Fe Lewis acidic sites within silicon skeleton and its contribution to Ketoprofen ozonation. <i>Separation and Purification Technology</i> , 2023, 309, 123113.	3.9	5
14663	Synthesis of phenazone based carboxamide under thiourea reaction conditions. Molecular and crystal structure, Hirshfeld surface analysis and intermolecular interaction energies. <i>Journal of Molecular Structure</i> , 2023, 1278, 134948.	1.8	3
14664	Formation of medium- and long-chain fatty alcohols in long-term stored oil and biodiesels revealed by chemical isotope labeling-liquid chromatography-high resolution mass spectrometry. <i>Industrial Crops and Products</i> , 2023, 193, 116171.	2.5	5
14665	Understanding the electro-cocatalytic peroxy monosulfate-based systems with BDD versus DSA anodes: Radical versus nonradical dominated degradation mechanisms. <i>Separation and Purification Technology</i> , 2023, 309, 123120.	3.9	8
14666	Application of facilitated transfer mechanisms of SEBS/[P(14)666][TMPP] composite membrane on CH ₄ /N ₂ separation. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109243.	3.3	1
14667	Investigation of the synergetic regulation of O ₂ /Ar preheating treatment and sodium salt addition on semichar combustion characteristics. <i>Fuel</i> , 2023, 338, 127269.	3.4	4
14668	AIE-based fluorescence probes with different torsional configurations for monitoring human serum albumin. <i>Sensors and Actuators B: Chemical</i> , 2023, 380, 133320.	4.0	13
14669	Electrophoretic coalescence behavior of oil droplets in oil-in-water emulsions containing SDS under DC electric field: A molecular dynamics study. <i>Fuel</i> , 2023, 338, 127258.	3.4	7
14670	The influence of double lanthanide metal atoms on the stability of germanium-based clusters. <i>Chemical Physics</i> , 2023, 567, 111819.	0.9	1
14671	Screening, ACE-inhibitory mechanism and structure-activity relationship of a novel ACE-inhibitory peptide from <i>Lepidium meyenii</i> (Maca) protein hydrolysate. <i>Food Bioscience</i> , 2023, 52, 102374.	2.0	13
14672	Spectral studies, crystal structures, DNA binding, and anticancer potentials of Pd(II) complexes with iminophosphine ligands: Experimental and computational methods. <i>Inorganica Chimica Acta</i> , 2023, 547, 121368.	1.2	3
14673	Comprehensive study of substituent effects on structure and photochromic properties of 1,3-benzoxazine-4-one spiropyrans. <i>Journal of Molecular Structure</i> , 2023, 1277, 134898.	1.8	6
14674	Microscopic mechanism for the effect of potassium on heterogeneous NO _x -char(N) interaction: A theoretical account. <i>Fuel Processing Technology</i> , 2023, 242, 107657.	3.7	3
14675	$\frac{1}{4}$ -Disulfido complexes of ruthenium(III) 1,1-dithiolate [{"(Me ₃ tacn)Ru} ₂ (η^2 -S ₂ COR)(η^2 -S ₂ C=O)(η^4 -S ₂)]PF ₆ (Me ₃ tacn=1,4,7-trimethyl-1,4,7-triazacyclononane; R=Alkyl). <i>Inorganica Chimica Acta</i> , 2023, 548, 121374.	1.2	0
14676	Effect of isopropyl side chain branching and different anions on electronic structure, vibrational spectra, and hydrogen bonding of isopropyl-imidazolium-based ionic liquids: Experimental and theoretical investigations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 291, 122325.	2.0	1
14677	DFT investigations and molecular docking as potent inhibitors of SARS-CoV-2 main protease of 4-phenylpyrimidine. <i>Journal of Molecular Structure</i> , 2023, 1277, 134895.	1.8	3
14678	Side-chain engineering on triphenylamine derivative-based hole-transport materials for perovskite solar cells: Theoretical simulation and experimental exploration. <i>Dyes and Pigments</i> , 2023, 212, 111097.	2.0	2

#	ARTICLE	IF	CITATIONS
14679	Understanding the pH-dependent interaction of anthocyanin with two food-derived transferrins. <i>Food Chemistry</i> , 2023, 410, 135473.	4.2	3
14680	Tailoring the solar cell efficiency of Y-series based non-fullerene acceptors through end cap modification. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 291, 122322.	2.0	4
14681	Estimation of electrostatic and covalent contributions to the enthalpy of H-bond formation in H-complexes of 1,2,3-benzotriazole with proton-acceptor molecules by IR spectroscopy and DFT calculations. <i>Journal of King Saud University - Science</i> , 2023, 35, 102530.	1.6	10
14682	Insights into the HCl formation and volatilization mechanism from organochlorine in coal: A DFT study. <i>Fuel</i> , 2023, 338, 127271.	3.4	6
14683	Effect of Electric Field Intensity on Microphysical Parameters of Natural Ester from the Perspective of Molecular Structure. , 2022, , .		0
14684	The Conformations of Isolated Gallic Acid: A Laser-Ablation Rotational Study. <i>Molecules</i> , 2023, 28, 159.	1.7	0
14685	Obtaining advanced insensitive energetic materials by regioselectively introducing N-oxide groups onto 6-trifluoromethyl-1,2,4,5-tetrazine-3-amine. <i>Energetic Materials Frontiers</i> , 2023, 4, 30-36.	1.3	5
14686	Density Functional Study on the Hydrogenation of Phosphorus Oxides: Structural, Electronic, and Spectral Properties. <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 2928-2937.	0.1	0
14687	Interfacial charge mismatch enhanced energetic crystals for efficient energy-release and improved safety. <i>Science China Materials</i> , 0, , .	3.5	0
14688	Corrosion inhibition mechanism of imidazole ionic liquids with high temperature in 20% HCl solution. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	7
14689	Rational Hapten Design and Establishment of Broad-spectrum Indirect Competitive Enzyme-linked Immunosorbent Assay for Benzimidazoles Monitoring in Milk. <i>Food Quality and Safety</i> , 0, , .	0.6	0
14690	Molecular structure, spectroscopic and DFT computational studies on 3,9-diazatetraasteranes. <i>Chemical Papers</i> , 0, , .	1.0	0
14691	Planar Elongated B12 Structure in M3B12 Clusters (M = Cu-Au). <i>Molecules</i> , 2023, 28, 236.	1.7	0
14692	Solvent Molecule Design Enables Excellent Charge Transfer Kinetics for a Magnesium Metal Anode. <i>ACS Energy Letters</i> , 2023, 8, 780-789.	8.8	15
14693	Hydrolysis Mechanism of Carbamate Methomyl by a Novel Esterase PestE: A QM/MM Approach. <i>International Journal of Molecular Sciences</i> , 2023, 24, 433.	1.8	1
14694	Design of Lanthanide Single-Chain Magnets Based on Tubular Segment Clusters. <i>Journal of Physical Chemistry C</i> , 2023, 127, 621-626.	1.5	0
14695	Vibrational spectroscopic, electronic influences, reactivity analysis and molecular docking studies of 2-Fluoro-4-iodo-5-methylpyridine. <i>Spectroscopy Letters</i> , 2023, 56, 14-27.	0.5	6
14696	Synthesis and Chemistry of Dihydridoborate Group 7 Metal Complexes with Varied N,E-Chelated Ligands (E = O, NH, or S). <i>Inorganic Chemistry</i> , 2023, 62, 160-169.	1.9	1

#	ARTICLE	IF	CITATIONS
14697	Enzyme inhibition, molecular docking, and density functional theory studies of new thiosemicarbazones incorporating the 4-hydroxy-3,5-dimethoxy benzaldehyde motif. <i>Archiv Der Pharmazie</i> , 2023, 356, .	2.1	16
14698	Construction of Polyaromatic Hydrocarbons Containing Sulfur and Nitrogen via Controllable Domino Reactions and DFT Studies. <i>Organic Letters</i> , 2023, 25, 140-145.	2.4	3
14699	Nonfused Dimethoxybenzene Electron Acceptors in Organic Solar Cells: From Molecular Design to Structure-Performance Relationship. <i>Journal of Physical Chemistry C</i> , 2023, 127, 110-124.	1.5	3
14700	Metal clusters/modified graphene composites with enhanced CO adsorption: a density functional theory approach. <i>Journal of Nanoparticle Research</i> , 2023, 25, .	0.8	1
14701	On the relationship between the strength of bonding between topological atoms and the exchange-correlation energy. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	3
14702	Synthesis and Crystal Structure of 3-(4-Cyano-3-nitro-1H-pyrazol-5-yl)-4-nitrofurazan: Comparison of the Influence of the NO ₂ and CN Groups on Crystal Packing and Density. <i>MolBank</i> , 2023, 2023, M1533.	0.2	0
14703	The Pincer Ligand Supported Ruthenium Catalysts for Acetylene Hydrochlorination: Molecular Mechanisms from Theoretical Insights. <i>Catalysts</i> , 2023, 13, 31.	1.6	0
14704	Solid-Electrolyte Interphase for Ultra-Stable Aqueous Dual-Ion Storage. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	3
14705	Tunable Photochromism of Spirooxazine in the Solid State: A New Design Strategy Based on the Hypochromic Effect. <i>Advanced Materials</i> , 2023, 35, .	11.1	20
14707	SARS-CoV-2 M _{pro} binding profile and drug-likeness of two novel thiazole derivatives: structural elucidation, DFT studies, ADME-T and molecular docking simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 11122-11136.	2.0	5
14708	Effect of the Al Doping on the Sensing Behaviour of Carbon Nanotubes Toward Carbazochrome: a Computational Study. <i>Afyon Kocatepe University Journal of Sciences and Engineering</i> , 2022, 22, 1279-1289.	0.1	0
14709	NON-COVALENT INTERATOMIC INTERACTIONS IN TETRAFLUORO-SUBSTITUTED ZINC PHTHALOCYANINE. <i>Journal of Structural Chemistry</i> , 2022, 63, 1923-1928.	0.3	0
14710	Physical Mechanism of Spectra in Carbon Nanobelts under Quantum Size Effect. <i>Nanomaterials</i> , 2023, 13, 159.	1.9	2
14711	Improved Wide-Temperature-Range Insulation Properties of Block Polypropylene by UV-Irradiated Cografting of Maleic Anhydride and 4- <i>tert</i> -Butylstyrene. <i>ACS Applied Polymer Materials</i> , 2023, 5, 247-258.	2.0	8
14712	Two New Alkaloids and a New Butenolide Derivative from the Beibu Gulf Sponge-Derived Fungus <i>Penicillium</i> sp. SCSIO 41413. <i>Marine Drugs</i> , 2023, 21, 27.	2.2	5
14713	Atmospheric chemistry of methoxyflurane: Reaction with Cl atoms and further degradation. <i>International Journal of Chemical Kinetics</i> , 2023, 55, 129-142.	1.0	0
14714	Synthesis, Spectroscopic, Quantum Chemical, and Molecular Docking Studies of 2-Cyano- <i>N</i> -Cyclopropylacetamide and 2-Cyano- <i>N</i> -(1-Phenylethyl)Acetamide. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-27.	1.4	1
14715	DFT Study Adsorption of Hydroxychloroquine for Treatment COVID-19 by SiC Nanotube and Al, Si Doping on Carbon Nanotube Surface: A Drug Delivery Simulation. <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 2953-2966.	0.1	1

#	ARTICLE	IF	CITATIONS
14716	Synthesis and structural characterization of new spiropyran containing conjugated vinyl-3D-indolium moiety and its hydrolysis product. <i>Chemistry of Heterocyclic Compounds</i> , 2022, 58, 712-720.	0.6	2
14717	Visible Light-Active Ternary Heterojunction Photocatalyst for Efficient CO ₂ Reduction with Simultaneous Amine Oxidation and Sustainable H ₂ O ₂ Production. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 914-931.	4.0	9
14718	A new insight on the NO ⁺ CO reaction at the electronic level: homogeneous, E-R, and L ⁺ H mechanisms. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	2
14719	Regulation of external electric field on the high-energy polynitrogen compound 1,5-diaminotetrazole-4N-oxide. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	2
14720	Photocatalysis Combined with Microalgae to Promote the Degradation and Detoxification of Tetracycline Hydrochloride. <i>Bulletin of Environmental Contamination and Toxicology</i> , 2023, 110, .	1.3	4
14721	Molecular docking/dynamics simulations, MEP analysis, bioisosteric replacement and ADME/T prediction for identification of dual targets inhibitors of Parkinson TM s disease with novel scaffold. In <i>Silico Pharmacology</i> , 2023, 11, .	1.8	4
14722	Role of halogen effects and cyclic imide groups in constructing red and near-infrared room temperature phosphorescence molecules: theoretical perspective and molecular design. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 6659-6673.	1.3	5
14723	Construction of Fluorinated Propane ⁺ Trap in Metal ⁺ Organic Frameworks for Record Polymer ⁺ Grade Propylene Production under High Humidity Conditions. <i>Advanced Materials</i> , 2023, 35, .	11.1	22
14724	Photo-activated autophagy-associated tumour cell death by lysosome impairment based on manganese-doped graphene quantum dots. <i>Journal of Materials Chemistry B</i> , 2023, 11, 2466-2477.	2.9	5
14725	1,4-Phenylene incorporated decaphyrin tetrarhodium(I) complex: Synthesis, structures, and chiroptical properties. <i>Journal of Porphyrins and Phthalocyanines</i> , 2023, 27, 1059-1066.	0.4	1
14726	New kind of electride sandwich complexes based on the cyclooctatetraene ligand M ⁺ ₁ ⁺ ₂ (⁺ ₈ -C ₈ H ₈) ₂ M ⁺ ₂ ⁺ ₄ (M ⁺ ₂ ⁺ ₄) 4710-4723.	1.3	4
14727	Anion photoelectron spectroscopy and quantum chemical calculations of bimetallic niobium-aluminum clusters NbAl _n ⁺ ₄ ⁺ ₀ (n = 3-12): Identification of half-encapsulated symmetric structure for NbAl ₁₂ ⁺ ₄ . <i>Physical Chemistry Chemical Physics</i> , 0, .	1.3	0
14728	Theoretical investigation on optical properties of M ⁺ bius carbon nanobelts in one- and two-photon absorption. <i>Frontiers of Physics</i> , 2023, 18, .	2.4	1
14729	Uncovering Triradicaloid Structures in S ₁ Benzene Photochemistry**. <i>ChemPhotoChem</i> , 2023, 7, .	1.5	3
14730	Mitigation of the Toxicity of Capsaicin on Anaerobic Codigestion of Food Waste and Waste Activated Sludge Using Calcium Peroxide: A Comprehensive Analysis Using Computational and Biological Approaches. <i>ACS Sustainable Chemistry and Engineering</i> , 2023, 11, 1448-1458.	3.2	3
14731	Effects of aprotic solvents on the physicochemical properties and ferric ion oxidation activity of iron-based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
14732	Efficient narrowband green OLEDs with TADF sensitizers combining multiple charge-transfer pathways. <i>Materials Chemistry Frontiers</i> , 2023, 7, 1128-1136.	3.2	4
14733	Special structural and dynamical interplay of cyano-based novel deep eutectic solvents. <i>New Journal of Chemistry</i> , 2023, 47, 5356-5366.	1.4	4

#	ARTICLE	IF	CITATIONS
14734	Structure effects of Pt ₁₅ clusters for the oxygen reduction reaction: first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 4764-4772.	1.3	2
14735	Molecular design of dual-emission rhodamine analogs. <i>Materials Chemistry Frontiers</i> , 2023, 7, 1137-1145.	3.2	2
14736	Solid state synthesis of a fluorescent Schiff base (E)-1-(perfluorophenyl)-N-(o-toly)methanimine followed by computational, quantum mechanical and molecular docking studies. <i>Results in Chemistry</i> , 2023, 5, 100819.	0.9	6
14737	Novel Design of Co-Poly(Hydrazide Imide) and Its Complex with Cu(I) for Membrane Separation of Methanol/Dimethyl Carbonate Mixture. <i>Membranes</i> , 2023, 13, 160.	1.4	3
14738	Potential of Single Transition Metal Atom Embedded C ₂ N as Efficient Catalysts for N ₂ O Reduction: Theoretical Investigation. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	1
14739	Hierarchical self-assembly of a radical naphthalenediimide-based N-heterocyclic carbene-Au macrocycle. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 1457-1464.	3.0	2
14740	Enhancing effect of choline chloride-based deep eutectic solvents with polyols on the aqueous solubility of curcumin—insight from experiment and theoretical calculation. <i>Chinese Journal of Chemical Engineering</i> , 2023, 59, 160-168.	1.7	1
14741	Selective and Efficient Synthesis of Pine Sterol Esters Catalyzed by Deep Eutectic Solvent. <i>Molecules</i> , 2023, 28, 993.	1.7	1
14742	Assembled Bisphenol A with cyclic oligosaccharide as the controlled release complex to reduce risky effects. <i>Environmental Science and Pollution Research</i> , 2023, 30, 43300-43319.	2.7	3
14743	A Novel Source of Radicals from UV/Dichloroisocyanurate for Surpassing Abatement of Emerging Contaminants Versus Conventional UV/Chlor(am)ine Processes. <i>Environmental Science & Technology</i> , 0, , .	4.6	2
14744	Oxidorhenium(V) and Rhenium(III) Complexes with Arylselenolato and tellurolato Ligands. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	1
14745	Host molecule enhanced aggregation induced emission of chiral silver nanoclusters for achieving highly efficient circularly polarized electroluminescence. <i>Nano Research</i> , 2023, 16, 7733-7741.	5.8	5
14746	Thermoinduced Metal-to-Metal Charge Transfer in Trinuclear Metal String Complex Ru ₂ M(dpa) ₄ Cl ₂ (M=Ni, Cu, dpa=Dipyridylamido). <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
14747	Theoretical Insights into the Optical and Excited State Properties of Donor-Phenyl Bridge-Acceptor Containing Through-Space Charge Transfer Molecules. <i>Journal of Physical Chemistry A</i> , 2023, 127, 886-893.	1.1	3
14748	Designing of asymmetric non-fullerene based acceptor materials by re-modification of spacers with PCEA for organic solar cell. <i>Optik</i> , 2023, 278, 170602.	1.4	7
14749	A Deep Understanding on the Effective Generation of Twisted Intramolecular Charge Transfer by Protonation in Thiazolo[5,4-d]thiazole Derivatives. <i>Journal of Physical Chemistry A</i> , 2023, 127, 902-912.	1.1	2
14751	Inorganic Solid Electrolyte Interphase Engineering Rationales Inspired by Hexafluorophosphate Decomposition Mechanisms. <i>Journal of Physical Chemistry C</i> , 2023, 127, 1744-1751.	1.5	4
14752	Electron-Coupled Proton Transfer Governed Magnetic Spin Couplings and Switching in Defect Nano Silicon Carbide. <i>Journal of Physical Chemistry C</i> , 2023, 127, 2012-2024.	1.5	0

#	ARTICLE	IF	CITATIONS
14753	Understanding the mechanism and regio- and stereo selectivity of [3+2] cycloaddition reactions between substituted azomethine ylide and 3,3,3-trifluoro-1-nitroprop-1-ene, within the molecular electron density theory. <i>Journal of Computational Chemistry</i> , 0, .	1.5	1
14754	Computational Investigation of a Series of Small Molecules as Potential Compounds for Lysyl Hydroxylase-2 (LH2) Inhibition. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 986-1001.	2.5	4
14755	CO ₂ Aggregation on Monoethanolamine: Observations from Rotational Spectroscopy. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	1
14756	OH radical-initiated single-electron transfer for accelerated degradation via carbocation intermediates. <i>Chemical Science</i> , 2023, 14, 2229-2236.	3.7	1
14757	Open-Cage Fullerene as a Selective Molecular Trap for LiF/[BeF] ⁺ . <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	12
14758	Intermolecular interactions between the heavy-atom analogues of acetylene T ₂ H ₂ (T = Si, Ge, Sn, Pb) and HCN. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	3
14760	Molecular structure and spectroscopic properties of two radicals of C ₄ H ₂ N: a DFT study. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	0
14762	Unusually Kinetically Inert Monocationic Neptunyl Complex with a Fluorescein-Modified 1,10-Phenanthroline-2,9-dicarboxylate Ligand: Specific Separation and Detection in Gel Electrophoresis. <i>Inorganic Chemistry</i> , 2023, 62, 730-738.	1.9	3
14763	Aryl Boronic Acids in Columnar Stacked Co-crystalline Materials: Key Factors Governing the Assembly with Quinones. <i>ChemPhysChem</i> , 0, .	1.0	0
14764	Unraveling Weak Interaction of Kinematic Viscosity of Fatty Acid Methyl Esters in Natural Ester Insulating Oils. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2023, 30, 528-535.	1.8	0
14765	Inquiring into geometric structures and electronic properties of sodium doped boron clusters: DFT study of NaB _n (<i>n</i> = 12) clusters. <i>Molecular Physics</i> , 2023, 121, .	0.8	3
14766	Effect of different end-capped donor moieties on non-fullerenes based non-covalently fused-ring derivatives for achieving high-performance NLO properties. <i>Scientific Reports</i> , 2023, 13, .	1.6	30
14767	Mechanisms and energetics for hydrogen abstraction of thymine photosensitized by benzophenone from theoretical principles. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 6467-6472.	1.3	2
14768	A fluoride-free siliceous STW-type zeolite synthesized using a designed organic structure-directing agent. <i>Chemical Communications</i> , 2023, 59, 1649-1652.	2.2	3
14769	Unraveling the effect of solvents on the excited state dynamics of C540A by experimental and theoretical study. <i>RSC Advances</i> , 2023, 13, 4924-4931.	1.7	2
14770	Increasing the limits of energy and safety in tetrazoles: dioximes as unusual precursors to very thermostable and insensitive energetic materials. <i>Journal of Materials Chemistry A</i> , 2023, 11, 12896-12901.	5.2	16
14771	Molecular dynamic, Hirshfeld surface, molecular docking and drug likeness studies of a potent anti-oxidant, anti-malaria and anti-inflammatory medicine: Pyrogallol. <i>Results in Chemistry</i> , 2023, 5, 100763.	0.9	4
14772	Assessing Solvate Prediction Approaches: A Case of Spironolactone. <i>Crystal Growth and Design</i> , 2023, 23, 832-841.	1.4	4

#	ARTICLE	IF	CITATIONS
14773	Side-Chain Methylthio-Based Position Isomerism of Hole-Transport Materials for Perovskite Solar Cells: From Theoretical Simulation to Experimental Characterization. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	8
14774	Stability and hydrogen storage properties of Sc ₆ O ₈ and Y ₆ O ₈ cage-like complexes. <i>International Journal of Hydrogen Energy</i> , 2023, .	3.8	0
14775	f-Aromatic MA ₆ S ₆ (M = Ni, Pd, Pt) Stars Containing Planar Hexacoordinate Transition Metals. <i>Molecules</i> , 2023, 28, 942.	1.7	3
14776	Tuning Molecular Electron Affinities against Atomic Electronegativities by Spatial Expansion of a System. <i>ChemPhysChem</i> , 2023, 24, .	1.0	4
14777	Experimental and theoretical analysis for the structural, FT-IR, NLO, NBO and RDG properties of lindane using DFT technique. <i>AIP Conference Proceedings</i> , 2023, , .	0.3	2
14778	Protonated methylcyclopropane is an intermediate providing complete ¹³ C-label scrambling at C ₄ olefin isomerization in zeolite. <i>Chem Catalysis</i> , 2023, 3, 100503.	2.9	1
14779	5-Vinyl-1H-tetrazole. <i>MolBank</i> , 2023, 2023, M1565.	0.2	0
14780	Mechanistic insights into aerobic oxidative cleavage of glycol catalyzed by an Anderson-type polyoxometalate [Mo ₆ O ₂₄] ⁵⁻ . <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	2
14781	Manifestation of Hydrogen Bonding and Exciton Delocalization on the Absorption and Two-Dimensional Electronic Spectra of Chlorosomes. <i>Journal of Physical Chemistry B</i> , 2023, 127, 1097-1109.	1.2	3
14782	Revisiting the Sweet Taste Receptor T1R2-T1R3 through Molecular Dynamics Simulations Coupled with a Noncovalent Interactions Analysis. <i>Journal of Physical Chemistry B</i> , 2023, 127, 1110-1119.	1.2	2
14783	Theoretical exploration of noncovalent interactions in Sc ₂ C ₂ @C ₂ (C ₂ = 40, 41, and 42)Š, [12]CPP, PF[12]CPP. <i>RSC Advances</i> , 2023, 13, 4553-4563.	1.7	1
14784	A Pyridyl-1,2-azaborine Ligand for Phosphorescent Neutral Iridium(III) Complexes. <i>Inorganic Chemistry</i> , 2023, 62, 2456-2469.	1.9	5
14785	Interpretable Machine Learning of Two-Photon Absorption. <i>Advanced Science</i> , 2023, 10, .	5.6	8
14786	Multifunctional Regulation of Highly Orientated Tin-Lead Alloyed Perovskite Solar Cells. <i>ACS Energy Letters</i> , 2023, 8, 1068-1075.	8.8	17
14787	Construction of High-Performance Energetic MOFs: C ₄ N ₈ O ₄ and C ₃ N ₄ O ₄ with Their Derivatives, Compared with Their Energetic Salts. <i>Crystal Growth and Design</i> , 2023, 23, 820-831.	1.4	4
14788	Discovery of N-Lactoyl-Trp as a Bitterness Masker via Structure-Based Virtual Screening and a Sensory Approach. <i>Journal of Agricultural and Food Chemistry</i> , 2023, 71, 2082-2093.	2.4	6
14789	z-Type Tilted Quasi-One-Dimensional Assembly of Actinide-Embedded Coinage Metal Near-Plane Superatoms and Their Optical Properties. <i>Advanced Science</i> , 2023, 10, .	5.6	3
14790	Packing-induced selectivity switching in molecular nanoparticle photocatalysts for hydrogen and hydrogen peroxide production. <i>Nature Nanotechnology</i> , 2023, 18, 307-315.	15.6	29

#	ARTICLE	IF	CITATIONS
14791	One-Dimensional 1D Conjugated Conductive Metal-Organic Framework with Dual Redox-Active Sites for High-Capacity and Durable Cathodes for Aqueous Zinc Batteries. <i>ACS Nano</i> , 2023, 17, 3077-3087.	7.3	31
14792	Two-dimensional semiconducting Cu(I)/Sb(III) bimetallic hybrid iodides with a double perovskite structure and photocurrent response. <i>Nanoscale</i> , 2023, 15, 5265-5273.	2.8	1
14793	Determination of the acidic structure and Lewis activity in an Fe-based ionic liquid with slope analysis of the quantitative pyridine-IR spectrum. <i>New Journal of Chemistry</i> , 2023, 47, 4761-4774.	1.4	0
14794	Preparation of multi-functional type coordination compounds: spanning the quantitative restriction of oxidizing groups. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 1475-1484.	3.0	3
14796	Computational study of the interaction of the psychoactive amphetamine with 1,2-indanedione and 1,8-diazafuoren-9-one as fingerprinting reagents. <i>RSC Advances</i> , 2023, 13, 4077-4088.	1.7	0
14797	Controlling the Triplet Potential Energy Surface of Bimetallic Platinum(II) Complex by Constructing Structure-Property Relationship: A Theoretical Exploration. <i>Inorganic Chemistry</i> , 2023, 62, 2440-2455.	1.9	2
14798	In vitro contraceptive activities, molecular docking, molecular dynamics, MM-PBSA, non-covalent interaction and DFT studies of bioactive compounds from <i>Aegle marmelos</i> . Linn., leaves. <i>Frontiers in Chemistry</i> , 0, 11, .	1.8	2
14799	Indication of 3 ¹⁰ -Helix Structure in Gas-Phase Neutral Pentaalanine. <i>Journal of Physical Chemistry A</i> , 2023, 127, 938-945.	1.1	0
14800	Inverse Sandwich Arene-Bridged Titanium Complexes Supported by a Bulky Tridentate [O, P, O] Ligand. <i>Organometallics</i> , 2023, 42, 1243-1247.	1.1	4
14801	Construction of Efficient D-A-Type Photocatalysts by N Bond Substitution for Water Splitting. <i>Macromolecules</i> , 2023, 56, 858-866.	2.2	7
14802	Assembly Rules and Dehydration Mechanism of an Unconventional Hydrate: On the Complexity of the Hydrates of Creatine Phosphate Sodium. <i>Crystal Growth and Design</i> , 0, , .	1.4	1
14803	Chemical insights from the Source Function reconstruction of scalar fields relevant to chemistry. , 2023, , 269-333.		0
14804	Valeramide and Halo-phenol in a Non-polar Liquid: DFT Based Characterization and Reactivity, Non-covalent Interaction, and Dielectric Relaxation Studies. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-26.	1.4	2
14805	Hydrophobic Deep eutectic Solvents based on cineole and organic acids. <i>Journal of Molecular Liquids</i> , 2023, 377, 121322.	2.3	3
14806	Selective Chelation of the Exotic Meitner- ¹⁹⁷ Auger Emitter Mercury ¹⁹⁷ om/g with Sulfur-Rich Macrocyclic Ligands: Towards the Future of Theranostic Radiopharmaceuticals. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	2
14807	Rational design of non-fullerene acceptors <i>via</i> side-chain and terminal group engineering: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7994-8004.	1.3	3
14808	Mechanistic insights into the pyrolysis of poly (vinyl chloride). <i>Journal of Polymer Research</i> , 2023, 30, .	1.2	3
14809	Reduction-Activatable Fluorogenic Nanobody for Targeted and Low-Background Bioimaging. <i>Analytical Chemistry</i> , 2023, 95, 2804-2811.	3.2	3

#	ARTICLE	IF	CITATIONS
14810	A new fan-like adaptive porous organic cage for the structure determination of liquid perfume molecules. <i>Organic Chemistry Frontiers</i> , 0, , .	2.3	0
14811	Density Functional Study to Investigate the Ability of $(ZnS)_n$ ($n = 1-12$) Clusters Removing HgO, HgCl, and HgCl ₂ via Electron Localization Function and Non-covalent Interactions Analyses. <i>Molecules</i> , 2023, 28, 1214.	1.7	1
14812	Crystal growth, optoelectronic and biological properties of acetamidinium compounds: experimental and computational approaches. <i>Journal of Materials Science: Materials in Electronics</i> , 2023, 34, .	1.1	5
14813	Simultaneous Hydrogen Bonds with Different Binding Modes: the Acceptor chooses but the Donor chooses. <i>Chemistry - A European Journal</i> , 0, , .	1.7	1
14814	Catalytic Enantioselective Allylboration and Related Reactions of Isatins Promoted by Chiral BINOLs: Scope and Mechanistic Studies. <i>Journal of Organic Chemistry</i> , 2023, 88, 1469-1492.	1.7	0
14815	Signatures of Chemical Dopants in Simulated Resonance Raman Spectroscopy of Carbon Nanotubes. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 1182-1191.	2.1	10
14816	Tetranuclear Copper(I) and Silver(I) Pyrazolate Adducts with 1,1'-Dimethyl-2,2'-bibenzimidazole: Influence of Structure on Photophysics. <i>Molecules</i> , 2023, 28, 1189.	1.7	3
14817	Perfect Core-shell Octahedral B_{38}^{+} , $Be@B_{38}$, and $Zn@B_{38}$ with an Octahedral Coordinate Center as Superatoms Following the Octet Rule. <i>ChemPhysChem</i> , 2023, 24, .	1.0	1
14818	Enhanced triplet-triplet annihilation upconversion luminescence through conformational restriction based on donor-acceptor heavy atom molecules. <i>ChemPhotoChem</i> , 0, , .	1.5	2
14819	2D coordination sheets based on tetranuclear cuprofullerene pentafluorobenzoate and their electronic properties. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 1731-1738.	3.0	3
14820	CO ₂ Aggregation on Monoethanolamine: Observation from Rotational Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 0, , .	7.2	2
14821	Monomer morphology selection rules for an accurate design of bulk heterojunction: An updated theoretical account. <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	0
14822	Design of A type carbon nanohoops with enhanced nonlinear optical response: a size-dependent effect study. <i>New Journal of Chemistry</i> , 2023, 47, 5390-5398.	1.4	3
14823	Synthesis, Structural and Theoretical Analyses of $C_{60}N_4I$ Halogen-Bonded Liquid Crystalline Complexes of 4-Cyano-4'-alkoxy Biphenyl Systems. <i>Crystal Growth and Design</i> , 0, , .	1.4	2
14824	Combined effects of the lewis acidity and electric field of proximal redox innocent metal ions on the redox potential of vanadyl Schiff base complexes: an experimental and theoretical study. <i>Dalton Transactions</i> , 2023, 52, 3097-3110.	1.6	2
14825	Adsorption of Molnupiravir anti-COVID-19 drug over $B_{12}N_{12}$ and $Al_{12}N_{12}$ nanocarriers: a DFT study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 12923-12937.	2.0	1
14826	Insight into the Varying Reactivity of Different Catalysts for CO ₂ Cycloaddition into Styrene Oxide: An Experimental and DFT Study. <i>International Journal of Molecular Sciences</i> , 2023, 24, 2123.	1.8	1
14827	Prediction of donor-acceptor-type novel noble gas complexes in the triplet electronic state. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 6987-6994.	1.3	2

#	ARTICLE	IF	CITATIONS
14828	Molecular Dynamics Study on the Reaction of RDX Molecule with Si Substrate. ACS Omega, 2023, 8, 4270-4277.	1.6	0
14830	A comparative analysis of the influence of hydrofluoroethers as diluents on solvation structure and electrochemical performance in non-flammable electrolytes. Journal of Materials Chemistry A, 2023, 11, 4111-4125.	5.2	8
14831	Synthesis and Theoretical and Photophysical Study on a Series of Neutral Ruthenium(II) Complexes with Donor–Metal–Acceptor Configuration. Inorganic Chemistry, 2023, 62, 1476-1487.	1.9	3
14832	Spirocyclic rhodamine B benzoisothiazole derivative: a multi-stimuli fluorescent switch manifesting ethanol-responsiveness, photo responsiveness, and acidochromism. RSC Advances, 2023, 13, 5134-5148.	1.7	2
14833	Theoretical Kinetic Studies on Thermal Decomposition of Glycerol Trinitrate and Trimethylolethane Trinitrate in the Gas and Liquid Phases. Journal of Physical Chemistry A, 2023, 127, 1283-1292.	1.1	2
14834	Theoretical study of the interaction of trimethylamine with aluminium nitride nanotube and gallium-doped aluminium nitride nanotube. Bulletin of Materials Science, 2023, 46, .	0.8	3
14835	In Silico Designing of Thieno[2,3- <i>b</i>]thiophene Core-Based Highly Conjugated, Fused-Ring, Near-Infrared Sensitive Non-fullerene Acceptors for Organic Solar Cells. ACS Omega, 2023, 8, 4767-4781.	1.6	8
14836	Prediction of the enantiomeric excess value for asymmetric transfer hydrogenation based on machine learning. Organic Chemistry Frontiers, 2023, 10, 1456-1462.	2.3	1
14837	Efficient thermally activated delayed fluorescence emitters with regioisomeric effects for red/near-infrared organic light-emitting diodes. Materials Chemistry Frontiers, 2023, 7, 1633-1641.	3.2	5
14838	Supramolecular Assemblies in Pyridine- and Pyrazole-Based Coordination Compounds of Co(II) and Ni(II): Characterization, Hirshfeld Analysis and Theoretical Studies. Crystals, 2023, 13, 203.	1.0	2
14839	Quantum modeling of dimethoxyl-indaceno dithiophene based acceptors for the development of semiconducting acceptors with outstanding photovoltaic potential. RSC Advances, 2023, 13, 4641-4655.	1.7	5
14840	Influence of non-covalent interactions on the coordination geometry of Ni(II) in Ni(II)–M(II) complexes (M = Zn and Hg) with a salen-type N ₂ O ₂ Schiff base ligand and thiocyanate ion as the coligand. CrystEngComm, 2023, 25, 1393-1402.	1.3	1
14841	Single and dual metal atom catalysts for enhanced singlet oxygen generation and oxygen reduction reaction. Journal of Materials Chemistry A, 2023, 11, 7513-7525.	5.2	6
14842	Mechanism of Radical Initiation and Transfer in Class Id Ribonucleotide Reductase Based on Density Functional Theory. Inorganic Chemistry, 2023, 62, 2561-2575.	1.9	0
14843	Intermolecular through-space charge transfer enabled by bicomponent assembly for ultrasensitive detection of synthetic cannabinoid JWH-018. Aggregate, 2023, 4, .	5.2	5
14844	Systematic Study of Podand Molecules for Synergistic Halogen and Hydrogen Bond-Driven Anion Recognition in the Solid State. Chemistry - an Asian Journal, 2023, 18, .	1.7	1
14845	Supramolecular Enhancement of Charge Transport through Pillar[5]arene-Based Self-Assembled Monolayers. Angewandte Chemie, 2023, 135, .	1.6	0
14846	A comparative DFT study on Al- and Si- doped single-wall carbon nanotubes (SWCNTs) for Ribavirin drug sensing and detection. Materials Science in Semiconductor Processing, 2023, 158, 107360.	1.9	3

#	ARTICLE	IF	CITATIONS
14847	Adjusting hydrophilicity of g-C ₃ N ₄ based heterojunction photocatalyst through sulfur-impregnation to enhancing degradation effect of tetracycline. <i>Materials Science in Semiconductor Processing</i> , 2023, 158, 107351.	1.9	0
14848	Effects of solvent polarity on the novel excited-state intramolecular thiol proton transfer and photophysical property compared with the oxygen proton transfer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 293, 122475.	2.0	29
14849	Unveiling the gemcitabine drug complexation with cucurbit[n]urils (n=6, 8): a computational analysis. <i>Structural Chemistry</i> , 2023, 34, 1869-1882.	1.0	0
14850	Migration detection of six aromatic amines in polyamide food contact materials by HPLC after molecularly imprinted polymer pipette tip solid phase extraction. <i>Food Packaging and Shelf Life</i> , 2023, 36, 101029.	3.3	4
14851	A novel series of thiosemicarbazone hybrid scaffolds: Design, synthesis, DFT studies, metabolic enzyme inhibition properties, and molecular docking calculations. <i>Journal of Molecular Structure</i> , 2023, 1280, 135077.	1.8	16
14852	Theoretical insight on the importance of CH \cdots O and NH \cdots O interactions in the crystal packing of a decavanadate synthesized from a simple V(IV) precursor. <i>Inorganica Chimica Acta</i> , 2023, 549, 121411.	1.2	0
14853	The chemical reactivity and antimalarial investigation of crystal structure (2E)-3-(biphenyl-4-yl)-1-(4-chlorophenyl)prop-2-en-1-one and hydroxyphenyl, nitrophenyl substituted chalcone derivative molecules. <i>Journal of Molecular Structure</i> , 2023, 1280, 135001.	1.8	3
14854	The influence of N \cdots N hydrogen bonding in π -stacked parallel displaced geometry of nitrobenzene dimers: Evidence using matrix isolation infrared spectroscopy and ab initio computations. <i>Journal of Molecular Structure</i> , 2023, 1279, 135022.	1.8	1
14855	A DFT study of hydrogen adsorption on Pt modified carbon nanocone structures: Effects of modification and inclination of angles. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 23077-23088.	3.8	5
14856	Quantitative structure-activity relationship models for predicting apparent rate constants of organic compounds with ferrate (VI). <i>Science of the Total Environment</i> , 2023, 871, 162043.	3.9	2
14857	Photo-induced heterogeneous regeneration of Fe(II) in Fenton reaction for efficient polycyclic antibiotics removal and in-depth charge transfer mechanism. <i>Journal of Colloid and Interface Science</i> , 2023, 638, 768-777.	5.0	4
14858	Highly efficient extractive desulfurization by specific functionalized porous ionic liquids via C-H \cdots N interactions. <i>Fuel Processing Technology</i> , 2023, 243, 107687.	3.7	13
14859	The impact of π - π stacking interactions on photo-physical properties of hydroxyanthraquinones. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 292, 122453.	2.0	2
14860	Dissecting amide-I vibrations in histidine dipeptide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 292, 122424.	2.0	0
14861	Improved surface flashover voltage of epoxy following polythiourea-assisted coating with high gas adsorption ability. <i>Applied Surface Science</i> , 2023, 618, 156546.	3.1	8
14862	A new Schiff base derived from 5-(thiophene-2-yl)oxazole as a fluorescence sensor for monitoring indium and ferric ions sequentially and its application. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 292, 122376.	2.0	1
14863	Computational approach to understanding the structures, properties, and supramolecular chemistry of pagoda[n]arenes. <i>Journal of Molecular Structure</i> , 2023, 1281, 135073.	1.8	1
14864	Influence of hydroxyl group in stabilizing the Schiff base crystal structure: Crystal structure, computational and molecular docking studies. <i>Journal of Molecular Structure</i> , 2023, 1280, 135054.	1.8	3

#	ARTICLE	IF	CITATIONS
14865	New thioether-hydrazone based ONS donor Schiff base and its Pd(II) complex: Synthesis, crystal structure, thermal analysis, hirshfeld surface analysis, quantum chemical studies and molecular docking. <i>Journal of Molecular Structure</i> , 2023, 1281, 135041.	1.8	0
14866	A theoretical insight into the mechanism of NO heterogeneous reduction on char surface: The catalytic effect of potassium. <i>Fuel</i> , 2023, 340, 127568.	3.4	3
14867	Density functional theory (DFT) computation of pristine and metal-doped MC59 (M = Au, Hf, Hg, Ir) fullerenes as nitrosourea drug delivery systems. <i>Materials Science in Semiconductor Processing</i> , 2023, 158, 107362.	1.9	20
14868	The characteristics of ultraviolet absorption and electronic excitation of sulfate at high concentrations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 293, 122455.	2.0	3
14869	Preparation, characterization, and crystal structures of novel sophocarpine salts with improvements on stability and solubility. <i>Journal of Molecular Structure</i> , 2023, 1279, 134992.	1.8	0
14870	Experimental and theoretical studies of a thiourea derivative: 1-(4-chloro-benzoyl)-3-(2-trifluoromethyl-phenyl)thiourea. <i>Journal of Molecular Structure</i> , 2023, 1279, 134996.	1.8	4
14871	Computational Investigation of Stability and Molecular Properties of C18BN Corannulene Molecules. <i>Russian Journal of Inorganic Chemistry</i> , 2022, 67, S158-S168.	0.3	1
14872	Effect of Ni-Doping on the Hydrogen Storage Properties of Nanoscale MgH ₂ . <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 3220-3231.	0.1	0
14873	Pressure-induced room-temperature phosphorescence enhancement based on purely organic molecules with a folded geometry. <i>Chemical Science</i> , 2023, 14, 2640-2645.	3.7	12
14874	Why does the cyclic pentazolate anion fail to undergo <i>N</i> -oxidization in oxone solution?. <i>New Journal of Chemistry</i> , 2023, 47, 5616-5620.	1.4	0
14875	Supramolecular detoxification of nitrogen mustard via "guest encapsulation by carboxylatopillar[5]arene. <i>Journal of Materials Chemistry B</i> , 2023, 11, 2706-2713.	2.9	6
14876	Exploring multifunctional applications of a luminescent covalent triazine polymer in acid vapour sensing, CO ₂ capture, dye removal, and turn-off fluorescence sensing of dichromate ions. <i>Materials Chemistry Frontiers</i> , 2023, 7, 1831-1840.	3.2	3
14877	Accelerated screening and assembly of promising MOFs with open Cu sites for isobutene/isobutane separation using a data-driven approach. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8608-8623.	1.3	3
14878	Terahertz spectroscopic characterization and DFT calculations of vanillin cocrystals with nicotinamide and isonicotinamide. <i>CrystEngComm</i> , 2023, 25, 2038-2051.	1.3	0
14879	The importance of spodium bonds, H-bonds and π -stacking interactions in the solid state structures of four zinc complexes with tetradentate secondary diamine ligands. <i>New Journal of Chemistry</i> , 2023, 47, 9346-9363.	1.4	4
14880	Influence of stabilisers on the catalytic activity of supported Au colloidal nanoparticles for the liquid phase oxidation of glucose to glucaric acid: understanding the catalyst performance from NMR relaxation and computational studies. <i>Green Chemistry</i> , 2023, 25, 2640-2652.	4.6	6
14881	New nitrosyl ruthenium complexes with combined activities for multiple cardiovascular disorders. <i>Dalton Transactions</i> , 2023, 52, 5176-5191.	1.6	2
14882	The dynamical temporal behaviors of guanine-cytosine coherent charge transfer. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10661-10670.	1.3	3

#	ARTICLE	IF	CITATIONS
14883	Structural analysis of potassium borate solutions. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 12207-12219.	1.3	2
14884	Effects of aggregation on the structures and excited-state absorption for zinc phthalocyanine. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10278-10287.	1.3	0
14885	High-performing, insensitive and thermally stable energetic materials from zwitterionic <i>gem</i> -dinitromethyl substituted C=C bonded 1,2,4-triazole and 1,3,4-oxadiazole. <i>Chemical Communications</i> , 2023, 59, 4324-4327.	2.2	15
14886	Carbonyl (C=O)/N-based thermally activated delayed fluorescent materials with high efficiency and fast reverse intersystem crossing rate: a theoretical design and study. <i>New Journal of Chemistry</i> , 2023, 47, 7686-7693.	1.4	2
14887	Halogen bonds regulating structures and optical properties of hybrid iodobismuthate perovskites. <i>Dalton Transactions</i> , 0, , .	1.6	2
14888	Mechanistic study on the structure–property relationship of flexible organic crystals. <i>CrystEngComm</i> , 2023, 25, 2600-2606.	1.3	3
14889	Modulation of chiral spectral deflection by van der Waals force-induced molecular electropolarization in catenane oligomers. <i>RSC Advances</i> , 2023, 13, 11055-11061.	1.7	1
14890	Combined experimental and theoretical studies of conformationally diverse (thio)semicarbazone-based semiconducting materials. <i>CrystEngComm</i> , 2023, 25, 2133-2143.	1.3	1
14891	<i>N</i> -Cyanomethylmethanimine tethered anthracene dimer: concise synthesis, conformational properties and photoinduced configurational isomerization. <i>New Journal of Chemistry</i> , 2023, 47, 6708-6720.	1.4	2
14892	Optimized Geometry, NBO, MEP, Docking Analysis and Antimicrobial Activity of (2R,3R)-Butanediol Bis(methanesulfonate). <i>Asian Journal of Chemistry</i> , 2023, 35, 748-754.	0.1	0
14893	To dimerize or not: <i>para</i> -aminothiophenol on a bismuth heterostructure. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 9569-9575.	1.3	0
14894	Diamondoid ether clusters in helium nanodroplets. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 11951-11958.	1.3	3
14895	Photo-induced defluorination acyl fluoride exchange as a fluorogenic photo-click reaction for photo-affinity labeling. <i>Chemical Science</i> , 2023, 14, 3630-3641.	3.7	1
14896	Visualization Analysis of Weak Interactions in Chemical Systems. , 2024, , 240-264.		10
14897	Atomic charges in molecules defined by molecular real space partition into atomic subspaces. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 9020-9030.	1.3	4
14898	Group-10 ĩ-hole ^d _z ² [M ^{II}] interactions: a theoretical study of model systems inspired by CSD structures. <i>Dalton Transactions</i> , 0, , .	1.6	2
14899	Experimental spectral investigations for structural, electronic, topological properties and molecular docking studies of 2-cyclohexylidene hydrazine carbaxamide. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100902.	1.3	1
14900	Molecular Dynamics Simulation of Adsorption and Absorption Behavior of Shale Oil in Realistic Kerogen Slits. <i>Energy & Fuels</i> , 2023, 37, 3654-3671.	2.5	5

#	ARTICLE	IF	CITATIONS
14901	Solubility and Antioxidant Activity of 1,2-Dihydro-2-Methyl-2-Phenyl-3H-Indole-3-One-1-Oxyl Hosted at Randomly Methylated- β -cyclodextrin: A Computational Investigation. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-13.	1.4	0
14902	Synthesis and Characterization of Novel Triphenylamine-Containing Electrochromic Polyimides with Benzimidazole Substituents. <i>Molecules</i> , 2023, 28, 2029.	1.7	3
14903	How temperature and hydrostatic pressure impact organic room temperature phosphorescence from H-aggregation of planar triarylboranes and the application in bioimaging. <i>Science China Chemistry</i> , 0, , .	4.2	2
14904	Excited-State Descriptors for High-Throughput Screening of Efficient Electro-Fluorescent Materials. <i>Chemistry of Materials</i> , 2023, 35, 1827-1833.	3.2	3
14905	Theoretical Insights into the Substitution Effect of Phenanthroline Derivatives on Am(III)/Eu(III) Separation. <i>Inorganic Chemistry</i> , 2023, 62, 2705-2714.	1.9	14
14906	Discovery of novel anti-cyanobacterial allelochemicals by multi-conformational QSAR approach. <i>Aquatic Toxicology</i> , 2023, 256, 106420.	1.9	2
14907	Role of anchoring groups on the light harvesting and optoelectronic properties of triphenylamine derivatives: insights from theory. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	1
14908	Tunable nonradiative recombination dynamics and charge injection of graphene quantum dots for energy conversion applications by controllable functionalization. <i>Physica Scripta</i> , 2023, 98, 045009.	1.2	2
14909	Consequences of Overfitting the van der Waals Radii of Ions. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 2064-2074.	2.3	4
14910	Lead Sequestration in Perovskite Photovoltaic Device Encapsulated with Water-Proof and Adhesive Poly(ionic liquid). <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 13637-13643.	4.0	3
14911	Three-Dimensional-Printed Device for In Situ Monitoring of an Organic Redox-Flow Battery via NMR/MRI. <i>Analytical Chemistry</i> , 2023, 95, 6020-6028.	3.2	1
14912	Regioisomeric Benzidine-Fullerenes: Tuning of the Diverse Hole-Distribution to Influence Charge Separation Patterns. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	1
14913	A study of the oxidation mechanism of the organic pigment indigo in grottoes murals by ozone under dark conditions. <i>Heritage Science</i> , 2023, 11, .	1.0	1
14914	Impact of Polarization Effect on Exciton Binding Energies and Charge Transport for the Crystals of Chlorinated ITIC Derivatives. <i>Journal of Physical Chemistry C</i> , 2023, 127, 5597-5603.	1.5	13
14915	Catalyst-Free Photochemical Activation of Peroxymonosulfate in Xanthene-Rich Systems for Fenton-Like Synergistic Decontamination: Efficacy of Proton Transfer Process. <i>Angewandte Chemie</i> , 0, , .	1.6	0
14916	Non-bonding interaction of dual atom catalysts for enhanced oxygen reduction reaction. <i>Nano Energy</i> , 2023, 108, 108218.	8.2	17
14917	Solvents incubated π - π stacking in hole transport layer for perovskite-silicon 2-terminal tandem solar cells with 27.21% efficiency. <i>Journal of Energy Chemistry</i> , 2023, 82, 25-30.	7.1	2
14918	Transition Metal-Decorated B ₁₂ N ₁₂ -X (X = Au, Cu, Ni, Os, Pt, and Zn) Nanoclusters as Biosensors for Carboplatin. <i>ACS Omega</i> , 2023, 8, 10006-10021.	1.6	24

#	ARTICLE	IF	CITATIONS
14919	Construction of a OD/3D AgI/MOF-808 photocatalyst with a one-photon excitation pathway for enhancing the degradation of tetracycline hydrochloride: Mechanism, degradation pathway and DFT calculations. <i>Chemical Engineering Journal</i> , 2023, 460, 141842.	6.6	22
14920	Benzotriazole-based structure in porous organic polymer enhancing O ₂ activation for high-efficient degradation of tetracycline under visible light. <i>Chemical Engineering Journal</i> , 2023, 460, 141810.	6.6	4
14921	Comparative analysis of the reactivity of anthocyanidins, leucoanthocyanidins, and flavonols using a quantum chemistry approach. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	1
14922	Molecularly imprinted MOFs-driven carbon nanofiber for sensitive electrochemical detection and targeted electro-Fenton degradation of perfluorooctanoic acid. <i>Separation and Purification Technology</i> , 2023, 310, 123257.	3.9	11
14923	Lactim or lactam? A theoretical study on the possibility of excited-state intramolecular proton transfer in hydroxyphenyl-imidazo-isoindoles. <i>Journal of Luminescence</i> , 2023, 260, 119850.	1.5	0
14924	â€œNanomagnet-inspiredâ€ design on molecularly imprinted nanofiber membrane: Mechanisms for improved transport selectivity of sufficient specific sites. <i>Journal of Membrane Science</i> , 2023, 672, 121467.	4.1	5
14925	Spectroscopic study on size-dependent optoelectronics of N-type ultra-high conductive polymer PBFDO. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, , 122744.	2.0	2
14926	Unveiling the thermodynamic and molecular mechanisms for the separation of diethoxymethane and ethanol azeotrope by deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2023, 376, 121451.	2.3	1
14927	Study of the Sensing Kinetics of G Protein-Coupled Estrogen Receptor Sensors for Common Estrogens and Estrogen Analogs. <i>Molecules</i> , 2023, 28, 3286.	1.7	2
14928	Contribution of air-water interface in removing PFAS from drinking water: Adsorption, stability, interaction and machine learning studies. <i>Water Research</i> , 2023, 236, 119947.	5.3	5
14929	Theoretical exploration of the mechanisms on the iron complexes catalyzed ammonia borane dehydrogenation and polyaminoborane formation. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 23633-23644.	3.8	1
14930	A green and novel strategy based on CO ₂ -responsive surfactant-functionalized multi-walled carbon nanotubes with microwave-ultrasound assistant to improve extraction and enrichment of phytochemicals from plant waste. <i>Industrial Crops and Products</i> , 2023, 194, 116294.	2.5	3
14931	Efficient nitrous oxide capture by cationic forms of FAU and CHA zeolites. <i>Chemical Engineering Journal</i> , 2023, 462, 142300.	6.6	1
14932	Humidity-resistant organic room-temperature phosphorescence materials synthesized using catalyst-free click reaction. <i>Chemical Engineering Journal</i> , 2023, 462, 142198.	6.6	4
14933	Tuning Solid-State Emission of 9-Anthraldehyde through Cocrystal Engineering. <i>Crystals</i> , 2023, 13, 595.	1.0	2
14934	Oxygen vacancy construction and in situ reduction of metal ions to enhance the photocatalytic performance of Bi ₅ Nb ₃ O ₁₅ . <i>Separation and Purification Technology</i> , 2023, 311, 123276.	3.9	5
14935	Microstructural Evolution of Zincâ€on Species from Aqueous to Hydrated Eutectic Electrolyte for Znâ€on Batteries. <i>ChemSusChem</i> , 2023, 16, .	3.6	2
14936	A sensitive fluorescence assay based on aggregation-induced emission by copper-free click reaction for rapid ctDNA detection. <i>Talanta</i> , 2023, 259, 124562.	2.9	2

#	ARTICLE	IF	CITATIONS
14937	Interaction of 5-Fluorouracil on the Surfaces of Pristine and Functionalized Ca ₁₂ O ₁₂ Nanocages: An Intuition from DFT. ACS Omega, 2023, 8, 13551-13568.	1.6	9
14938	Efficient boron-based electrolytes constructed by anionic and interfacial co-regulation for rechargeable magnesium batteries. Chemical Engineering Journal, 2023, 461, 141901.	6.6	8
14939	Indirect Nuclear Spin-Spin Exchange Coupling through Solvated Electron in Small Sizes of Cyclic and Cage-Shaped Perfluoroalkanes. ChemPhysChem, 2023, 24, .	1.0	1
14940	Enhanced NH ₃ permeation of bis[3-(trimethoxysilyl)propyl] amine membranes via coordination with metals. Journal of Membrane Science, 2023, 678, 121665.	4.1	3
14941	A deep eutectic solvent binary-phase system for alkaloid extraction from Chinese herb Evodia lepta residue and its mechanism. Journal of Cleaner Production, 2023, 398, 136645.	4.6	4
14942	Thermal stable poly-dioxolane based electrolytes via a robust crosslinked network for dendrite-free solid-state li-metal batteries. Chemical Engineering Journal, 2023, 461, 141973.	6.6	11
14943	Experimental and theoretical analyses and investigation of intermolecular interactions and antibacterial activity of a novel proton transfer compound:8-hydroxyquinolinium oxalate monohydrate. Heliyon, 2023, 9, e14703.	1.4	1
14944	The Effect of Miscibility and Morphology of Porphyrin Donors and Non-Fullerene Acceptors on Exciton Dissociation Processes: A Quantum Chemical and Molecular Dynamics Study. ChemPhotoChem, 2023, 7, .	1.5	1
14945	Inorganic wide-bandgap perovskite subcells with dipole bridge for all-perovskite tandems. Nature Energy, 2023, 8, 610-620.	19.8	63
14946	He adsorption and sensing properties of graphene nanoflakes doped with Mo and Nb. Physica Scripta, 0, , .	1.2	1
14947	A Synthetic Strategy for the Preparation of Fused [5,6,5,5]-Tetracyclic Energetic Compounds. Organic Letters, 2023, 25, 2461-2465.	2.4	8
14948	Experimental and Theoretical Investigation of the Synchronicity of Ambident Silyloxypyrone-Based (5 +) Tj ETQq1 1,0,784314 rgBT /Ole	1.7	1
14949	Exploring the deagglomerating behaviors of selected additives on oxidized asphaltenes using the steered molecular dynamics approach. Journal of Molecular Liquids, 2023, 375, 121327.	2.3	4
14950	Weak intra and intermolecular interactions via aliphatic hydrogen bonding in piperidinium based ionic Liquids: Experimental, topological and molecular dynamics studies. Journal of Molecular Liquids, 2023, 375, 121354.	2.3	5
14951	Waste additives as biopolymers for the modification of bitumen: Mechanical performance and structural analysis characterization. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2023, 663, 131079.	2.3	2
14952	Theoretical studies of new iridium-based terpolymer donors for high-efficiency triplet-material-based organic photovoltaics: Incorporation of different iridium(III) complexes. Materials Chemistry and Physics, 2023, 302, 127780.	2.0	1
14953	Insight into electrochemically boosted trace Co(II)-PMS catalytic process: Sustainable Co(IV)/Co(III)/Co(II) cycling and side reaction blocking. Journal of Hazardous Materials, 2023, 448, 130905.	6.5	21
14954	Phosphatidylcholine in the tear film of the eye: Enhanced topical delivery of fluorometholone to the eye. Inorganic Chemistry Communication, 2023, 150, 110506.	1.8	3

#	ARTICLE	IF	CITATIONS
14955	Molecular insight into the structure of heterometallic metal-organic frameworks MIL-53-M (M=Al and Tj ETQqO O O rgBT /Overlock 10 Inorganic Chemistry Communication, 2023, 150, 110531.	1.8	0
14956	Soil amended with Algal Biochar Reduces Mobility of deicing salt contaminants in the environment: An atomistic insight. Chemosphere, 2023, 323, 138172.	4.2	6
14957	A non-peptide chymotrypsin activatable probe for 3D-photoacoustic and NIR fluorogenic imaging of deep tumor. Sensors and Actuators B: Chemical, 2023, 382, 133553.	4.0	2
14958	Mixing behavior of 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide and 1-Ethyl-3-methylimidazolium tetrafluoroborate binary ionic liquids mixtures. Chemical Physics, 2023, 569, 111858.	0.9	2
14959	Designing Donor-Acceptor-Donor (D-A-D) Type Molecules for Efficient Hole-Transporting in Perovskite Solar Cells – A DFT Study. ChemistrySelect, 2023, 8, .	0.7	0
14960	A mechanism study of methylene blue adsorption on seaweed biomass derived carbon: From macroscopic to microscopic scale. Chemical Engineering Research and Design, 2023, 172, 1132-1143.	2.7	29
14961	Influence of ligands on lithium salt properties: A comprehensive approach to the structure-function relationship. Journal of Power Sources, 2023, 565, 232881.	4.0	2
14962	Highly reinforce the interface stability using 2-Phenyl-1H-imidazole-1-sulfonate electrolyte additive to enhance the high temperature performance of LiNi0.8Co0.1Mn0.1O2/graphite batteries. Journal of Energy Chemistry, 2023, 80, 10-22.	7.1	5
14963	The effect of alkyl chain length on imidazole chloroaluminate ionic liquid/Pt(1 1 1) interface and aluminum deposition: A DFT-D3 study. Chemical Physics, 2023, 568, 111842.	0.9	1
14964	Localized high-concentration carbonate electrolyte creating functional in situ interfaces: Side reaction inhibition for lithium sulfur batteries. Journal of Power Sources, 2023, 563, 232783.	4.0	4
14965	Construction of a QCM sensor for detecting diethylstilbestrol in water based on the computational design of molecularly imprinted polymers. Arabian Journal of Chemistry, 2023, 16, 104601.	2.3	2
14966	Theoretical exploration of new particle formation from glycol aldehyde in the atmosphere – A temperature-dependent study. Computational and Theoretical Chemistry, 2023, 1222, 114057.	1.1	0
14967	The binding mechanism of benzophenone-type UV filters and human serum albumin: The role of site, number, and type of functional group substitutions. Environmental Pollution, 2023, 324, 121342.	3.7	10
14968	Overestimation of O2 role in N-doped carbon materials/peroxymonosulfate system: The misleading of furfuryl alcohol quenching effect. Chemosphere, 2023, 324, 138264.	4.2	3
14969	Photophysical and photochemical properties of heterocyclic analogs of 1,4-cyclohexadiene: Experimental and theoretical studies. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 439, 114624.	2.0	1
14970	Chemo- and regioselectivities of the TBAF-catalyzed C F bond allylation of trifluoromethylalkenes: A theoretical view. Molecular Catalysis, 2023, 542, 113111.	1.0	0
14971	Robust superhydrophobic SiO2/epoxy composite coating prepared by one-step spraying method for corrosion protection of aluminum alloy: Experimental and theoretical studies. Materials and Design, 2023, 228, 111833.	3.3	12
14972	Converting commonly-used paper into nano-engineered fluorescent biomass-based platform for rapid ClO ⁻ quantitative detection in living cells and water sources. Chemosphere, 2023, 324, 138227.	4.2	3

#	ARTICLE	IF	CITATIONS
14973	Toward high-performance associative extraction by forming deep eutectic solvent: A component pairing and mechanism study. <i>Chemical Engineering Science</i> , 2023, 272, 118602.	1.9	0
14974	POSS@TiCl ₄ nanoparticles: A minimalism styled Ziegler-Natta catalytic system. <i>Journal of Catalysis</i> , 2023, 421, 384-392.	3.1	1
14975	A hydrogel electrolyte with ultrahigh ionic conductivity and transference number benefit from Zn ²⁺ "highways" for dendrite-free Zn-MnO ₂ battery. <i>Chemical Engineering Journal</i> , 2023, 463, 142535.	6.6	20
14976	A novel insight into the bimolecular concerted interaction in lignin pyrolysis: Tautomer-assisted hydrogen transfer mechanism. <i>Chemical Engineering Journal</i> , 2023, 463, 142513.	6.6	6
14977	Directed synthesis of nylon 5X key monomer cadaverine with alkaline metal modified Ru@FAU catalysts. <i>Applied Catalysis A: General</i> , 2023, 658, 119172.	2.2	2
14978	Effect of SO ₂ on HCl removal over ethanol-hydrated CaO adsorbent: Mechanism of competitive adsorption and product layer shielding. <i>Chemical Engineering Journal</i> , 2023, 464, 142516.	6.6	9
14979	Pectin grafted with resorcinol and 4-hexylresorcinol: Preparation, characterization and application in meat preservation. <i>International Journal of Biological Macromolecules</i> , 2023, 237, 124212.	3.6	3
14980	Adsorption-enhanced catalytic oxidation for long-lasting dynamic degradation of organic dyes by porous manganese-based biopolymeric catalyst. <i>International Journal of Biological Macromolecules</i> , 2023, 237, 124152.	3.6	4
14981	Behavior and fate of short chain chlorinated paraffins (SCCPs) in different oxidation reactions. <i>Chemical Engineering Journal</i> , 2023, 464, 142557.	6.6	0
14982	A combined experimental and theoretical study of covalent vs noncovalent dimer formation in vanadium(V) complexes with Schiff base ligands. <i>Polyhedron</i> , 2023, 235, 116335.	1.0	1
14983	One-pot production of 5-methylfurfural (5-MF) and enhanced dewaterability of waste activated sludge by hydrothermal treatment with natural deep eutectic solvents (NADES): Experimental and theoretical studies. <i>Chemical Engineering Journal</i> , 2023, 464, 142575.	6.6	8
14984	A range of bifunctional vermiculite-based adsorbents for simultaneous removal of Congo red and permanganate. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 665, 131280.	2.3	2
14985	Recovery of chlorogenic acid from the DES-based extract of <i>Eucommia ulmoides</i> leaves by molecularly imprinted solid-phase extraction. <i>Industrial Crops and Products</i> , 2023, 195, 116406.	2.5	3
14986	Lactam node as a two-fold functional unit for achieving highly efficient and tunable dual-state emitters. <i>Dyes and Pigments</i> , 2023, 213, 111198.	2.0	4
14987	Kinetics, mechanism, and tautomerism in ametryn acid hydrolysis: From molecular structure to environmental impacts. <i>Chemosphere</i> , 2023, 324, 138278.	4.2	1
14988	Diamondoid as potential nonlinear optical material by superalkali doping: A first principles study. <i>Diamond and Related Materials</i> , 2023, 135, 109826.	1.8	9
14989	Conformers of 1,4-dioxane and their hydrogen bond complexation with methanol. <i>Vibrational Spectroscopy</i> , 2023, 126, 103519.	1.2	1
14990	Diffusion-assisted displacive transformation in Yttrium-doped Sb ₂ Te ₃ phase change materials. <i>Acta Materialia</i> , 2023, 249, 118809.	3.8	3

#	ARTICLE	IF	CITATIONS
14991	Atomic insights into the mechanism of trace water influence on lipase catalysis in organic media. <i>Chemical Engineering Journal</i> , 2023, 464, 142610.	6.6	3
14992	Application of mass spectrometry fragmentation patterns for rapid screening and structure identification of fentanyl analogues in suspicious powder. <i>Forensic Chemistry</i> , 2023, 33, 100485.	1.7	4
14993	Triple-decker complexes comprising heterocyclic middle-deck with coinage metals. <i>Journal of Organometallic Chemistry</i> , 2023, 990, 122667.	0.8	1
14994	Enantioseparation and mechanism study on baclofen by capillary electrophoresis and molecular modeling. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2023, 229, 115371.	1.4	0
14995	A novel binary solid-liquid biphasic functionalized ionic liquids for efficient CO ₂ capture: Reversible polarity and low energy penalty. <i>Separation and Purification Technology</i> , 2023, 313, 123486.	3.9	5
14996	Intermolecular interactions in ethanol solution of OABA: Raman, FTIR, DFT, M062X, MEP, NBO, FMO, AIM, NCI, RDG analysis. <i>Journal of Molecular Liquids</i> , 2023, 377, 121552.	2.3	55
14997	Improvement in the storage stability of camphorquinone-based photocurable materials in sunlight via Ziegler-Natta photoisomerization of photomask agent. <i>Progress in Organic Coatings</i> , 2023, 178, 107455.	1.9	0
14998	Study on intermolecular hydrogen bond of uric acid water-clusters. <i>Chemical Physics Letters</i> , 2023, 818, 140424.	1.2	0
14999	Analysis of the dissolution behavior and solubility of Rotigotine form II in different mono-solvents. <i>Journal of Molecular Liquids</i> , 2023, 377, 121532.	2.3	4
15000	Rational control of π -conjugation and CT component in hybridized local and charge transfer molecules for high performance deep blue emitters. <i>Dyes and Pigments</i> , 2023, 213, 111185.	2.0	2
15001	Unpaired electrons-induced geochemical activity of native sulfur in energy-triggered ring-opening process. <i>Geochimica Et Cosmochimica Acta</i> , 2023, 348, 355-368.	1.6	0
15002	H \cdots Bond interactions in water multimers and water multimers \cdots Pyridine complexes: Natural bond orbital and reduced density gradient isosurface analyses. <i>Journal of Molecular Liquids</i> , 2023, 377, 121524.	2.3	6
15003	Enzymatic hydrolysis lignin dissolution and low-temperature solvolysis in ethylene glycol. <i>Chemical Engineering Journal</i> , 2023, 463, 142256.	6.6	3
15004	Mechanisms and origins of stereoselectivity involved in NHC-catalyzed [3+3] Annulation of 2-bromoaldehydes and β -ketoamides: A DFT study. <i>Molecular Catalysis</i> , 2023, 542, 113135.	1.0	0
15005	Extraction and separation of Li ⁺ from high-ratio Mg/Li salt lake brines by [C2mim][NTf ₂] ionic liquid and a homemade extractor. <i>Desalination</i> , 2023, 553, 116450.	4.0	7
15006	Theoretical investigation into activation of hydroperoxides by excited quinones under ultraviolet irradiation. <i>Chemical Engineering Journal</i> , 2023, 463, 142423.	6.6	0
15007	Highly symmetrical B12@Mg ₂₀ C12 with icosahedral B12 motif: A potential hydrogen storage medium. <i>Results in Physics</i> , 2023, 48, 106390.	2.0	0
15008	Novel 2-amino-2-methyl-1-propanol-based biphasic solvent for energy-efficient carbon dioxide capture using tetraethylenepentamine as a phase change regulator. <i>Energy</i> , 2023, 270, 126930.	4.5	9

#	ARTICLE	IF	CITATIONS
15009	A versatile AIE probe with mitochondria targeting for dual-channel detection of superoxide anion and viscosity. <i>Analytica Chimica Acta</i> , 2023, 1253, 341099.	2.6	6
15010	Nitrobenzoate as a flotation depressant for arsenopyrite: A theoretical study of the structure-reactivity relationship. <i>Journal of Molecular Liquids</i> , 2023, 377, 121493.	2.3	3
15011	Oxygen-mediated dielectric barrier discharge plasma for enhanced degradation of chlorinated aromatic compounds. <i>Separation and Purification Technology</i> , 2023, 313, 123445.	3.9	5
15012	Design of new bithieno thiophene (BTTI) central core-based small molecules as efficient hole transport materials for perovskite solar cells and donor materials for organic solar cells. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2023, 291, 116392.	1.7	24
15013	DFT assessments of BN, AlN, and GaN decorated carbon cage scaffolds for sensing the thiamazole drug. <i>Diamond and Related Materials</i> , 2023, 135, 109800.	1.8	1
15014	Study on the reaction mechanism of C8+ aliphatic hydrocarbons obtained directly from biomass by hydrolysis vapor upgrading. <i>Chemical Engineering Journal</i> , 2023, 464, 142639.	6.6	6
15015	Influencing pathways and toxicity changes of pre-ozonation on carcinogenic NDEA formation from greenhouse gas adsorbent DEAPA in subsequent disinfection processes. <i>Science of the Total Environment</i> , 2023, 873, 162355.	3.9	2
15016	Investigating the structural and electronic properties of anionic calcium-doped magnesium clusters. <i>Journal of Molecular Structure</i> , 2023, 1282, 135195.	1.8	0
15017	Tuning the surface electronic structure of WS ₂ with Zn- and Cu-phthalocyanine for improved hydrogen evolution reaction: Experimental and DFT investigation. <i>FlatChem</i> , 2023, 39, 100499.	2.8	4
15018	Preparation of the starch-lipid complexes by ultrasound treatment: Exploring the interactions using molecular docking. <i>International Journal of Biological Macromolecules</i> , 2023, 237, 124187.	3.6	7
15019	Synthesis, characterization, DFT studies, and adsorption properties of sulfonated starch synthesized in deep eutectic solvent. <i>International Journal of Biological Macromolecules</i> , 2023, 238, 124083.	3.6	1
15020	A novel technology for producing high-purity V ₂ O ₅ from hazardous vanadium-containing solutions using precipitation and solvent extraction. <i>Chemical Engineering Research and Design</i> , 2023, 173, 567-578.	2.7	4
15021	FeN ₄ -embedded warped nanographene as a potential candidate for scavenging and detecting sulfur-based gases: A DFT study. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109705.	3.3	0
15022	Aging affects isomer-specific occurrence of dechlorane plus in soil profiles: A case study in a geographically isolated landfill from the Tibetan Plateau. <i>Science of the Total Environment</i> , 2023, 878, 163119.	3.9	3
15023	<i>Journal of Molecular Liquids</i> , 2023, 380, 121714.	2.3	9
15024	The rapid and sensitive detection of trace copper ions by L-cysteine capped ZnS nanoparticle fluorescent probe and the insight into micro-mechanism: Experiments and DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 294, 122570.	2.0	2
15025	The application of a novel phenothiazine-based organic dye with N719 in efficient parallel tandem dye-sensitized solar cells. <i>Synthetic Metals</i> , 2023, 295, 117344.	2.1	3
15026	Mechanism analysis of fuel-N oxidation during ammonia-coal co-combustion: Influence of H ₂ O. <i>Fuel</i> , 2023, 342, 127747.	3.4	7

#	ARTICLE	IF	CITATIONS
15027	Novel strategy for copper precipitation from cupric complexes wastewater: Catalytic oxidation or reduction self-decomplexation?. Journal of Hazardous Materials, 2023, 452, 131183.	6.5	2
15028	Research on 1,10-phenanthroline quaternary ammonium salt composite corrosion inhibitors for oilfield acidizing at high temperatures and high HCl concentrations. , 2023, 225, 211663.		1
15029	Insight into mechanochemical destruction of PFOA by BaTiO ₃ : An electron-dominated reduction process. Journal of Hazardous Materials, 2023, 450, 131028.	6.5	4
15030	Novel rapid coordination of ascorbic acid 2-phosphate and iron(III) as chromogenic substrate system based on Fe ₂ O ₃ nanoparticle and application in immunoassay for the colorimetric detection of carcinoembryonic antigen. Talanta, 2023, 258, 124414.	2.9	3
15031	A novel phase change absorbent with ionic liquid as promoter for low energy-consuming CO ₂ capture. Separation and Purification Technology, 2023, 315, 123740.	3.9	6
15032	Heteroatom substitution controlled luminescent property and excited state intramolecular proton transfer (ESIPT) process of novel benzothiazole-based fluorophore: A TD-DFT investigation. Journal of Molecular Structure, 2023, 1281, 135132.	1.8	2
15033	Theoretical study of lithium oxide clusters adsorbed on anatase TiO ₂ surface. Surfaces and Interfaces, 2023, 38, 102856.	1.5	1
15034	Synthesis, solvent polarity(polar and nonpolar), structural and electronic properties with diverse solvents and biological studies of (E)-3-((3-chloro-4-fluorophenyl) imino) indolin-2-one. Journal of Molecular Liquids, 2023, 380, 121709.	2.3	9
15035	Insights into $\hat{1}23$ -adrenoceptor agonism through comprehensive in silico investigation. Computational Biology and Chemistry, 2023, 104, 107836.	1.1	0
15036	Constructing aloe-emodin/FeOOH organic-inorganic heterojunction for synergetic photocatalysis-Fenton eliminating antibiotic pollutants. Journal of Environmental Chemical Engineering, 2023, 11, 109775.	3.3	1
15037	Impact of silica nanoparticles architectures on the photosensitization of O ₂ by immobilized Rose Bengal. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 440, 114648.	2.0	6
15038	Excellent high-temperature dielectric energy storage of flexible all-organic polyetherimide/poly(arylene ether urea) polymer blend films. Journal of Power Sources, 2023, 570, 233053.	4.0	12
15039	A copolyether with pendant cyclic carbonate segment for PEO-based solid polymer electrolyte. Journal of Power Sources, 2023, 570, 233049.	4.0	4
15040	A novel heavy-atom-free lysosome-targeted BODIPY as triplet photosensitizer based on SOCT-ISC mechanism for photodynamic therapy. Dyes and Pigments, 2023, 214, 111214.	2.0	5
15041	Nitrogen-doped carbon materials prepared using different organic precursors as catalysts of peroxymonosulfate to degrade sulfamethoxazole: First-time performance leading to the incorrect selection of the best catalyst. Chemosphere, 2023, 326, 138442.	4.2	1
15042	MIL-125(Ti)-derived double vacancy-induced enhanced visible-light-driven TiO ₂ p-n homojunction for photocatalytic elimination of OFL and Cr(VI). Journal of Environmental Chemical Engineering, 2023, 11, 109721.	3.3	2
15043	CaPt ₄ P ₆ , first calcium-containing representative of the ternary pyrite-derived pnictides of the BaPt ₄ As ₆ type: Synthesis, crystal, and electronic structure. Journal of Solid State Chemistry, 2023, 322, 123969.	1.4	0
15044	Designing and theoretical study of benzocarbazole-based D- π -D type small molecules donor for organic solar cells. Journal of Molecular Graphics and Modelling, 2023, 121, 108455.	1.3	4

#	ARTICLE	IF	CITATIONS
15045	Nanofiltration membrane comprising structural regulator Cyclen for efficient Li ⁺ /Mg ²⁺ separation. <i>Desalination</i> , 2023, 556, 116575.	4.0	20
15046	Dual-reaction center catalyst based on common metals Cu-Mg-Al for synergistic peroxymonosulfate adsorption-activation in Fenton-like process. <i>Applied Catalysis B: Environmental</i> , 2023, 327, 122468.	10.8	20
15047	Insights into multi-pathway peroxymonosulfate activation by copper-doped Ca/Mn perovskite oxides for diethyl phthalate degradation. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109845.	3.3	0
15048	Computational studies of chalcogen doped on graphene vs. chalcogen doped on CNT and their role in the catalytic performance of electrochemical CO ₂ reduction. <i>Materials Today Communications</i> , 2023, 35, 105631.	0.9	0
15049	4-(4-methoxyphenyl)-6-methyl-3-phenyl-4H-1,2,4-oxadiazin-5(6H)-one: Synthesis, crystal structure, Hirshfeld surface analysis, noncovalent, ADMET studies and biological evaluation. <i>Journal of Molecular Structure</i> , 2023, 1282, 135197.	1.8	1
15050	Crystal structure studies, Hirshfeld surface analysis, 3D energy frameworks, computational studies and docking analysis of a 2-(4-nitrophenyl)-2-oxoethyl 2-methoxybenzoate. <i>Journal of Molecular Structure</i> , 2023, 1282, 135215.	1.8	0
15051	First, second and third order NLO response of alkaline earth metals doped C ₆₀ O ₆ Li ₆ organometallic complexes. <i>Chemical Physics</i> , 2023, 570, 111894.	0.9	7
15052	Theoretical insights into the excited-state single and double proton transfer processes of DEASH in water. <i>Chemical Physics</i> , 2023, 570, 111882.	0.9	7
15053	Molecular dynamics study on the structure and antifouling performance of aromatic polyamide membrane with sulfonamide group. <i>Materials Today Communications</i> , 2023, 35, 105674.	0.9	0
15054	Oxygen-containing functional groups enhance uranium adsorption by aged polystyrene microplastics: Experimental and theoretical perspectives. <i>Chemical Engineering Journal</i> , 2023, 465, 142730.	6.6	11
15055	Non-porous covalent organic polymers enable ultrafast removal of cationic dyes via carbonyl/hydroxyl-synergistic electrostatic adsorption. <i>Separation and Purification Technology</i> , 2023, 315, 123689.	3.9	7
15056	Quantum chemical investigation of Z-shaped heptazethrenes derivatives with detailed structural parameters and singlet fission for photovoltaic applications. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 121, 108432.	1.3	8
15057	Efficient tuning of various coumarin based donor dyes with diketopyrrolopyrrole by forming D-A ⁺ -A structure for high-efficiency solar cells: A DFT/ TD-DFT study. <i>Chemical Data Collections</i> , 2023, 45, 101017.	1.1	3
15058	Construction and validation of the average molecular structure model of the bio-oil from solvent-thermal liquefaction of sawdust using molecular characterization and molecular simulation. <i>Journal of Molecular Liquids</i> , 2023, 379, 121689.	2.3	1
15059	Controlled supramolecular interactions for targeted release of Amiodarone drug through Graphyne to treat cardiovascular diseases: An in silico study. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 121, 108452.	1.3	2
15060	Porous aromatic frameworks as HF resistant adsorbents for SF ₆ separation at elevated pressure. <i>Separation and Purification Technology</i> , 2023, 315, 123657.	3.9	3
15061	Oxidative desulfurization of thiophene derivatives with L-proline/benzene sulfonic acid deep eutectic solvent and their interaction: An experimental and computational study. <i>Journal of Cleaner Production</i> , 2023, 406, 136878.	4.6	4
15062	Comparison of two pyrazole derived fluorescent probes for the recognition of Ga ³⁺ . <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 440, 114656.	2.0	1

#	ARTICLE	IF	CITATIONS
15063	Eliminating ciprofloxacin antibiotic contamination from water with a novel submerged thermal plasma technology. <i>Chemosphere</i> , 2023, 326, 138470.	4.2	5
15064	Hydroxylation of some emerging disinfection byproducts (DBPs) in water environment: Halogenation induced strong pH-dependency. <i>Journal of Hazardous Materials</i> , 2023, 452, 131233.	6.5	1
15065	Understanding of three different polyvinylpyrrolidone (PVP) based battery binders blends on graphene surfaces from first principles via DFT simulations. <i>Materials Chemistry and Physics</i> , 2023, 301, 127548.	2.0	3
15066	Chitosan derivatives as promising green corrosion inhibitors for carbon steel in acidic environment: Inhibition performance and interfacial adsorption mechanism. <i>Journal of Colloid and Interface Science</i> , 2023, 640, 1052-1067.	5.0	13
15067	Long-term environmental stability of bromide coupled mechanical modified fly ash after mercury adsorption. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109622.	3.3	1
15068	Direct observation on argon tagging nitrobenzene radical anion in gas phase: Infrared photodissociation spectroscopy and theoretical calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 294, 122482.	2.0	2
15069	Fe and Au-codoping of molybdenum carbide (MoC) nanosheet for hydrogen adsorption. <i>Materials Science in Semiconductor Processing</i> , 2023, 159, 107402.	1.9	3
15070	Adsorption of thiotepa anticancer by the assistance of aluminum nitride nanocage scaffolds: A computational perspective on drug delivery applications. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 666, 131276.	2.3	0
15071	Machine learning prediction of deep eutectic solvents pretreatment of lignocellulosic biomass. <i>Industrial Crops and Products</i> , 2023, 196, 116431.	2.5	8
15072	Chemical reactivity, solvent effects, spectroscopic (FTIR, Raman, SERS, UV-Visible), Hirshfeld analyses and antimalarial investigation of 3-Acetylbenzoic acid. <i>Chemical Physics Impact</i> , 2023, 6, 100190.	1.7	3
15073	Insight into micropollutant abatement during ultraviolet light-emitting diode combined electrochemical process: Reaction mechanism, contributions of reactive species and degradation routes. <i>Science of the Total Environment</i> , 2023, 876, 162798.	3.9	2
15074	Structural evolution, electronic and magnetic properties investigation of V ₃ Si _n (n=14-18) clusters based on photoelectron spectroscopy and density functional theory calculations. <i>Chemical Physics Letters</i> , 2023, 820, 140423.	1.2	6
15075	Positional isomerism mediated the self-assembly and optical properties of amphiphilic cyanostyrene-based mesogens. <i>Journal of Luminescence</i> , 2023, 258, 119810.	1.5	6
15076	Interaction of barley β-glucan with food dye molecules – An insight from pulse dipolar EPR spectroscopy. <i>Carbohydrate Polymers</i> , 2023, 309, 120698.	5.1	3
15077	A comprehensive method of ionic liquid screening and experimental verification for simultaneous separation of multiple sulfides from oil. <i>Separation and Purification Technology</i> , 2023, 315, 123714.	3.9	2
15078	Dynamic adsorption separation of c-C ₄ F ₈ /C ₃ F ₈ for effective purification of perfluoropropane electronic gas. <i>Chemical Engineering Science</i> , 2023, 273, 118656.	1.9	5
15079	First-principle study on the lattice-directed missing linker defect in zirconium based metal-organic framework (MOF-801): Electronic properties and interaction with hydrogen. <i>Materials Today Communications</i> , 2023, 35, 105967.	0.9	2
15080	Metronidazole photodegradation under solar light with UiO-66-NH ₂ photocatalyst: Mechanisms, pathway, and toxicity assessment. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109744.	3.3	0

#	ARTICLE	IF	CITATIONS
15081	Bidirectional selection of the functional properties and environmental friendliness of organophosphorus (OP) pesticide derivatives: Design, screening, and mechanism analysis. <i>Science of the Total Environment</i> , 2023, 879, 163043.	3.9	5
15082	A comparative analysis of UV-vis transitions in hetaryl and ferrocenyl thioketones. <i>Chemical Physics</i> , 2023, 570, 111901.	0.9	1
15083	Structure, stability, and properties of cyclo[18]carbon-Zinc super sandwich complexes (C18-Zn-C18). <i>Journal of Organometallic Chemistry</i> , 2023, 991, 122668.	0.8	3
15084	Reversible hydrogen storage on multiple Ti-doped B12C6N6 nanocage. <i>Journal of Energy Storage</i> , 2023, 62, 106910.	3.9	3
15085	Theoretical investigation of the borazine B9N9 monocyclic ring. <i>Chemical Physics Letters</i> , 2023, 821, 140476.	1.2	5
15086	In-depth unveiling the interfacial adsorption mechanism of triazine derivatives as corrosion inhibitors for carbon steel in carbon dioxide saturated oilfield produced water. <i>Journal of Colloid and Interface Science</i> , 2023, 639, 107-123.	5.0	8
15087	Enhanced degradation of monobrominated diphenyl ether by sophorolipid modified nanoscale zerovalent iron: Reactivity, electron selectivity, and mechanism. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109827.	3.3	0
15088	Unrevealing the phase transition of high-performing high-nitrogen energetic material 1,5-diaminotetrazole-4: N-oxide via first-principles studies. <i>Materials Today Communications</i> , 2023, 35, 105940.	0.9	0
15089	Therapeutic efficiency of B3O3 quantum dot as a targeted drug delivery system toward Foscarnet anti-HIV drug. <i>Computational and Theoretical Chemistry</i> , 2023, 1224, 114107.	1.1	4
15090	Investigation of linear and second-order nonlinear optical properties of donor-acceptor interaction derivatives based on acceptor DCPPr core. <i>Journal of Molecular Structure</i> , 2023, 1282, 135203.	1.8	0
15091	Thiazole-pyrazoline hybrids as potential antimicrobial agent: Synthesis, biological evaluation, molecular docking, DFT studies and POM analysis. <i>Journal of Molecular Structure</i> , 2023, 1282, 135191.	1.8	17
15092	Effects of sucrose degradation product furfural on cyanidin-3-O-glucoside: Mechanism of action, stability, and identification of products in sugar solutions. <i>Food Research International</i> , 2023, 168, 112788.	2.9	1
15093	Two-dimensional titanium nitride as a highly active electrocatalyst for ammonia production via NO electroreduction. <i>Materials Today Communications</i> , 2023, 35, 105715.	0.9	1
15094	Exploring the structural, photophysical and optoelectronic properties of a diaryl heptanoid curcumin derivative and identification as a SARS-CoV-2 inhibitor. <i>Journal of Molecular Structure</i> , 2023, 1281, 135110.	1.8	6
15095	Experimental and quantum chemical investigations on the generation mechanism of Al-V intermediate alloy by aluminothermic reduction of NaVO3. <i>Journal of Alloys and Compounds</i> , 2023, 945, 169252.	2.8	0
15096	A theoretical study of the ESIPT mechanism for the 2-butyl-4-hydroxyisoindoline-1, 3-dione probe. <i>Computational and Theoretical Chemistry</i> , 2023, 1224, 114104.	1.1	1
15097	Highly efficiently selective separation of zirconium from scandium by TRPO modified adsorbent. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109906.	3.3	2
15098	Fluorescent properties based on ESIPT and TICT of novel acylhydrazone-based probe and its sensing mechanism for Al ³⁺ : A TD-DFT investigation. <i>Journal of Molecular Liquids</i> , 2023, 379, 121639.	2.3	1

#	ARTICLE	IF	CITATIONS
15099	The molecular salt of pyrimethamine and fenbufen for enhancing dissolubility via an assisted efficacy-increasing approach of dual-drug salt formation: A combined study including theory analysis and experiment validation. <i>Journal of Molecular Structure</i> , 2023, 1284, 135455.	1.8	0
15100	Extraction of bioactive compounds from cinnamon residues with deep eutectic solvents and its molecular mechanism. <i>Chemical Engineering Science</i> , 2023, 273, 118630.	1.9	8
15101	Understanding the mechanism for initial deposition under the coupling effect of sodium and calcium during boiler operation: The first-principles study and thermodynamic analysis. <i>Materials Letters</i> , 2023, 340, 134160.	1.3	0
15102	Establishing TA-Pb/Cu and SA-Pb/Cu interface catalyst shells on HMX surfaces via in situ coprecipitation to ameliorate the performances of HMX. <i>Arabian Journal of Chemistry</i> , 2023, 16, 104720.	2.3	4
15103	Design of donor-acceptor small molecules based on diazaisoindigo unit: Synthesis, theoretical calculations and photophysical studies. <i>Dyes and Pigments</i> , 2023, 214, 111197.	2.0	2
15104	Triplet state generation followed by the excited-state intramolecular proton transfer in 3-sulfanylchromen-4-one. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 441, 114700.	2.0	4
15105	Boron-rich triphenylene COF based electrides having excellent nonlinear optical activity. <i>Materials Science in Semiconductor Processing</i> , 2023, 160, 107468.	1.9	4
15106	Why and how could an aliphatic bridge allow for a long-range photoinduced charge separation in Tröger's bases derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 441, 114699.	2.0	2
15107	A novel C6-sulfonated celastrol analog as a tyrosinase and melanin inhibitor: Design, synthesis, biological evaluation and molecular simulation. <i>Journal of Molecular Structure</i> , 2023, 1283, 135288.	1.8	3
15108	New semiconductor halocadmte [CdnXm](2n ⁺ m) crystal structure, molecular conformation and theoretical investigations. <i>Journal of Solid State Chemistry</i> , 2023, 322, 123954.	1.4	2
15109	New insights into the pH dependence of anthocyanin-protein interactions by a case study of cyanidin-3-O-glucoside and bovine serum albumin. <i>Food Hydrocolloids</i> , 2023, 140, 108649.	5.6	8
15110	Performance enhancement of catechin-graphene quantum dot nanocomposites functionalized with carboxyl and doped/decorated with boron towards dye-sensitized solar cell applications: DFT and TD-DFT calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 121, 108427.	1.3	5
15111	Potential differentiation of successive SARS-CoV-2 mutations by RNA: DNA hybrid analyses. <i>Biophysical Chemistry</i> , 2023, 297, 107013.	1.5	0
15112	Co nanoparticles modified N-doped carbon nanosheets array as a novel bifunctional photothermal membrane for simultaneous solar-driven interfacial water evaporation and persulfate mediating water purification. <i>Applied Catalysis B: Environmental</i> , 2023, 330, 122556.	10.8	16
15113	Computational characteristics of the structure-activity relationship of inhibitors targeting Pks13-TE domain. <i>Computational Biology and Chemistry</i> , 2023, 104, 107864.	1.1	0
15114	Thoughtful design of a covalent organic framework with tailor-made polarity and pore size for the enrichment of bisphenols and their derivatives: Extraction performance, adsorption mechanism and toxicity evaluation. <i>Environmental Pollution</i> , 2023, 326, 121475.	3.7	8
15115	Synthesis, crystal structure, computational investigation, molecular docking analysis and anti-lung cancer activity of novel (Z)-3-amino-2-(cyclohexylidenehydrazono)thiazolidin-4-one. <i>Journal of Molecular Structure</i> , 2023, 1285, 135462.	1.8	3
15116	Combined experimental and theoretical studies of bis-chalcone: Estimation of non-covalent interactions. <i>Journal of Molecular Structure</i> , 2023, 1282, 135189.	1.8	2

#	ARTICLE	IF	CITATIONS
15117	Design, synthesis and characterization of organic second-order nonlinear optical crystal materials DOBS. <i>Journal of Molecular Structure</i> , 2023, 1282, 135237.	1.8	1
15118	IR and UV-VIS spectroscopic characterization of norbadione A and study of the electronic properties of other pigments derived from pulvinic acid. <i>Journal of Molecular Structure</i> , 2023, 1285, 135491.	1.8	0
15119	Theoretical study into effects of different substituents on the structure and properties of Keto-RDX compounds. <i>Computational and Theoretical Chemistry</i> , 2023, 1224, 114111.	1.1	1
15120	The prediction and assessment of properties for high energy density fuel “Adamantane derivatives: The combined DFT and molecular dynamics simulation. <i>Fuel</i> , 2023, 343, 127975.	3.4	1
15121	Starch-guar gum-ferulic acid molecular interactions alter the ordered structure and ultimate retrogradation properties and in vitro digestibility of chestnut starch under extrusion treatment. <i>Food Chemistry</i> , 2023, 416, 135803.	4.2	11
15122	Simulation for fluorescence detection of O4-methylthymidine with definite photophysical characteristics. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 296, 122691.	2.0	1
15123	Molecular engineering of bicarbazole-based donor molecules with remarkable photovoltaic parameters for organic solar cells. <i>Optik</i> , 2023, 281, 170818.	1.4	6
15124	Microscopic stabilization mechanism of nanoparticle-laden droplets under external electric fields: A molecular dynamics study. <i>International Journal of Heat and Mass Transfer</i> , 2023, 209, 124113.	2.5	5
15125	Deep insight into the charge-transfer cocrystals: Decreasing structural overlap induced bathochromically shift emission. <i>Dyes and Pigments</i> , 2023, 215, 111277.	2.0	0
15126	Structural, electronic, nonlinear optical properties and spectroscopic study of noble metals doped C60 fullerene using M06-2X. <i>Computational and Theoretical Chemistry</i> , 2023, 1224, 114114.	1.1	1
15127	High fixed carbon and low ash hydrochar production from sewage sludge with addition of phloroglucinol: Theoretical modeling of reaction mechanism using density functional theory. <i>Fuel Processing Technology</i> , 2023, 244, 107703.	3.7	1
15128	Carbon composites for rapid and effective photodegradation of 4-halogenophenols: characterization, removal performance, and computational studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 441, 114753.	2.0	3
15129	Mechanism-driven moderate alkalinity release for efficient recovery of high-purity cobalt and nickel from spent lithium-ion batteries. <i>Separation and Purification Technology</i> , 2023, 315, 123645.	3.9	4
15130	Enhanced degradation performance and mineralization of ciprofloxacin by ionizing radiation combined with g-C3N4/CDs. <i>Radiation Physics and Chemistry</i> , 2023, 208, 110958.	1.4	3
15131	A comprehensive discussion on photophysical properties of dihydropyridines: Experimental and theoretical studies. <i>Journal of Molecular Structure</i> , 2023, 1281, 135167.	1.8	1
15132	Study on the structural characteristics and interaction mechanisms of ionic liquid mixtures with a common imidazolium cation. <i>Journal of Molecular Liquids</i> , 2023, 380, 121743.	2.3	8
15133	A Zn-based metal coordination cluster Zn ₅ used for solid phase microextraction of ten phenolic compounds from water and soil. <i>Journal of Hazardous Materials</i> , 2023, 453, 131382.	6.5	7
15134	Carbazole-based thermally activated delayed fluorescent emitters for efficient pure blue organic light-emitting diodes. <i>Organic Electronics</i> , 2023, 118, 106795.	1.4	2

#	ARTICLE	IF	CITATIONS
15135	Exciton dissociation and transfer behavior and surface reaction mechanism in Donor-acceptor organic semiconductor photocatalytic separation of uranium. <i>Applied Catalysis B: Environmental</i> , 2023, 332, 122751.	10.8	13
15136	Highly selective chemosensor for the sensitive detection of Hg ²⁺ in aqueous media and its cell imaging application. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 296, 122648.	2.0	8
15137	Theoretical study on the mechanism of aggregation-induced emission in red thermally activated delayed fluorescence molecules: trans/cis-arrangement effect. <i>Organic Electronics</i> , 2023, 119, 106811.	1.4	0
15138	Design, synthesis and characterization of a novel oxygen-containing heterocycle crystal with NLO properties. <i>Optik</i> , 2023, 282, 170851.	1.4	0
15139	The enhanced charge separation over dual Z-scheme MoS ₂ @g-C ₃ N ₄ /ZIF-8(Zn) photocatalyst: The boosted Fenton activation model and DFT calculation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 441, 114756.	2.0	6
15140	Theoretical insights into the spectroscopic properties of ferrocenyl hetaryl ketones. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 296, 122635.	2.0	0
15141	Electronic structure and detonation property prediction of pentazolates derivatives: Aminopentazole, diaminopentazole cations, azopentazole, and 1,2-diazopentazole. <i>Journal of Molecular Structure</i> , 2023, 1285, 135420.	1.8	5
15142	All organic transport materials (TMs) based QLEDs: Revisiting molecular electron TMs with mapping hole TMs via cross-linking strategy. <i>Organic Electronics</i> , 2023, 119, 106816.	1.4	1
15143	Toward better Halon substitutes: Effects of H content on pyrolytic and fire-suppressing mechanisms of ozone-friendly fluorinated alkanes. <i>Journal of Molecular Structure</i> , 2023, 1285, 135506.	1.8	1
15144	Mononuclear copper(II) complexes with mechanochromic thermally activated delayed fluorescence behaviour based on switchable hydrogen bonds. <i>Polyhedron</i> , 2023, 237, 116391.	1.0	1
15145	Mechanism of sugar degradation product 5-hydroxymethylfurfural reducing the stability of anthocyanins. <i>Food Chemistry</i> , 2023, 419, 136067.	4.2	0
15146	Two Cd(II)-MOFs containing pyridylbenzimidazole ligands as fluorescence sensors for sensing enrofloxacin, nitrofurazone and Fe ³⁺ . <i>Journal of Molecular Structure</i> , 2023, 1285, 135488.	1.8	3
15147	Synthesis and luminescence properties of the four-coordinate N-heterocyclic carbene (NHC) copper(I) complexes with different bisphosphine ligands. <i>Journal of Molecular Structure</i> , 2023, 1285, 135504.	1.8	0
15148	Sustainable self-powered degradation of antibiotics using Fe ₃ O ₄ @MoS ₂ /PVDF modified pipe with superior piezoelectric activity: Mechanism insight, toxicity assessment and energy consumption. <i>Applied Catalysis B: Environmental</i> , 2023, 331, 122655.	10.8	10
15149	Synthesis of cardanol grafted hydrophilic polymers and its mechanism of coal dust inhibition. <i>Fuel</i> , 2023, 345, 128112.	3.4	3
15150	Fluorescent deactivation behaviors based on ESIPT and TICT of novel double target fluorescent probe and its sensing mechanism for Al ³⁺ /Mg ²⁺ : A TD-DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 297, 122718.	2.0	1
15151	3,4,5-Trimethoxycinnamic acid in aqueous co-solvent solutions of isopropanol/acetone/methanol/ethanol: Solubility, preferential solvation and intermolecular interactions. <i>Journal of Chemical Thermodynamics</i> , 2023, 183, 107055.	1.0	0
15152	High atom utility of robust Ca-Co bimetallic catalyst for efficient Fenton-like catalysis in advanced oxidation processes. <i>Applied Catalysis B: Environmental</i> , 2023, 331, 122698.	10.8	11

#	ARTICLE	IF	CITATIONS
15153	Tailored pH-triggered surfactant for stepwise separation of a three-component mineral system. <i>Separation and Purification Technology</i> , 2023, 316, 123753.	3.9	1
15154	A molecular dynamics study on polybenzimidazole based proton exchange membrane with dual proton conductors. <i>Journal of Membrane Science</i> , 2023, 677, 121618.	4.1	4
15155	Hypochlorous acid-activated near-infrared fluorescent probe for in vivo/exogenous detection and dairy toxicity evaluation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 296, 122661.	2.0	3
15156	Main/side chain asymmetric molecular design enhances charge transfer of two-dimensional conjugated polymer/g-C ₃ N ₄ heterojunctions for high-efficiency photocatalytic sterilization and degradation. <i>Journal of Colloid and Interface Science</i> , 2023, 641, 619-630.	5.0	8
15157	Direct synthesis of high silica SSZ-16 zeolite with extraordinarily superior performance in NH ₃ -SCR reaction. <i>Applied Catalysis B: Environmental</i> , 2023, 332, 122746.	10.8	5
15158	The isolation of anthocyanin monomers from blueberry pomace and their radical-scavenging mechanisms in DFT study. <i>Food Chemistry</i> , 2023, 418, 135872.	4.2	8
15159	Bisacodyl in aqueous co-solvent solutions of isopropanol/methanol/ethanol: Solubility modeling, preferential solvation and density functional theory study. <i>Journal of Chemical Thermodynamics</i> , 2023, 183, 107054.	1.0	3
15160	Molecular insights into ions permeation and destruction behavior in methane hydrate driven by electrostatic fields. <i>Fuel</i> , 2023, 346, 128211.	3.4	4
15161	New cationic spiropyrans with photoswitchable NIR fluorescence. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 297, 122712.	2.0	4
15162	Diphenyl imidazole-based fluorescent chemosensor for Al ³⁺ and its Al ³⁺ complex toward water detection in food products. <i>Food Chemistry</i> , 2023, 420, 136138.	4.2	4
15163	Insights into interaction mechanism between xanthan gum and galactomannan based on density functional theory and rheological properties. <i>Food Chemistry</i> , 2023, 418, 135990.	4.2	3
15164	Enhanced electrocatalytic cathodic degradation of 2,4-dichlorophenoxyacetic acid based on a synergistic effect obtained from Co single atoms and Cu nanoclusters. <i>Applied Catalysis B: Environmental</i> , 2023, 332, 122748.	10.8	7
15165	Co-modification of carbon and cyano defect in g-C ₃ N ₄ for enhanced photocatalytic peroxydisulfate activation: Combined experimental and theoretical analysis. <i>Separation and Purification Technology</i> , 2023, 316, 123844.	3.9	1
15166	Experimental and theoretical investigation on piperazine-1,4-dium bis (2,5-dichlorophenoxyacetate) single crystal: A potential candidate for nonlinear optical applications. <i>Journal of Molecular Structure</i> , 2023, 1285, 135520.	1.8	4
15167	Effects of different hydrogen bond donors on the extraction of gasoline additive ethanol using deep eutectic solvents formed by choline chloride and dihydric alcohol or dicarboxylic acid as extractant. <i>Fuel</i> , 2023, 346, 128382.	3.4	3
15168	A novel use of an oxime molecule as supramolecular tecton. Synthesis of a Pt (II) 2D network. <i>Journal of Molecular Structure</i> , 2023, 1285, 135485.	1.8	0
15169	Mechanism of acid-catalyzed pyrolysis of levoglucosan: Formation of anhydro-disaccharides. <i>Fuel</i> , 2023, 345, 128242.	3.4	13
15170	Spectral investigation, TD-DFT study, Hirshfeld surface analysis, NCI-RDG, HOMO-LUMO, chemical reactivity and NLO properties of 1-(4-fluorobenzyl)-5-bromolindolin-2,3-dione. <i>Journal of Molecular Structure</i> , 2023, 1285, 135492.	1.8	12

#	ARTICLE	IF	CITATIONS
15171	Complexation determines the removal of multiple tetracyclines by ferrate. Separation and Purification Technology, 2023, 316, 123804.	3.9	9
15172	D-O-A based organic phosphors for both aggregation-induced electrophosphorescence and host-free sensitization. Nature Communications, 2023, 14, .	5.8	6
15173	Scissor-like Au ₄ Cu ₂ Cluster with Phosphorescent Mechanochromism and Thermochromism. Molecules, 2023, 28, 3247.	1.7	0
15174	Hierarchical Self-Assembly of Organic-Inorganic Hybrid Nanosheets to Construct Tubular Superstructures for Photocatalytic Degradation. ACS Applied Nano Materials, 2023, 6, 6270-6278.	2.4	2
15175	Molecular dynamics simulations, molecular docking study, and scaled quantum calculations of 5-hydroxy-2-nitrobenzaldehyde. Indian Journal of Physics, 0, , .	0.9	5
15176	Photochemical diversification of strong C(sp ³)-H bonds enabled by allyl bromide and sodium fluoride. , 2023, 2, 766-777.		8
15177	Tailoring the draw solution chemistry in the integrated electro-Fenton and forward osmosis for enhancing emerging contaminants removal: Performance, DFT calculation and degradation pathway. Science of the Total Environment, 2023, 872, 162155.	3.9	3
15178	Iridium/Zinc-Co-Catalyzed Ring-Opening Reactions of Oxabicyclic Alkenes with Indole Nucleophiles: A Combined Experimental and Theoretical Study. Organometallics, 2023, 42, 780-792.	1.1	2
15179	Improved degradation of iohexol using electro-enhanced activation of persulfate by a Cu _x O-loaded carbon felt with carbon nanotubes as an interlayer. Separation and Purification Technology, 2023, 312, 123336.	3.9	3
15180	Atomically dispersed nano Au clusters stabilized by Zr on the TS-1 surface: Significant enhancement of catalytic oxidation ability using H ₂ and O ₂ . Applied Surface Science, 2023, 619, 156733.	3.1	2
15181	Complexes of NgHNg ⁺ (Ng=He, Ne, Ar) with He: Theoretical insights into structure, stability, and bonding character. Chemical Physics Letters, 2023, 819, 140443.	1.2	1
15182	Experimental and computational investigation of complexing agents on copper dissolution for chemical mechanical polishing process. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2023, 664, 131142.	2.3	4
15183	Degradation efficiency and mechanism of 2,2,4,4-tetrabromodiphenyl ether (BDE-47) by thermally activated persulfate system. Chemosphere, 2023, 325, 138396.	4.2	1
15184	Fine tuning the optoelectronic properties of Dibenzo[b,d]Furan-Centered linear hole transporting materials for perovskite solar cells. Journal of Physics and Chemistry of Solids, 2023, 178, 111337.	1.9	11
15185	A novel dopamine electrochemical sensor based on 3D flake nickel oxide/ cobalt oxide @porous carbon nanosheets/carbon nanotubes/electrochemical reduced of graphene oxide composites modified glassy carbon electrode. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2023, 666, 131284.	2.3	10
15186	Tremella-like Boron-doped hierarchical CN and dispersion Co phthalocyanine assembling heterojunction for photocatalytic hydrogen evolution. Chemical Engineering Journal, 2023, 465, 142775.	6.6	2
15187	A density functional theory investigation on norepinephrine interaction with amino acids and alcohols. Journal of Molecular Structure, 2023, 1283, 135305.	1.8	1
15188	Synthesis, spectroscopic, and molecular interaction study of lead(II) complex of DL-alanine using experimental techniques and quantum chemical calculations. Journal of Molecular Structure, 2023, 1283, 135208.	1.8	4

#	ARTICLE	IF	CITATIONS
15189	Reinforced photoinduced behavior of a low-cost mechanochemical synthesized Fe-doped B12As ₂ nanocrystals. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109913.	3.3	0
15190	Synthesis, crystal structure, DFT calculations, and Hirshfeld surface analysis of an NNN pincer type compound. <i>Journal of Molecular Structure</i> , 2023, 1283, 135252.	1.8	3
15191	Praziquanamine enantiomers: Crystal structure, Hirshfeld surface analysis, and quantum chemical studies. <i>Journal of Molecular Structure</i> , 2023, 1283, 135343.	1.8	2
15192	Development and catalytic mechanism of ionic liquid catalysts for polyoxymethylene dimethyl ethers. <i>Chemical Physics Letters</i> , 2023, 822, 140471.	1.2	2
15193	Disparate toxicity mechanisms of parabens with different alkyl chain length in freshwater biofilms: Ecological hazards associated with antibiotic resistome. <i>Science of the Total Environment</i> , 2023, 881, 163168.	3.9	2
15194	An electronic structure investigation of excited state intramolecular proton transfer in amino-benzazole derivatives: Relative energies and electron density descriptors. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 441, 114738.	2.0	2
15195	Studies towards investigation of Naphthoquinone-based scaffold with crystal structure as lead for SARS-CoV-19 management. <i>Journal of Molecular Structure</i> , 2023, 1283, 135256.	1.8	2
15196	Constructing high-efficiency aggregation-induced delayed fluorescence molecules and OLEDs applying C-H \cdots N hydrogen bond manipulation strategy. <i>Dyes and Pigments</i> , 2023, 215, 111298.	2.0	4
15197	Switching the reaction mechanisms and pollutant degradation routes through active center size-dependent Fenton-like catalysis. <i>Applied Catalysis B: Environmental</i> , 2023, 329, 122569.	10.8	40
15198	Methoxy triphenylamine hexaazatrinaphthylene based small molecules as donor material for photovoltaic applications. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 122, 108486.	1.3	1
15199	Electronic effect of substituents regulates the photocatalytic activity of PhC ₂ Cu. <i>Journal of Alloys and Compounds</i> , 2023, 949, 169885.	2.8	0
15200	Nanoarchitectonics of Co ₉ S ₈ /Zn _{0.5} Cd _{0.5} S nanocomposite for efficient photocatalytic hydrogen evolution. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 667, 131404.	2.3	3
15201	Potent heteroaromatic hydrazone based 1,2,4-triazine motifs: synthesis, anti-oxidant activity, cholinesterase inhibition, quantum chemical and molecular docking studies. <i>Journal of Molecular Structure</i> , 2023, 1284, 135383.	1.8	2
15202	Polymethine chain modified trimethine cyanine based fluorescent probe to selectively light up G-quadruplexes DNA in mitochondria. <i>Dyes and Pigments</i> , 2023, 215, 111286.	2.0	0
15203	Removal of methylene blue by using sodium alginate-based hydrogel; validation of experimental findings via DFT calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 122, 108468.	1.3	12
15204	High-symmetry core-shell B12@Ca ₂₀ C12: A nanocluster-based hydrogen storage material. <i>Applied Surface Science</i> , 2023, 626, 157233.	3.1	0
15205	Efficient full dechlorination of chlorinated ethenes on single enzyme-like Co ^{IV} N ₄ sites in nitrogen-doped carbons. <i>Applied Catalysis B: Environmental</i> , 2023, 328, 122459.	10.8	4
15206	Photophysical properties of Pt(II) and Pd(II) complexes for two-photon photodynamic therapy: A computational investigation. <i>Dyes and Pigments</i> , 2023, 215, 111283.	2.0	1

#	ARTICLE	IF	CITATIONS
15207	Investigation on non-radioactive behavior of an acylhydrazone-based fluorescent probe: Coexistence of PET and TICT mechanisms. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 295, 122603.	2.0	2
15208	Therapeutic potential of oxo-triarylmethyl (oxTAM) as a targeted drug delivery system for nitrosourea and fluorouracil anticancer drugs; A first principles insight. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 122, 108469.	1.3	11
15209	Insights into the uses of two azine decorated d10-MOFs for corrosion inhibition application on mild steel surface in saline medium: Experimental as well as theoretical investigation. <i>Journal of Molecular Liquids</i> , 2023, 381, 121789.	2.3	11
15210	Prolonging oxidation stability of peony (<i>Paeonia suffruticosa</i> Andr.) seed oil by endogenous lipid concomitants: Phospholipids enhance antioxidant capacity by improving the function of tocopherol. <i>Industrial Crops and Products</i> , 2023, 197, 116552.	2.5	1
15211	Enhanced π -conjugation in hybridized local and charge transfer state by intramolecular hydrogen bonding to construct efficient red emitters for OLEDs and cellular imaging. <i>Dyes and Pigments</i> , 2023, 215, 111290.	2.0	0
15212	Computational underpinnings for the dimerization of para-aminothiophenol to dimercaptoazobenzene on copper surface. <i>Chemical Physics</i> , 2023, 571, 111910.	0.9	1
15213	Electrocatalytic hydrogen evolution on the MoS ₂ /C60 heterostructure: Reaction mechanism and activity improvement. <i>Applied Surface Science</i> , 2023, 624, 157163.	3.1	1
15214	Enhancement of peroxymonosulfate activation by humic acid-modified sludge biochar: Role of singlet oxygen and electron transfer pathway. <i>Chemosphere</i> , 2023, 329, 138690.	4.2	5
15215	Effect of green solvents, molecular structure and topological studies on 4-amino-1- β -D-ribofuranosyl-1,3,5 triazin-2(1H)-one - anti-blood cancer agent. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100912.	1.3	5
15216	Simultaneous removal of levofloxacin and sulfadiazine in water by dielectric barrier discharge (DBD) plasma: Enhanced performance and degradation mechanism. <i>Chemical Engineering Research and Design</i> , 2023, 171, 459-469.	2.7	11
15217	C ⁺ H Activation by Iron-Vanadium Bimetallic Oxide Cluster Anions FeV ₃ O ₁₀ and FeV ₅ O ₁₅ : A Comparison with Scandium-Vanadium Oxide Clusters. <i>ChemPhysChem</i> , 0, , .	1.0	0
15218	Covalent interaction, solvent effects, electrochemical, and spectroscopic characterization of novel (4Z)-4-{2-[amino(hydroxy)methyl]hydrazinylidene}-2,6-di(furan-2-yl)-3-methylpiperidin-1-ol derivative-anti-microbial activity study. <i>Journal of Molecular Liquids</i> , 2023, 374, 121272.	2.3	5
15219	Discovery, synthesis and mechanism study of 2,3,5-substituted [1,2,4]-thiadiazoles as covalent inhibitors targeting 3C-Like protease of SARS-CoV-2. <i>European Journal of Medicinal Chemistry</i> , 2023, 249, 115129.	2.6	6
15220	Different competition mechanism between ESPT and TICT process regulated by protic and aprotic solvent in DHP. <i>Journal of Molecular Liquids</i> , 2023, 375, 121278.	2.3	3
15221	(E)-4-((4-chlorobenzylidene)amino)-N-(thiazole-2yl) benzenesulfonamide: Synthesis, characterization and electronic structure theory and docking studies. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100910.	1.3	2
15222	Arsenic-Involving Intermolecular Interactions in Crystal Structures: The Dualistic Behavior of As(III) as Electron-Pair Donor and Acceptor. <i>Crystal Growth and Design</i> , 2023, 23, 1033-1048.	1.4	0
15223	Asymmetric counteranion-directed photoredox catalysis. <i>Science</i> , 2023, 379, 494-499.	6.0	22
15224	The dodeca-coordinated La ^{III} C ₈ H ₄ molecular wheels: conflicting aromaticity versus double aromaticity. <i>RSC Advances</i> , 2023, 13, 3071-3078.	1.7	0

#	ARTICLE	IF	CITATIONS
15225	Theoretical study on the influence of the extra N in transition metal-N4 embedded graphene as efficient CO2 reduction catalysts. <i>Applied Surface Science</i> , 2023, 616, 156494.	3.1	1
15226	Pristine and X-doped (X=As, N) phosphorene as platform materials to the removal of phenol: A theoretical insight. <i>Journal of Molecular Liquids</i> , 2023, 374, 121280.	2.3	4
15227	Photosensitizers Dispersed on Nanosized Triterpenoid Matrix with Deaggregation-Enhanced Singlet Oxygen Production. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 4973-4983.	4.0	5
15228	Bifunctional solvent-driven hydrodechlorination of 1,2-dichlorohexafluorocyclopentene and mechanism study. <i>Journal of Fluorine Chemistry</i> , 2023, 266, 110091.	0.9	0
15229	The quest of the most stable structure of a carboxyfullerene and its drug delivery limits: A DFT and QTAIM approach. <i>Computational and Theoretical Chemistry</i> , 2023, 1221, 114036.	1.1	1
15230	Computational investigations on the 4-cyanopyridine adsorbed on ZnO-graphene oxide nanocomposite toward the efficient performance of surface-enhanced Raman scattering. <i>Diamond and Related Materials</i> , 2023, 133, 109693.	1.8	0
15231	Constant oxidation of atrazine in Fe(III)/PDS system by enhancing Fe(III)/Fe(II) cycle with quinones: Reaction mechanism, degradation pathway and DFT calculation. <i>Chemosphere</i> , 2023, 317, 137883.	4.2	18
15232	Imidazo[1,2-a]quinazolines as novel, potent EGFR-TK inhibitors: Design, synthesis, bioactivity evaluation, and in silico studies. <i>Bioorganic Chemistry</i> , 2023, 133, 106383.	2.0	3
15233	Degradation of sulfamethoxazole in microbubble ozonation process: Performance, reaction mechanism and toxicity assessment. <i>Separation and Purification Technology</i> , 2023, 311, 123262.	3.9	5
15234	Revealing the supramolecular interactions of the bis(azopyrenyl) dibenzo-18-crown-6-ether system. <i>Journal of Molecular Liquids</i> , 2023, 374, 121298.	2.3	1
15235	Metal and nitrogen co-doped carbon dots in the sensitized solar cells. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	0
15236	Insights into the CO ₂ Capture Capacity of Covalent Organic Frameworks. <i>ChemPhysChem</i> , 2023, 24, .	1.0	2
15237	Synthesis, Crystal, and Electronic Structure of (HpipeH ₂) ₂ [Sb ₂ I ₁₀](I ₂), with I ₂ Molecules Linking Sb ₂ X ₁₀ Dimers into a Polymeric Anion: A Strategy for Optimizing a Hybrid Compound's Band Gap. <i>International Journal of Molecular Sciences</i> , 2023, 24, 2201.	1.8	3
15238	Simultaneous Stabilization of Lithium Anode and Cathode using Hyperconjugative Electrolytes for High-voltage Lithium Metal Batteries. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	3
15239	Simultaneous Stabilization of Lithium Anode and Cathode using Hyperconjugative Electrolytes for High-voltage Lithium Metal Batteries. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	8
15241	Aromatic volatile organic compounds absorption with phenyl-based deep eutectic solvents: A molecular thermodynamics and dynamics study. <i>AIChE Journal</i> , 2023, 69, .	1.8	11
15242	Carbonyl and defect of metal-free char trigger electron transfer and O ₂ in persulfate activation for Aniline aerofloat degradation. <i>Water Research</i> , 2023, 231, 119659.	5.3	35
15243	Excitation of quantum-sized (CuS) _n clusters for NIR-II photothermal application: Insights from experiment and DFT calculation. <i>Journal of Alloys and Compounds</i> , 2023, 941, 169005.	2.8	1

#	ARTICLE	IF	CITATIONS
15244	Boosted photocatalytic performance on molecule/semiconductor hybrid materials: conversion of sunlight energy into hydrogen fuel. <i>New Journal of Chemistry</i> , 2023, 47, 4636-4643.	1.4	1
15245	Mechanistic insights into the conformational switch in profilin-1 subject to collective effects of mutation and histidine tautomerism. <i>International Journal of Biological Macromolecules</i> , 2023, 230, 123403.	3.6	1
15246	Improving the solubility of tetrahydropalmatine by introducing sulfonic acid by forming pharmaceutical salts of tetrahydropalmatine with supramolecular helical structure via CAHBs. <i>Journal of Drug Delivery Science and Technology</i> , 2023, 80, 104207.	1.4	0
15247	Pore surface engineering of covalent organic frameworks by simultaneously appending amine group and tailoring pore size for efficient adsorption of diclofenac sodium. <i>Chemical Engineering Journal</i> , 2023, 459, 141561.	6.6	11
15248	Thermal hazard risk and decomposition mechanism identification of 1-Hexyl-2,3-dimethylimidazolium nitrate: Combined thermal analysis experiment and DFT emulation. <i>Chemical Engineering Research and Design</i> , 2023, 172, 38-47.	2.7	4
15249	A Two-Dimensional Porphyrin Coordination Supramolecular Network Cathode for High-Performance Aqueous Dual-Ion Battery. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	1
15250	Experimental and theoretical studies on the extraction behavior of Cf(C_8) by NTAamide(C_8) ligand and the separation of Cf(C_8)/Cm(C_8). <i>RSC Advances</i> , 2023, 13, 3781-3791.	1.7	2
15251	A Two-Dimensional Porphyrin Coordination Supramolecular Network Cathode for High-Performance Aqueous Dual-Ion Battery. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	10
15252	Enhanced Efficiency of Exciplex Emission from a 9-Phenylfluorene Derivative. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 7236-7246.	4.0	5
15253	Anion recognition using enhanced halogen bonding through intramolecular hydrogen bonds – a computational insight. <i>New Journal of Chemistry</i> , 2023, 47, 4439-4447.	1.4	4
15254	A Comparison of Non-Covalent Interactions in the Crystal Structures of two C_6H_6 -Alkane Complexes of Rh Exhibiting Contrasting Stabilities in the Solid State.. <i>Faraday Discussions</i> , 0, , .	1.6	1
15255	Properties of $\text{CF}_3\text{SO}_2\text{F}$ under the influence of external electric field: A DFT study. <i>Results in Physics</i> , 2023, 45, 106248.	2.0	1
15256	Boat and Chair Shaped Hexahalogen Synthons. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	3
15257	Adsorption and photocatalytic degradation process of oxytetracycline using mesoporous Fe-TiO ₂ based on high-resolution mass spectrometry. <i>Chemical Engineering Journal</i> , 2023, 460, 141618.	6.6	17
15258	Molecular encapsulation of bioactive ingredients from Xuefu Zhuyu decoction by cyclodextrin-assisted extraction. <i>Journal of Drug Delivery Science and Technology</i> , 2023, 81, 104219.	1.4	0
15259	Microbial biotransformation mechanisms of PFPiAs in soil unveiled by metagenomic analysis. <i>Journal of Hazardous Materials</i> , 2023, 448, 130896.	6.5	0
15260	Comparative study of the efficiency of silicon carbide, boron nitride and carbon nanotube to deliver cancerous drug, azacitidine: A DFT study. <i>Computers in Biology and Medicine</i> , 2023, 154, 106593.	3.9	7
15261	Through-Space Conjugated Molecule with Dual Delayed Fluorescence and Room-Temperature Phosphorescence for High-Performance OLEDs. , 2023, 5, 664-672.		12

#	ARTICLE	IF	CITATIONS
15262	Degradation of sulpiride in water by the UV/chlorine process: kinetics, reaction mechanism, and transformation pathways. <i>Environmental Science: Water Research and Technology</i> , 2023, 9, 1090-1098.	1.2	0
15263	Interâ€Alkaliâ€Metal Dative Bond in the MMN ₃ ⁺ (M=Alkali Metal) Cluster. <i>ChemPhysChem</i> , 2023, 24, .	1.0	0
15264	Adsorption behaviour and mechanism of Avermectin-based pesticides in soil driven by H-bonds formed between the compounds and humus. <i>Chemical Engineering Journal</i> , 2023, 459, 141647.	6.6	4
15265	Experimental and theoretical vibrational spectroscopic, quantum chemical analysis, and electronic properties investigations of novel ruthenium complexes (RuLCl ₂ ·2H ₂ O; L: 4,4'-Dimethoxy-2,2'-Bipyridine,) Tj ETQq1 1 0.784314 rgB	1.0	0
15266	Openâ€Cage Fullerene as a Selective Molecular Trap for LiF/[BeF] ⁺ . <i>Angewandte Chemie</i> , 2023, 135, .	1.6	0
15267	Polyamide nanofiltration membrane fabricated with ultra-low concentration triaminoguanidine showing efficient desalination performance. <i>Journal of Membrane Science</i> , 2023, 672, 121449.	4.1	6
15268	Study and Applications of Tetrasubstituted Hypervalent Seleniumâ€Halogen Species in Catalytic Electrophilic Halogenations. <i>ACS Catalysis</i> , 2023, 13, 2386-2395.	5.5	4
15269	A Tetrahedral Bisacridine Donor Enables Fast Radiative Decay in Thermally Activated Delayed Fluorescence Emitter. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	8
15270	Is chitin a promising hydrogen storage material? A thorough quantum mechanical study. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 16779-16789.	3.8	2
15271	First row transition metal doped B12P12 and Al12P12 nanocages as excellent single atom catalysts for the hydrogen evolution reaction. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 16663-16677.	3.8	19
15272	Structural, Spectral, Molecular Docking, and Molecular Dynamics Simulations of Phenylthiophene-2-Carboxylate Compounds as Potential Anticancer Agents. <i>Polycyclic Aromatic Compounds</i> , 2024, 44, 238-260.	1.4	20
15273	Pyrrrolizidine alkaloids from <i>Jacobaea vulgaris</i> Gaertn and theoretical studies on intramolecular interactions. <i>Natural Product Research</i> , 0, , 1-6.	1.0	1
15274	A Tetrahedral Bisacridine Donor Enables Fast Radiative Decay in Thermally Activated Delayed Fluorescence Emitter. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	0
15275	Synthesis, Vibrational Analysis, Electronic Structure Property Investigation and Molecular Simulation of Sulphonamideâ€Based Carboxamides against <i>Plasmodium</i> Species. <i>ChemistrySelect</i> , 2023, 8, .	0.7	5
15276	Cation functional group effect on SO ₂ absorption in amino acid ionic liquids. <i>Frontiers in Chemistry</i> , 0, 11, .	1.8	0
15277	Mechanism of Li ⁺ /Na ⁺ separation by crown ether and butyrate acid root. <i>Rare Metals</i> , 2023, 42, 1238-1248.	3.6	3
15278	Tanzawaic Acid Derivatives from the Marine-Derived <i>Penicillium steckii</i> as Inhibitors of RANKL-Induced Osteoclastogenesis. <i>Journal of Natural Products</i> , 2023, 86, 1171-1178.	1.5	4
15279	Absorption of dichloromethane in deep eutectic solvents: Experimental and computational thermodynamics. <i>Separation and Purification Technology</i> , 2023, 311, 123281.	3.9	5

#	ARTICLE	IF	CITATIONS
15280	Electronic and Crystal Packing Effects in Terms of Static and Kinetic Force Field Features: Picolinic Acid N-Oxide and Methimazole. <i>Crystal Growth and Design</i> , 2023, 23, 1726-1742.	1.4	9
15281	Insight into the stabilization mechanism of imidazole-based ionic liquids at the interface of the carbon nanotubes: A computational study. <i>Journal of Molecular Liquids</i> , 2023, 375, 121320.	2.3	0
15282	Understanding lead and mercury adsorption by post-synthetically modified linkers in UiO-66 MOF. A computational theoretical study. <i>Molecular Simulation</i> , 2023, 49, 481-488.	0.9	1
15283	Anti-aging mechanism and rheological properties of lignin, quercetin, and gallic acid as antioxidants in asphalt. <i>Construction and Building Materials</i> , 2023, 369, 130560.	3.2	12
15284	Supramolecular Enhancement of Charge Transport through Pillar[5]arene-Based Self-Assembled Monolayers. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	4
15285	Computer-Aided Screening and Revealing Action Mechanism of Green Tea Polyphenols Intervention in Alzheimer's Disease. <i>Foods</i> , 2023, 12, 635.	1.9	2
15286	Azido azole-1,3,4-triazine fused energetic materials: A bioinspired strategy for tuning thermal stability and sensitivity of metal-free primary explosives via hierarchical hydrogen-bond self-assembly. <i>Chemical Engineering Journal</i> , 2023, 459, 141689.	6.6	4
15287	Methylthiazole Schiff base functionalized SBA-15 for high-performance Pb(II) capture and separation. <i>Microporous and Mesoporous Materials</i> , 2023, 351, 112476.	2.2	6
15288	Robust and Promising Electrocatalytic Oxygen Evolution Reaction by Activated Cu-Co Amorphous Nanosheets. <i>ACS Sustainable Chemistry and Engineering</i> , 2023, 11, 2541-2553.	3.2	15
15289	Sensing functions of an iron-doped boron nitride nanocone towards acetaminophen and its thio/thiol analogs: A DFT outlook. <i>Diamond and Related Materials</i> , 2023, 133, 109749.	1.8	10
15290	Amorphous Nitrogen-Doped Carbon Nanocages with Excellent SERS Sensitivity and Stability for Accurate Identification of Tumor Cells. <i>Analytical Chemistry</i> , 2023, 95, 4671-4681.	3.2	6
15291	Multi-Hydration Induced Zwitterionic Hydrogel with Open Environment Stability for Chemical Sensing. , 2023, 2, .		0
15292	The Structural Basis of African Swine Fever Virus pS273R Protease Binding to E64 through Molecular Dynamics Simulations. <i>Molecules</i> , 2023, 28, 1435.	1.7	1
15293	Emergence of a proton exchange-based isomerization and lactonization mechanism in the plant coumarin synthase COSY. <i>Nature Communications</i> , 2023, 14, .	5.8	3
15294	Redox-Active Polymers as Robust Electron-Shuttle Co-Catalysts for Fast Fe ³⁺ /Fe ²⁺ Circulation and Green Fenton Oxidation. <i>Environmental Science & Technology</i> , 2023, 57, 3334-3344.	4.6	15
15295	Electronic Structures and NLO Properties of a Series of TMDs Lateral-Core-Shell Heterostructures Quantum Dots. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	0
15296	Spectral analysis (FT-IR, FT-Raman, UV and NMR), molecular docking, ADMET properties and computational studies: 2-Hydroxy-5-nitrobenzaldehyde. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100927.	1.3	9
15297	Experimental and Theoretical Study of Tetrel Bonding and Noncovalent Interactions in Hemidirected Lead(II) Phosphorodithioates: An Implication on Crystal Engineering. <i>Crystal Growth and Design</i> , 2023, 23, 2138-2154.	1.4	2

#	ARTICLE	IF	CITATIONS
15298	Chiral copper-hydride nanoclusters: synthesis, structure, and assembly. Dalton Transactions, 2023, 52, 3371-3377.	1.6	8
15299	Novel electro-fluorescent materials with hybridized local and charge-transfer (HLCT) excited state for highly efficient non-doped pure blue OLEDs. Organic Chemistry Frontiers, 2023, 10, 1485-1494.	2.3	7
15300	Mechanistic Insights into Substrate Positioning That Distinguish Non-heme Fe(II)/ β -Ketoglutarate-Dependent Halogenases and Hydroxylases. ACS Catalysis, 2023, 13, 2489-2501.	5.5	10
15301	Supramolecular structure and isomeric transformations of N- <i>t</i> -butyl-N ϵ ² -trifluoromethanesulfonacetamide. Structural Chemistry, 0, , .	1.0	1
15302	Facile fabrication of cobalt doped manganese oxide with hierarchical porosity for peroxymonosulfate activation: Performance investigation, mechanistic insight to degrade organic pollutants in water and DFT study. Journal of Hazardous Materials Advances, 2023, 9, 100244.	1.2	3
15303	A conceptual DFT and information-theoretic approach towards QSPR modeling in polychlorobiphenyls. Journal of Mathematical Chemistry, 2023, 61, 1143-1164.	0.7	2
15304	Tuning Ion Transport at the Anode ϵ Electrolyte Interface via a Sulfonate ϵ Rich Ion ϵ Exchange Layer for Durable Zinc ϵ Iodine Batteries. Advanced Energy Materials, 2023, 13, .	10.2	42
15305	Highly selective extraction of aromatics from aliphatics using an <i>N</i> -methylpyrrolidone ϵ based protic ionic liquid. Canadian Journal of Chemical Engineering, 2023, 101, 5967-5976.	0.9	1
15306	Distal Mutations in the β -Clamp of DNA Polymerase III* Disrupt DNA Orientation and Affect Exonuclease Activity. Journal of the American Chemical Society, 2023, 145, 3478-3490.	6.6	2
15307	Regulation of external electric field on sensitivity of ICM energetic materials. Journal of Molecular Modeling, 2023, 29, .	0.8	1
15308	Reduced Nucleophilicities Δ \langle sub \rangle B \rangle of Lewis Bases B: Is Δ \langle sub \rangle B \rangle Independent of Whether B is Involved in a Hydrogen Bond or a Halogen Bond?. ChemPlusChem, 2023, 88, .	1.3	0
15309	Light Absorption by Cinnamaldehyde Constituents of Biomass Burning Organic Aerosol Modeled Using Time-Dependent Density Functional Theory. ACS Earth and Space Chemistry, 2023, 7, 490-500.	1.2	2
15310	The interaction between nucleotide bases and nano carbon: The dimension dominates. Surfaces and Interfaces, 2023, 37, 102715.	1.5	3
15311	Investigation on Gold ϵ Ligand Interaction for Complexes from Gold Leaching: A DFT Study. Molecules, 2023, 28, 1508.	1.7	3
15312	Exploring an intermolecular Ge/B frustrated Lewis pair from a multicentre Zintl Lewis base. Theoretical Chemistry Accounts, 2023, 142, .	0.5	2
15313	Decomposition mechanisms of nuclear-grade cationic exchange resin by advanced oxidation processes: Statistical molecular fragmentation model and DFT calculations. Journal of Environmental Sciences, 2024, 135, 433-448.	3.2	3
15314	Deciphering the Selectivity of the Electrochemical CO \langle sub \rangle 2 \rangle Reduction to CO by a Cobalt Porphyrin Catalyst in Neutral Aqueous Solution: Insights from DFT Calculations. ChemistryOpen, 2023, 12, .	0.9	1
15315	Enhanced reversible hydrogen storage performance of Mg-decorated g-C ₂ N: First principles calculations. Computational Materials Science, 2023, 220, 112046.	1.4	4

#	ARTICLE	IF	CITATIONS
15316	Competition Between the Two π -Holes in the Formation of a Chalcogen Bond. <i>ChemPhysChem</i> , 2023, 24, .	1.0	5
15317	Theoretical Mechanistic Investigation of the Dynamic Kinetic Resolution of N-Protected Amino Acid Esters using Phase-Transfer Catalysts. <i>Journal of Organic Chemistry</i> , 2023, 88, 7748-7754.	1.7	2
15318	Making and Breaking σ -Insight into the Symmetry of Salen Analogues. <i>Symmetry</i> , 2023, 15, 424.	1.1	2
15319	Torsional Rotation in Ditopic Receptor Host and its Complex Formation with Resorcinol Guest: A Computational Study. <i>ChemPhysChem</i> , 0, , .	1.0	1
15320	Theoretical exploration of polynitrogen compounds N_6 , N_8 , N_{10} , and N_6 ions based on N_3^+ and $cyclo-N_5^+$. <i>Journal of Energetic Materials</i> , 0, , 1-19.	1.0	3
15321	Dinuclear Phenoxo-Bridged Nickel(II) and Copper(II) Complexes of Phenolate-Based Tripodal Ligand: Theoretical and Experimental Insights. <i>Polycyclic Aromatic Compounds</i> , 2024, 44, 313-332.	1.4	1
15322	Anti-inflammatory Quinoline Alkaloids from the Roots of <i>Waltheria indica</i> . <i>Journal of Natural Products</i> , 2023, 86, 276-289.	1.5	1
15323	Electron Presolvation in Tetrahydrofuran-Incorporated Supramolecular Sodium Entities. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1402-1412.	1.1	3
15324	Hetero-Polar Sextuple Bond: A Relativistic Quantum Chemical Study**. <i>ChemPhysChem</i> , 0, , .	1.0	1
15325	Single-electron sodium bonds: Substituent effects. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	2
15326	Hydrogen molecule adsorption and sensing on lanthanide (La) doped/decorated carbon nanotube and graphene structures. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2023, 41, .	0.9	1
15327	Visible-light-driven photocatalytic degradation of tetracycline hydrochloride by Z-scheme $Ag_3PO_4/1T@2H-MoS_2$ heterojunction: Degradation mechanism, toxicity assessment, and potential applications. <i>Journal of Hazardous Materials</i> , 2023, 448, 130951.	6.5	34
15328	Charge-Separated States Determined Photoinduced Electron Transfer Efficiency in a D-D-A System in an External Electric Field. <i>Journal of Physical Chemistry C</i> , 2023, 127, 2805-2817.	1.5	2
15329	Noncovalent $n \rightarrow \pi^*$, $C\cdots H\cdots \pi$, and $C\cdots H\cdots O$ interaction mediated supramolecular assembly in a $Re(CO)_3$ (trifluoroacetate) complex bearing a bulky tetraazaphenanthrene ligand: a combined CSD study and theoretical calculations. <i>CrystEngComm</i> , 2023, 25, 1803-1816.	1.3	2
15330	Direct Catalytic Enantioselective Reaction of β -Isocyanoacetonitriles with Ketimines Using Cinchona Alkaloid Amide-Cu(II) Catalysts. <i>Organic Letters</i> , 2023, 25, 1040-1044.	2.4	0
15331	Room-Temperature Conversion of Methane to Methanediol by $[FeO_2]^+$. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 1633-1640.	2.1	2
15332	Neutral Monodentate and Hypervalent Chalcogen Bond Catalysis on the Intramolecular Rauhut-Currier Reaction of Bis(enones): A DFT Study. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	1
15333	Modulating the strength of acceptor in D-A-D type hole transport materials for efficient inverted perovskite solar cells. <i>Chemical Physics</i> , 2023, 568, 111847.	0.9	0

#	ARTICLE	IF	CITATIONS
15334	Molecular Mechanism of Conformational Crossover of Mefenamic Acid Molecules in scCO ₂ . <i>Materials</i> , 2023, 16, 1403.	1.3	1
15335	(8-Hydroxyquinoline) Gallium(III) Complex with High Antineoplastic Efficacy for Treating Colon Cancer via Multiple Mechanisms. <i>ACS Omega</i> , 2023, 8, 6945-6958.	1.6	4
15336	An Oxytocin Sensor Based on an Organic Field-Effect Transistor Functionalized with a Molecularly Imprinted Polymer. , 2022, , .		0
15337	Visible-light induced photocatalytic degradation of estrone (E1) with hexagonal copper selenide nanoflakes in water. <i>Chemical Engineering Research and Design</i> , 2023, 172, 1-15.	2.7	1
15338	Enhanced catalytic performance of hierarchical Zn/ZSM-5 with balanced acidities synthesized utilizing ZIF-14 as porogen and Zn source in methanol to aromatics. <i>Chemical Engineering Science</i> , 2023, 270, 118542.	1.9	2
15339	Luminescence properties and excitation behavior of ICG-conjugated nanoparticles for optical theranostics. <i>Optical Materials</i> , 2023, 137, 113541.	1.7	0
15340	Discrete Singular Metallophilic Interaction in Stable Large 12-Membered Binuclear Silver and Gold Metallamacrocycles of Amido-Functionalized Imidazole and 1,2,4-Triazole-Derived N-Heterocyclic Carbenes. <i>ACS Omega</i> , 2023, 8, 6439-6454.	1.6	0
15341	Virtual Screening and Multi-targets Investigation of Novel Diazine Derivatives as Potential Xanthine Oxidase Inhibitors Based on QSAR, Molecular Docking, ADMET Properties, Dynamics Simulation and Network Pharmacology. <i>Medicinal Chemistry</i> , 2023, 19, 704-716.	0.7	2
15342	Theoretical Studies of Mutual Effects between 6â€mâ€r Hemiketalization and 26â€mâ€r Lactonization in Pimaricin Thioesterase. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	1
15343	The Development and Design Strategy of Leucine-Rich Repeat Kinase 2 Inhibitors: Promising Therapeutic Agents for Parkinsonâ€™s Disease. <i>Journal of Medicinal Chemistry</i> , 2023, 66, 2282-2307.	2.9	7
15344	Reconstructed Cd(0001) Surface Induced by Adsorption of Triphenyl Bismuth. <i>Coatings</i> , 2023, 13, 394.	1.2	0
15345	Effect of cyclodextrins inclusion complexes into absorption and emission spectra of P-methylaminobenzoate derivatives: A DFT and TD-DFT investigation. <i>Journal of Fluorescence</i> , 2023, 33, 1457-1467.	1.3	1
15346	Structural Insights into the Antiparallel G-Quadruplex in the Presence of K ⁺ and Mg ²⁺ Ions. <i>Journal of Physical Chemistry B</i> , 2023, 127, 1499-1512.	1.2	1
15347	Experimental and DFT Research on the Effects of O ₂ /CO ₂ and O ₂ /H ₂ O Pretreatments on the Combustion Characteristics of Char. <i>Molecules</i> , 2023, 28, 1638.	1.7	0
15348	A combined experimental and theoretical study of RuO ₂ /TiO ₂ heterostructures as a photoelectrocatalyst for hydrogen evolution. <i>Dalton Transactions</i> , 2023, 52, 3472-3481.	1.6	1
15349	Contributing to Biochemistry and Optoelectronics: Pyrrolo[1â€²,2â€²:2,3]imidazo[1,5-a]indoles and Cyclohepta[4,5]pyrrolo[1,2-c]pyrrolo[1,2-a]imidazoles via [3+2] Annulation of Acylethynylcycloalka[b]pyrroles with ¹³ C-1-Pyrrolines. <i>International Journal of Molecular Sciences</i> , 2023, 24, 3404.	1.8	3
15350	Computational Evidence of the Incipient Oxocarbenium Ion as a "Hidden Intermediate" During the Cyclization of Hydroxyenol Ether into Spiroketal Under Mild Acidic Condition. <i>Chemistry - A European Journal</i> , 0, , .	1.7	0
15351	Ultrafast optical limiting ability of <i>trans</i> -stilbene enhanced and broadened by a donor-acceptor structure. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7508-7518.	1.3	2

#	ARTICLE	IF	CITATIONS
15352	Reactivity of a model of B3P3-doped nanographene with up to three CO ₂ molecules. <i>Scientific Reports</i> , 2023, 13, .	1.6	4
15353	Preparation of nano disperse dyes using sulfomethylated lignin: Effects of sulfonic group contents. <i>International Journal of Biological Macromolecules</i> , 2023, 234, 123605.	3.6	6
15354	Electrochemical Removal of Ni ²⁺ EDTA Mediated by Chlorine and Hydroxyl Radicals on BDD Anodes. <i>ACS ES&T Water</i> , 2023, 3, 827-837.	2.3	12
15355	Novel class of crown ether functionalized ionic liquids with multiple binding sites for efficient separation of lithium isotopes. <i>Journal of Molecular Liquids</i> , 2023, 376, 121412.	2.3	4
15356	Theoretical Study on the Origin of Abnormal Regioselectivity in Ring-Opening Reaction of Hexafluoropropylene Oxide. <i>Molecules</i> , 2023, 28, 1669.	1.7	0
15357	New functionalized thioxanthone derivatives as type I photoinitiators for polymerization under UV-Vis LEDs. <i>New Journal of Chemistry</i> , 2023, 47, 5330-5337.	1.4	12
15358	Reaction Site Designation by Intramolecular Electric Field in Tröger's Base-Derived Conjugated Microporous Polymer for Near-Unity Selectivity of CO ₂ Photoconversion. <i>Advanced Materials</i> , 2023, 35, .	11.1	13
15359	Evolution of Solute-Water Interactions in the Benzaldehyde-(H ₂ O) ₆ Clusters by Rotational Spectroscopy. <i>Journal of the American Chemical Society</i> , 2023, 145, 4119-4128.	6.6	11
15360	Mechanistic insight into the degradation of 1H-benzotriazole and 4-methyl-1H-benzotriazole by H_2O_2 -based advanced oxidation process and toxicity assessment. <i>Environmental Science and Pollution Research</i> , 2023, 30, 49150-49161.	2.7	1
15361	X-Ray Crystallography, Spectral Analysis, DFT Studies, and Molecular Docking of (C ₉ H ₇) ₂ ETQO ₂ on <i>Staphylococcus aureus</i> (MRSA). <i>Polycyclic Aromatic Compounds</i> , 2024, 44, 178-200.	1.4	9
15362	Intramolecular interactions (O-H TM ...O, C-H TM ...N, N-H TM ...N) in isomers of neutral, cation, and anion dopamine molecules: A DFT study on the influence of solvents (water and ethanol). <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	0
15363	Absorption of ethylene dichloride with imidazolium-based ionic liquids. <i>Journal of Molecular Liquids</i> , 2023, 376, 121449.	2.3	0
15364	Effect of TiO ₂ nanoparticles on the mass transfer process of absorption of toluene: Experimental investigation and molecular dynamics simulation. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109474.	3.3	2
15365	Investigation of difluorobenzene bridged cross-conjugated benzodithiophene-based small molecules with efficient photovoltaic parameters. <i>Journal of Materials Science: Materials in Electronics</i> , 2023, 34, .	1.1	1
15366	Solvent potential effects (topological aspects, electron excitation), spectral characterization and biological attributes of NLO active 1-(2,4-dinitrophenyl)-2-((E)-3-phenylallylidene) hydrazine: Multiple anti tuberculosis agent. <i>Journal of Molecular Liquids</i> , 2023, 376, 121439.	2.3	19
15367	Exploring durability and environmental impact of cementitious composites modified by fluoroalkyl-silane based additive. <i>Construction and Building Materials</i> , 2023, 370, 130665.	3.2	2
15368	Local dynamics in a hydrogen-bonded organic framework for adaptive guest accommodation with programmable luminescence. <i>CheM</i> , 2023, 9, 1241-1254.	5.8	15

#	ARTICLE	IF	CITATIONS
15370	Substituent effect on controlled release of fragrant aldehydes from pH-triggered nicotinoylhydrazone-based precursors. <i>Molecular Systems Design and Engineering</i> , 0, , .	1.7	0
15371	Multi-energetic group synergy driven design and synthesis of [1,2,4]triazolo[5,1- <i>c</i>][1,2,4]triazine-fused energetic compounds. <i>Materials Chemistry Frontiers</i> , 2023, 7, 1046-1057.	3.2	3
15372	Enhancing cation storage performance of layered double hydroxides by increasing the interlayer distance. <i>Journal of Chemical Physics</i> , 2023, 158, 094703.	1.2	1
15373	Synthesis of Disubstituted Carboxonium Derivatives of Closo-Decaborate Anion [2,6-B10H8O2CC6H5] ^â : Theoretical and Experimental Study. <i>Molecules</i> , 2023, 28, 1757.	1.7	1
15374	Investigation of the Spatial Structure of Flufenamic Acid in Supercritical Carbon Dioxide Media via 2D NOESY. <i>Materials</i> , 2023, 16, 1524.	1.3	7
15375	Insights into elusive and cooperative multi-oxidant mechanisms in enabling catalytic methane-to-methanol conversion over atomically dispersed metals. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 1838-1851.	3.0	2
15376	Heuristic-Based Alkaline Hydrolysis Mechanism of Nitrate Ester (Nitrocellulose Monomer) and Nitroamine (Hexogen) Compounds: Electrostatic Attraction Effect of the Nitro Group. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1609-1618.	1.1	1
15377	Molecular Understanding and Practical In Silico Catalyst Design in Computational Organocatalysis and Phase Transfer Catalysisâ”Challenges and Opportunities. <i>Molecules</i> , 2023, 28, 1715.	1.7	2
15378	DFT mechanistic studies of boronâ”silicon exchange reactions between silyl-substituted arenes and boron bromides. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 6714-6725.	1.3	0
15379	Energetics and Ionicâ”Electronic and Geometric Variabilities of Hydroxylammonium-Based Salts. <i>Crystal Growth and Design</i> , 2023, 23, 1821-1831.	1.4	1
15380	Machine Learning Prediction of Hydration Free Energy with Physically Inspired Descriptors. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 1877-1884.	2.1	2
15381	Mechanistic insights into catalyst-dependent divergent cycloaddition reactions via discrimination between diazo compounds. <i>Organic Chemistry Frontiers</i> , 2023, 10, 1606-1616.	2.3	2
15382	New Low-Dimensional Organicâ”Inorganic Lead Halide Hybrid Systems Directed by Imidazo[1,5- <i>a</i>]pyridinium-Based Cation or Imines: Synthesis, Structures, Non-Covalent Interactions and Optical Properties. <i>Crystals</i> , 2023, 13, 307.	1.0	1
15383	Cyclic and linear germynes as ligands: DFT study. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	0
15384	The combination of polyphenols and phospholipids as an efficient platform for delivery of natural products. <i>Scientific Reports</i> , 2023, 13, .	1.6	5
15385	A <i>d</i> - ₃ - <i>p</i> -Conjugated System with High Mobility and Strong Emission Simultaneously. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	4
15386	Modulating the Energetics of Câ”H Bond Activation in Methane by Utilizing Metalated Porphyrinic Metalâ”Organic Frameworks. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 1832-1839.	2.1	4
15387	A localized high concentration carboxylic ester-based electrolyte for high-voltage and low temperature lithium batteries. <i>Chemical Engineering Journal</i> , 2023, 461, 141904.	6.6	7

#	ARTICLE	IF	CITATIONS
15389	Vibrational Spectroscopies, Global Reactivity, Molecular Docking, Thermodynamic Properties and Linear and Nonlinear Optical Parameters of Monohydrate Arsenate Salt of 4-Aminopyridine. <i>Chemistry Africa</i> , 2023, 6, 1897-1912.	1.2	6
15390	Enhanced TSG stability through co-assembly with C3G: the mechanism behind processing <i>Polygonum multiflorum</i> Thunb with black beans via supramolecular analysis. <i>Food and Function</i> , 2023, 14, 4204-4212.	2.1	2
15391	Solvent-solute interactions, electronic properties, topological and biological explorations of 6-Bromo-7-methylimidazo[1,2-a]pyridine. <i>Journal of Molecular Liquids</i> , 2023, 376, 121437.	2.3	7
15392	Characterization of the interaction between boscalid and tannic acid and its effect on the antioxidant properties of tannic acid. <i>Journal of Food Science</i> , 2023, 88, 1325-1335.	1.5	4
15393	Energetic Salts Based on a Bicyclic Nitrogen-Rich Compound with Good Molecular Stability. <i>Crystal Growth and Design</i> , 2023, 23, 1466-1476.	1.4	2
15394	A Spiro Phosphamide Catalyzed Enantioselective Proton Transfer of Ylides in a Free Carbene Insertion into N-H Bonds. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	10
15396	The ability of pre-magnetized zero-valent iron for peroxymonosulfate activation to remove ofloxacin. <i>Chemical Engineering Journal</i> , 2023, 461, 141825.	6.6	9
15397	A Spiro Phosphamide Catalyzed Enantioselective Proton Transfer of Ylides in a Free Carbene Insertion into N-H Bonds. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	0
15398	Efficient oxygen reduction using a polymorphic tungsten catalyst. <i>Cell Reports Physical Science</i> , 2023, 4, 101288.	2.8	3
15399	Facile Transformation from Rofecoxib to a New Near-Infrared Lipid Droplet Fluorescent Probe and Its Investigations on AIE Property, Solvatochromism and Mechanochromism. <i>Molecules</i> , 2023, 28, 1814.	1.7	0
15400	Square Planar Pt(II) Ion as Electron Donor in Pnictogen Bonding Interactions. <i>Inorganics</i> , 2023, 11, 80.	1.2	2
15401	Solubility measurement and molecular simulation of unsolvated and solvated estrogen receptor agonist (R)-equol in binary solvents (alcohols+ <i>n</i> -heptane) from 273.15K to 333.15K. <i>Journal of Molecular Liquids</i> , 2023, 376, 121460.	2.3	7
15402	Insensitive High-Energy Density Materials Based on Azazole-Rich Rings: 1,2,4-Triazole N-Oxide Derivatives Containing Isomerized Nitro and Amino Groups. <i>International Journal of Molecular Sciences</i> , 2023, 24, 3918.	1.8	3
15403	Insights into the mechanism of cumene catalytic oxidation using ionic liquid [Bmim]OH. <i>Molecular Catalysis</i> , 2023, 538, 113008.	1.0	0
15404	Study on host-guest interaction of aroma compounds/ β -cyclodextrin inclusion complexes. <i>LWT - Food Science and Technology</i> , 2023, 178, 114589.	2.5	5
15405	Orbital Polarization-Dependent Fragment Twist-Induced Intramolecular Electric-Field-Driven Charge Transfer. <i>Molecules</i> , 2023, 28, 1801.	1.7	0
15406	Regioisomeric Benzidine-Fullerenes: Tuning of the Diverse Hole-Distribution to Influence Charge Separation Patterns. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	4
15407	Porous and Stable Zn-Series Metal-Organic Frameworks as Efficient Catalysts for Grafting Wood Nanofibers with Polycaprolactone via a Copolymerization Approach. <i>Inorganic Chemistry</i> , 2023, 62, 3464-3473.	1.9	5

#	ARTICLE	IF	CITATIONS
15408	Designing Excess Electron Compounds by Substituting Alkali Metals to a Small and Versatile Tetracyclic Framework: A Theoretical Perspective. <i>ACS Omega</i> , 2023, 8, 7978-7988.	1.6	3
15409	Stability Mechanism of Menthol and Fatty Acid Based Hydrophobic Eutectic Solvents: Insights from Nonbonded Interactions. <i>ACS Sustainable Chemistry and Engineering</i> , 2023, 11, 3539-3556.	3.2	7
15410	Improving the TADF in Corannulene-Based Emitters via Tuning the Strength of Donor and Acceptor Groups. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	0
15411	Design, Synthesis, Biological Evaluation, and Molecular Dynamics Simulation of Influenza Polymerase PB2 Inhibitors. <i>Molecules</i> , 2023, 28, 1849.	1.7	3
15412	High capacity adsorption of oxytetracycline by lignin-based carbon with mesoporous structure: Adsorption behavior and mechanism. <i>International Journal of Biological Macromolecules</i> , 2023, 234, 123689.	3.6	14
15413	Rational Design to Activate Tetrafluoromethane by Two-Coordinate Borinium. <i>Inorganic Chemistry</i> , 2023, 62, 3518-3524.	1.9	0
15414	Complexation between rice starch and cellulose nanocrystal from black tea residues: Gelatinization properties and digestibility in vitro. <i>International Journal of Biological Macromolecules</i> , 2023, 234, 123695.	3.6	7
15415	Photochemical formation and reversible base-induced cleavage of a phosphagallene. <i>Chemical Science</i> , 2023, 14, 3018-3023.	3.7	5
15416	Study on the Synergistic Antioxidant Effect of Coal Inhibitors and the DFT Calculation. <i>Combustion Science and Technology</i> , 0, , 1-20.	1.2	0
15417	Challenging the Limitations of Tetranitro Biimidazole through Introducing a <i>gem</i> -Dinitromethyl Scaffold. <i>Organic Letters</i> , 2023, 25, 1290-1294.	2.4	9
15418	The location of the chemical bond. Application of long covalent bond theory to the structure of silica. <i>Frontiers in Chemistry</i> , 0, 11, .	1.8	0
15419	Metalloporphyrinyl-Phosphonates with Serrated Chain Structures: Exfoliation and NIR Photothermal Effect. <i>ACS Applied Electronic Materials</i> , 2023, 5, 887-895.	2.0	2
15420	Nano-deterioration of steel passivation film: chloride attack in material defects. <i>Materials and Structures/Materiaux Et Constructions</i> , 2023, 56, .	1.3	11
15421	Migration of tocopherols from the oil phase to the oil-water interface using phospholipids improved the oxidative stability of O/W emulsions. <i>Food Chemistry</i> , 2023, 414, 135719.	4.2	3
15422	Does side chain group of anion affect absorption of SO ₂ in amino acid ionic liquid?. <i>Journal of Molecular Liquids</i> , 2023, 376, 121479.	2.3	2
15423	Single Crystal Investigations, Hirshfeld Surface Analysis, DFT Studies, Molecular Docking, Physico-Chemical Characterization, and Biological Activity of a Novel Non-Centrosymmetric Compound with a Copper Transition Metal Precursor. <i>ACS Omega</i> , 2023, 8, 7738-7748.	1.6	3
15424	Intrinsic Charge Transport for DTzTI-Based All-Acceptor Homopolymer n-Type Organic Semiconductors: Roles of Conjugation Length and Orbital Delocalization. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4273-4282.	1.5	2
15425	Endohedral group-14 clusters Au@X ₁₂ (X=Ge, Sn, Pb) and their anions: A first-principles study. <i>Journal of Molecular Liquids</i> , 2023, 376, 121477.	2.3	4

#	ARTICLE	IF	CITATIONS
15426	Mg(σ -Fe) and Mg(O) σ -Mg(σ) covalent bonding in the Mg ₄ Fe(CO) ₄ ⁺ ($n = 1, 2$) anion complexes: an infrared photodissociation spectroscopic and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7697-7703.	1.3	5
15427	Centrosymmetric Nickel(II) Complexes Derived from Bis-(Dithiocarbamate)piperazine with 1,1 σ -Bis-(Diphenylphosphino)ferrocene and 1,2-Bis-(Diphenylphosphino)ethane as Ancillary Ligands: Syntheses, Crystal Structure and Computational Studies. <i>Crystals</i> , 2023, 13, 343.	1.0	2
15428	A new class of amide-based organogels: from oil spill recovery to self-assembly structure analysis. <i>Journal of Materials Chemistry A</i> , 2023, 11, 6181-6190.	5.2	1
15429	Super stable, highly ion-conductive and transparent eutecto-/hydro-gel promotes wearable electronic and visual strain sensing. <i>Chemical Engineering Journal</i> , 2023, 461, 141965.	6.6	5
15430	Praseodymium Metallacrown-Based NMR Probe for Enantioselective Discrimination of Mandelate Anions in Water. <i>Inorganic Chemistry</i> , 2023, 62, 3827-3835.	1.9	3
15431	AlEgens/Mitochondria Nanohybrids as Bioactive Microwave Sensitizers for Non-Thermal Microwave Cancer Therapy. <i>Advanced Healthcare Materials</i> , 2023, 12, .	3.9	4
15432	Electrolyte design principles for developing quasi-solid-state rechargeable halide-ion batteries. <i>Nature Communications</i> , 2023, 14, .	5.8	11
15433	Theoretical prediction of nanomolar and sequence-selective binding of synthetic supramolecular cucurbit[7]uril to N-terminal Leu-containing tripeptides. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7893-7900.	1.3	0
15434	Synthesis, Supramolecular Structural Investigations of Co(II) and Cu(II) Azido Complexes with Pyridine-Type Ligands. <i>Crystals</i> , 2023, 13, 346.	1.0	0
15435	First-principle insights of initial hydration behavior affected by copper impurity in alite phase based on static and molecular dynamics calculations. <i>Journal of Cleaner Production</i> , 2023, 398, 136478.	4.6	2
15436	Does a halogen bond require positive potential on the acid and negative potential on the base?. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7184-7194.	1.3	5
15437	Computational Exploration of Dirhodium Complex-Catalyzed Selective Intermolecular Amination of Tertiary vs. Benzylic C-H Bonds. <i>Molecules</i> , 2023, 28, 1928.	1.7	1
15438	Can Copper(I) and Silver(I) be Hydrogen Bond Acceptors?. <i>Chemistry - A European Journal</i> , 0, , .	1.7	0
15439	Enhancing selective adsorption of CO ₂ through encapsulating FeTPPs into Cu-BTC. <i>Chemical Engineering Journal</i> , 2023, 461, 141977.	6.6	12
15440	Phase Evolution on the Hydrogen Adsorption Kinetics of NiFe-Based Heterogeneous Catalysts for Efficient Water Electrolysis. <i>Small Methods</i> , 2023, 7, .	4.6	55
15441	Halogen Bond Involving Supramolecular Assembly Utilizing Carbon as a Nucleophilic Partner of Non-covalent Interaction. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	5
15442	Synthesis and Biological Evaluation of Octahydroquinazolinones as Phospholipase A ₂ and Protease Inhibitors: Experimental and Theoretical Exploration. <i>Molecules</i> , 2023, 28, 1944.	1.7	1
15443	Mechanism Analysis of PFHxS Purification in Water Using Nanofiltration under the Coexistence of Sodium Alginate and Ca ²⁺ Based on DFT. <i>Water (Switzerland)</i> , 2023, 15, 792.	1.2	0

#	ARTICLE	IF	CITATIONS
15444	Effect of molecular weight on the properties of water-soluble terpolymers for heavy oil viscosity reduction. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2023, 144, 104738.	2.7	6
15445	Methoxylated Modification of Glutathione-Mediated Metabolism of Halobenzoquinones In Vivo and In Vitro. <i>Environmental Science & Technology</i> , 2023, 57, 3581-3589.	4.6	0
15446	Chemical sensing ability of aminated graphdiyne (GDY-NH ₂) toward highly toxic organic volatile pollutants. <i>Computational and Theoretical Chemistry</i> , 2023, 1222, 114079.	1.1	3
15447	Adsorption of juglone on pure and boron-doped C ₂₄ fullerene-like nano-cage: A density functional theory investigation. <i>Computational and Theoretical Chemistry</i> , 2023, 1222, 114077.	1.1	5
15448	Computational Insights into Sensing Mechanism for Al ³⁺ in a New Acylhydrazone Fluorescent Probe Based on Excited-State Intramolecular Proton Transfer (ESIPT) and Twisted Intramolecular Charge Transfer (TICT). <i>Journal of Physical Chemistry A</i> , 2023, 127, 1857-1865.	1.1	3
15449	NHC-Stabilised Parent Triptentyltrielanes. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	1
15450	Synthesis of a Wheel-Shaped Nanographdiyne. <i>Journal of the American Chemical Society</i> , 2023, 145, 5400-5409.	6.6	20
15451	Highly Efficient Purely Organic Phosphorescence Light-Emitting Diodes Employing a Donor-Acceptor Skeleton with a Phenoxaselenine Donor. <i>Advanced Science</i> , 2023, 10, .	5.6	14
15452	BODIPY-Perylene Charge Transfer Compounds; Sensitizers for Triplet-Triplet Annihilation Up-conversion. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	5
15453	Metal ion-decorated hexasilaprismane and its derivative as a molecular container for the separation of CO ₂ from flue gas molecules: a computational study. <i>Dalton Transactions</i> , 2023, 52, 4336-4348.	1.6	0
15454	Carboxyl substituted Bambus[6]uril as a novel macrocyclic receptor for cyanide anion: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2023, 1222, 114081.	1.1	1
15455	Oxidopyridinium Cycloadditions Revisited: A Combined Computational and Experimental Study on the Reactivity of 1-(2-Pyrimidyl)-3-oxidopyridinium Betaine. <i>Journal of Organic Chemistry</i> , 2023, 88, 3193-3207.	1.7	3
15457	Weak Interactions Initiate C-H and C-C Bond Dissociation of Ethane on Nb ⁺ Clusters. <i>ChemPhysChem</i> , 2023, 24, .	1.0	0
15458	Theoretical Investigation on 1-Ethyl-3-Methylimidazolium Fluoride: A Density Functional Theory Study. <i>Science of Advanced Materials</i> , 2022, 14, 1732-1740.	0.1	0
15461	Femtosecond Time-Resolved Observation of Relaxation and Wave Packet Dynamics of the S ₁ State in Electronically Excited o-Fluoroaniline. <i>Molecules</i> , 2023, 28, 1999.	1.7	0
15462	In-source fragmentation of nucleosides in electrospray ionization towards more sensitive and accurate nucleoside analysis. <i>Analyst</i> , 2023, 148, 1500-1506.	1.7	1
15463	Tunable Photoinduced Charge Transfer at the Interface between Benzoselenadiazole-Based MOF Linkers and Thermally Activated Delayed Fluorescence Chromophore. <i>Journal of Physical Chemistry B</i> , 2023, 127, 1819-1827.	1.2	3
15464	A comparative study on nonlinear optical properties of zinc porphyrins analogs: Coordination atoms and group effects. <i>International Journal of Quantum Chemistry</i> , 0, .	1.0	0

#	ARTICLE	IF	CITATIONS
15465	Therapeutic Potential of B ₁₂ N ₁₂ -X (X = Au, Os, and Pt) Nanostructured as Effective Fluorouracil (5Fu) Drug Delivery Materials. ACS Applied Bio Materials, 2023, 6, 1146-1160.	2.3	23
15466	Algorithms and Software. Theoretical Chemistry and Computational Modelling, 2023, , 301-315.	0.2	0
15467	Exploring quantum computational, molecular docking, and molecular dynamics simulation with MMGBSA studies of ethyl-2-amino-4-methyl thiophene-3-carboxylate. Journal of Biomolecular Structure and Dynamics, 0, , 1-19.	2.0	3
15468	Neutral, Heteroleptic [Cu(I)(PPh ₃) ₂ (4 <i>H</i> -imidazolato)] Complexes: Ligand Exchange Reactivity, Redox Properties, Excited-State Dynamics. Chemistry - A European Journal, 2023, 29, .	1.7	0
15469	Facile Synthesis of Energetic Multi-Heterocyclic Compound via a Promising Intramolecular Integration Strategy. Crystal Growth and Design, 2023, 23, 2721-2729.	1.4	2
15470	Design and synthesis of phenylene-bridged isoxazole and tetrazole-1-ol based energetic materials of low sensitivity. Dalton Transactions, 2023, 52, 3449-3457.	1.6	7
15471	Application of lithium and a few relevant electrolytes evaluated as secondary batteries studied using molecular descriptors, band structure and DOS. Journal of Materials Science, 2023, 58, 4005-4019.	1.7	6
15472	Group 13 salphen compounds (In, Ga and Al): a comparison of their structural features and activities as catalysts for cyclic carbonate synthesis. Dalton Transactions, 2023, 52, 5882-5894.	1.6	4
15473	Exploration of photovoltaic behavior of fused triphenylamine moiety as core donor with modified acceptors: Star-shaped D-  -A conjugated systems. Materials Chemistry and Physics, 2023, 299, 127528.	2.0	2
15474	Supramolecular Interactions-Assisted Polymorphism and Unique Mechanofluorochromism in 9,10-Bis((<i>E</i>)-trifluoromethyl)styryl)anthracene. Chemistry - A European Journal, 2023, 29, .	1.7	7
15475	Probing the Mechanisms of Inhibitors Binding to Presenilin Homologue Using Molecular Dynamics Simulations. Molecules, 2023, 28, 2076.	1.7	2
15476	Molecular Dynamics Simulation of CO ₂ Hydrate Growth in NaCl Aqueous Solution. SPE Production and Operations, 2023, 38, 471-477.	0.4	1
15477	Design of high-performance circularly polarized multiple resonance-based TADF materials via participatory chiral perturbation. Journal of Materials Chemistry C, 2023, 11, 4033-4041.	2.7	6
15478	Mechanism and security of UV driven sodium percarbonate for sulfamethoxazole degradation using DFT and metabolomic analysis. Environmental Pollution, 2023, 323, 121352.	3.7	6
15479	Red-Emitting Dithienothiophene S,S-Dioxide Dyes for Cellular Membrane Staining. Materials, 2023, 16, 1806.	1.3	1
15480	One-Step Synthesis of White-Light-Emitting Carbon Dots for White LEDs with a High Color Rendering Index of 97. Advanced Science, 2023, 10, .	5.6	39
15481	Radical Pairing Interactions and Donor-Acceptor Interactions in Cyclobis(paraquat-p-phenylene) Inclusion Complexes. Molecules, 2023, 28, 2057.	1.7	0
15482	Electronic, intermolecular, quantum computational investigations, molecular docking and simulation studies of the potent antiviral drug EIDD-2801. Journal of the Indian Chemical Society, 2023, 100, 100953.	1.3	2

#	ARTICLE	IF	CITATIONS
15483	Enhanced performance of Pd-[DBU][Cl]/AC mercury-free catalysts in acetylene hydrochlorination. Chinese Journal of Catalysis, 2023, 46, 137-147.	6.9	1
15484	Synthesis and Activity of Aurone and Indanone Derivatives. Medicinal Chemistry, 2023, 19, .	0.7	1
15486	Direct Incorporation of Dinitrogen into an Aliphatic C-H Bond. Journal of the American Chemical Society, 2023, 145, 6773-6780.	6.6	3
15487	Multi-componential metal intercalated graphite hybrids synthesized by co-intercalation polymerization towards high-efficient microwave absorptions. Nano Research, 2023, 16, 6369-6379.	5.8	8
15488	Deformation constraints of graphene oxide nanochannels under reverse osmosis. Nature Communications, 2023, 14, .	5.8	19
15489	A Superphane-based carcerand for arsenic detoxification via imprisoning arsenate. Cell Reports Physical Science, 2023, 4, 101295.	2.8	3
15490	Unconventional Dual Donor-Acceptor Topologies of Aromatic Rings in Amine-Based Polymeric Tetrahedral Zn(II) Compounds Involving Unusual Non-Covalent Contacts: Antiproliferative Evaluation and Theoretical Studies. Crystals, 2023, 13, 382.	1.0	2
15491	Efficient Circularly Polarized Electroluminescence from Achiral Luminescent Materials**. Angewandte Chemie, 2023, 135, .	1.6	1
15492	The Role of the Transient Atropisomerism and Chirality of Flurbiprofen Unveiled by Laser-Ablation Rotational Spectroscopy. Chemistry - A European Journal, 2023, 29, .	1.7	0
15494	Mechanistic study of the formation of arbutin polymorphs and solvates. CrystEngComm, 2023, 25, 2075-2084.	1.3	3
15495	Electrochemical Opening of Impermeable Nanochannels in Laminar Graphene Membranes for Ultrafast Nanofiltration. Environmental Science & Technology, 2023, 57, 3843-3852.	4.6	5
15496	Re12C80: A pentagonal hexecontahedron molecule. Chemical Physics Letters, 2023, 816, 140392.	1.2	0
15497	Isolation, Structure Elucidation, and First Total Synthesis of Quinomycins K and L, Two New Octadepsipeptides from the Maowei Sea Mangrove-Derived Streptomyces sp. B475. Marine Drugs, 2023, 21, 143.	2.2	0
15498	Quantum Computational, Spectroscopic (FT-IR, FT-Raman, NMR, and UV-Vis) Hirshfeld Surface and Molecular Docking-Dynamics Studies on 5-Hydroxymethyluracil (Monomer and Trimer). Molecules, 2023, 28, 2116.	1.7	2
15499	Efficient Circularly Polarized Electroluminescence from Achiral Luminescent Materials**. Angewandte Chemie - International Edition, 2023, 62, .	7.2	14
15500	Unveiling Structural Diversity of Uranyl Compounds of Aprotic 4,4'-Bipyridine N_2O_2 -Dioxide Bearing O-Donors. ACS Omega, 2023, 8, 8894-8909.	1.6	1
15501	Alteration of the central core of a DF-PCIC chromophore to boost the photovoltaic applications of non-fullerene acceptor based organic solar cells. RSC Advances, 2023, 13, 6530-6547.	1.7	7
15502	Evolution of carbamazepine under solar irradiation in the presence of chlorine: Efficiency, influences, degradation pathways and ecotoxicity. Chemical Engineering Journal, 2023, 461, 142106.	6.6	8

#	ARTICLE	IF	CITATIONS
15503	Atroposelective desymmetrization of 2-arylresorcinols via Tsuji-Trost allylation. <i>Communications Chemistry</i> , 2023, 6, .	2.0	1
15504	Drug repurposing and molecular mechanisms of the antihypertensive drug candesartan as a TMEM16A channel inhibitor. <i>International Journal of Biological Macromolecules</i> , 2023, 235, 123839.	3.6	0
15505	Comparative study of raw and HNO ₃ -modified porous carbon from waste printed circuit boards for sulfadiazine adsorption: Experiment and DFT study. <i>Chinese Chemical Letters</i> , 2023, 34, 108272.	4.8	6
15506	A quantum chemical computation and model investigation for autoignition kinetic of a long chain oxygenate: Tri-propylene glycol methyl ether. <i>Fuel</i> , 2023, 343, 127933.	3.4	0
15507	Phosphorus-Enhanced and Calcium-Retarded Transport of Ferrihydrite Colloid: Mechanism of Electrostatic Potential Changes Regulated via Adsorption Speciation. <i>Environmental Science & Technology</i> , 2023, 57, 4219-4230.	4.6	26
15508	Enhanced Ultra-Long Room Temperature Phosphorescence by Intermolecular Donor-Acceptor Interaction in Polymer Network. <i>Advanced Optical Materials</i> , 2023, 11, .	3.6	3
15509	The Multiplicity of π - π Interactions of Fused-Ring Electron Acceptor Polymorphs on the Exciton Migration and Charge Transport. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 2331-2338.	2.1	4
15510	Spiro-Conjugation in Narrow-Bandgap Nonfullerene Acceptors Enables Broader Spectral Response and Higher Detectivity for Near-Infrared Organic Photodetectors. <i>Advanced Optical Materials</i> , 2023, 11, .	3.6	6
15511	Trapping of Small Molecules within Single or Double Cyclo[18]carbon Rings. <i>Molecules</i> , 2023, 28, 2157.	1.7	1
15512	Ligand-enabled silver-catalyzed carbene insertion into the N-H bond of aliphatic and electron-rich aromatic amines. <i>Organic Chemistry Frontiers</i> , 2023, 10, 1746-1753.	2.3	2
15513	The decisive role of adsorbed OH* in low-potential CO electro-oxidation on single-atom catalytic sites. , 2023, 5, .		2
15514	DENSITY FUNCTIONAL THEORY INVESTIGATION ON DRUG-DRUG INTERACTIONS: ESCITALOPRAM AND SALICYLIC ACID. <i>EskiÅehir Teknik Åniversitesi Bilim Ve Teknoloji Dergisi B - Teorik Bilimler</i> , 0, , .	0.0	1
15515	A perspective on the role of anions in highly concentrated aqueous electrolytes. <i>Energy and Environmental Science</i> , 2023, 16, 1480-1501.	15.6	37
15516	A boronic acid conjugation integrates antitumor drugs into albumin-binding prodrugs-based nanoparticles with robust efficiency for cancer therapy. <i>Nano Research</i> , 0, , .	5.8	1
15517	Hydrated electrons as nodes in porous clathrate hydrates. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	1
15518	Tuning excited state electronic structure and charge transport in covalent organic frameworks for enhanced photocatalytic performance. <i>Nature Communications</i> , 2023, 14, .	5.8	111
15519	Comparative study of the hydrogen bonding interactions between ester-functionalized/non-functionalized imidazolium-based ionic liquids and DMSO. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8789-8798.	1.3	5
15520	Self-Assembly of the Tetraphenylethylene-Capped Diserine through a Hierarchical Assembly Process. <i>Bioconjugate Chemistry</i> , 2023, 34, 562-571.	1.8	0

#	ARTICLE	IF	CITATIONS
15521	The study on gas phase dehydrogenation reactions of transition metal cation and ethylene. <i>Molecular Physics</i> , 2023, 121, .	0.8	1
15522	Catalytic activity of OH functionalized N-doped graphene in oxygen reduction reaction for fuel cell applications: a DFT study. <i>Applied Physics A: Materials Science and Processing</i> , 2023, 129, .	1.1	7
15523	Modified UiO-66-Br Microphotocatalyst with High Electron Mobility Enhances Tetracycline Degradation. <i>Langmuir</i> , 2023, 39, 3678-3691.	1.6	5
15524	Mechanism and Origins of Site-Selectivity of Template-Directed C-H Insertion of Quinolines. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	2
15525	Peroxidase-like Nanozymes for Point-of-Care SERS Sensing and Wound Healing. <i>ACS Applied Bio Materials</i> , 2023, 6, 1272-1282.	2.3	3
15526	Electrical Breakdown Mechanism of ENB-EPDM Cable Insulation Based on Density Functional Theory. <i>Polymers</i> , 2023, 15, 1217.	2.0	2
15527	Porous Covalent Organic Framework Based Hydrogen-Bond Nanotrap for the Precise Recognition and Separation of Gold. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	2
15528	Porous Covalent Organic Framework Based Hydrogen-Bond Nanotrap for the Precise Recognition and Separation of Gold. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	17
15529	A novel silica-reinforced P(AM/AMPS/SA/TM-SiO ₂) microspheres for selective adsorption of methylene blue from aqueous solution. <i>Separation and Purification Technology</i> , 2023, 313, 123495.	3.9	5
15530	Unlocking the potential of ovalene: A dual-purpose sensor and drug enhancer. <i>Journal of Molecular Liquids</i> , 2023, 377, 121540.	2.3	8
15531	Importance of Noncovalent Interactions Involving Sulfur Atoms in Thiopeptide Antibiotics—Glycothiohexide I± and Nocathiacin I. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2081-2090.	1.1	0
15532	Impact of External Electronic Perturbations on Single-Walled Carbon Nanotube Electronic Structure: Scanning Tunneling Spectroscopy and Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4651-4659.	1.5	2
15533	Ladderphane copolymers for high-temperature capacitive energy storage. <i>Nature</i> , 2023, 615, 62-66.	13.7	82
15534	Investigation of NLO properties and molecular docking of 3, 5-dinitrobenzoic acid with some benzamide derivatives. <i>International Journal of Computational Materials Science and Engineering</i> , 0, , .	0.5	0
15535	Intermolecular interactions of cytosine DNA nucleoside base with Gallic acid and its Methylgallate and Ethylgallate derivatives. <i>ChemistrySelect</i> , 2023, 8, .	0.7	17
15536	Pyridine Ionic Liquid-Based Deep Eutectic Solvents Selectively Separating Toluene from Alkanes. <i>Energy & Fuels</i> , 2023, 37, 4233-4243.	2.5	2
15537	Synthesis, Molecular, and Supramolecular Structures of Two Azide-Bridged Cd(II) and Cu(II) Coordination Polymers. <i>Symmetry</i> , 2023, 15, 619.	1.1	1
15538	An exotic 3-center/4-electron carbon-carbon pi long-bond: Is it tangible?. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	0

#	ARTICLE	IF	CITATIONS
15539	Photoluminescent Properties and Mechanism of Novel Cyanine-Boron difluoride Curcuminoid Hybrids as Red/Near Infrared and Endoplasmic Reticulum-Targeting Dyes. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	1
15540	Morphological Regulation Mechanism of Tubular Ferrous Oxalate: Theoretical and Experimental Study. <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
15541	A simply visual and rapidly colorimetric detection of Hg ²⁺ in cosmetics based on gold nanoparticles modified by sulfadiazine. <i>Optical Materials</i> , 2023, 137, 113622.	1.7	2
15543	QM Calculations Revealed that Outer-Sphere Electron Transfer Boosted O-O Bond Cleavage in the Multiheme-Dependent Cytochrome <i>bd</i> Oxygen Reductase. <i>Inorganic Chemistry</i> , 2023, 62, 4066-4075.	1.9	1
15544	Effect of intermolecular interaction of the charge-transfer complex between molecular tweezers and C ₆₀ /C ₇₀ on second-order nonlinear optical properties. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8799-8808.	1.3	0
15545	Experimental and Theoretical Investigation of Hydrogen-Bonding Interactions in Cocrystals of Sulfaguanidine. <i>Crystal Growth and Design</i> , 2023, 23, 2306-2320.	1.4	5
15547	Aggregation Triggers Red/Near-Infrared Light Hydrogen Production of Organic Dyes with High Efficiency. <i>ACS Catalysis</i> , 2023, 13, 3723-3734.	5.5	10
15548	Assessment of the performance of six indices in predicating the aromaticity of planar porphyrinoids. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	0
15549	Synthesis of a π -Extended Double [9]Helicene. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	11
15550	Optimization of Spatial Arrangement and Optical Nonlinearity of Chalcone Crystals by Halogen Substituted Donor Groups. <i>Crystal Growth and Design</i> , 2023, 23, 2583-2592.	1.4	1
15551	Insights into the regioselectivity and diastereoselectivity of the Nazarov cyclization of 3-alkenyl-2-indolylmethanol with tryptophol. <i>Organic Chemistry Frontiers</i> , 2023, 10, 1721-1730.	2.3	2
15552	Turning dead leaves into an active multifunctional material as evaporator, photocatalyst, and bioplastic. <i>Nature Communications</i> , 2023, 14, .	5.8	27
15553	Reactivity and Selectivity of the Diels-Alder Reaction of Anthracene in [Pd ₆ L ₄] ¹²⁺ Supramolecular Cages: A Computational Study. <i>Inorganic Chemistry</i> , 2023, 62, 4330-4340.	1.9	2
15554	An ESIPT-based NIR-fluorescent probe for exosome labeling and in situ imaging. <i>Chinese Chemical Letters</i> , 2023, 34, 108273.	4.8	0
15555	A Series of Singlet-Triplet Inverted TADF Fluorescent Probes with High Stability, Low Molecular Weight, and Synthesis Accessibility. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	2
15556	C3-selective C-H thiolation of quinolines <i>via</i> an <i>N</i> -arylmethyl activation strategy. <i>Organic Chemistry Frontiers</i> , 2023, 10, 2324-2331.	2.3	2
15557	Computational and experimental studies of salvianolic acid A targets 3C protease to inhibit enterovirus 71 infection. <i>Frontiers in Pharmacology</i> , 0, 14, .	1.6	0
15558	TWO-DIMENSIONAL Cu(II) 5-IODOISOPHTHALATE WITH A 1,2-BIS(4-PYRIDYL)ETHYLENE LINKER: CRYSTAL STRUCTURE AND FEATURES OF ELECTRONIC STRUCTURE. <i>Journal of Structural Chemistry</i> , 2023, 64, 112-120.	0.3	0

#	ARTICLE	IF	CITATIONS
15559	Synthesis of a π - π Extended Double [9]Helicene. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	0
15560	Molecular Insights into Cyclodextrin-Adamantane-Modified Copolymer Host-Guest Interactions. <i>Langmuir</i> , 2023, 39, 3619-3627.	1.6	2
15561	A novel strategy for producing low-sugar pomegranate jam with better anthocyanin stability: Combination of high-pressure processing and low methoxyl & amidated pectin. <i>LWT - Food Science and Technology</i> , 2023, 179, 114625.	2.5	1
15562	Afterglow OLEDs incorporating bright closely stacked molecular dimers with ultra-long thermally activated delayed fluorescence. <i>Matter</i> , 2023, 6, 1231-1248.	5.0	10
15563	Ligand-Receptor Interactions of Lamivudine: A View from Charge Density Study and QM/MM Calculations. <i>Biomedicines</i> , 2023, 11, 743.	1.4	2
15564	Computational insight into gold(π)-catalyzed intramolecular regioselectivity of tryptamine-ynamide cycloisomerizations. <i>Organic and Biomolecular Chemistry</i> , 2023, 21, 2610-2619.	1.5	0
15565	Brønsted Acids Promote Olefin Oxidations by Bioinspired Nonheme Co(^{III})(PhIO)(OH) Complexes: A Role for Low-Barrier Hydrogen Bonds. <i>Journal of the American Chemical Society</i> , 2023, 145, 5739-5749.	6.6	9
15566	Cobalt-catalyzed radical-mediated carbon-carbon scission via a radical-type migratory insertion. <i>Chemical Science</i> , 2023, 14, 3352-3362.	3.7	5
15567	Anti-Quenching NIR Aggregates of Benzo[c]thiophene Fluorophore for Highly Efficient Bioimaging and Phototheranostics. <i>Advanced Materials</i> , 2023, 35, .	11.1	28
15568	Benzoxazole-Based Hybridized Local and Charge-Transfer Deep-Blue Emitters for Solution-Processable Organic Light-Emitting Diodes and the Influences of Hexahydrophthalimido. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 13415-13426.	4.0	4
15569	Nature and Strength of Sulfur-Centered Hydrogen Bond in Methanethiol Aqueous Solutions. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2265-2273.	1.1	1
15570	Mechanistic insights into H ₃ B-NMe ₂ dehydrogenation by Co-based complexes: a DFT perspective. <i>New Journal of Chemistry</i> , 2023, 47, 6661-6672.	1.4	1
15572	Activation of metal-involved halogen bonds and classical halogen bonds in gold(π) catalysis. <i>Dalton Transactions</i> , 2023, 52, 4517-4525.	1.6	3
15573	Electron heat transport in low-rank lignite: combining experimental and computational methods. <i>Journal of Thermal Analysis and Calorimetry</i> , 2023, 148, 4759-4768.	2.0	3
15574	From M ₆ to M ₁₂ , M ₁₉ and M ₃₈ molecular alloy Pt-Ni carbonyl nanoclusters: selective growth of atomically precise heterometallic nanoclusters. <i>Dalton Transactions</i> , 2023, 52, 3623-3642.	1.6	2
15575	Exploring electronic energy level structure and excited electronic states of β -carotene using DFT. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 9373-9381.	1.3	5
15576	Design and Synthesis of Nitro Cage Heterocycles as Energetic Materials Derived from Pentacycloundecane (PCUD) Systems. <i>Asian Journal of Organic Chemistry</i> , 2023, 12, .	1.3	0
15577	Salification-driven strategy toward the hydrophobic molecular salt of the antifungal drug 5-fluorocytosine and protocatechuic acid with triple-helix structure offers an innovative insight for conquering adverse drug reactions. <i>CrystEngComm</i> , 2023, 25, 1951-1964.	1.3	4

#	ARTICLE	IF	CITATIONS
15578	Synthesis, X-ray characterization and DFT calculations of a series of 3-substituted 4,5-dichloroisothiazoles. <i>CrystEngComm</i> , 2023, 25, 1976-1985.	1.3	0
15579	Theoretical descriptions of novel silicon analogs of cyclo[18]carbon. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	1
15580	Tunable Fluorescent Artificial Receptor Biosensor Based on Programmable Lanthanide Metal-Organic Framework for Highly Selective Neurotransmitter Detection. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	13
15581	Near-infrared absorbing acceptor with suppressed triplet exciton generation enabling high performance tandem organic solar cells. <i>Nature Communications</i> , 2023, 14, .	5.8	35
15582	Neglected acidity pitfall: boric acid-anchoring hole-selective contact for perovskite solar cells. <i>National Science Review</i> , 2023, 10, .	4.6	11
15583	Amide-Functional, Li ₃ N/Li-Rich Heterostructured Electrode Electrolyte Interphases for 4.6V Li LiCoO ₂ Batteries. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	31
15584	Acid-tailored self-assembled perylene diimide supramolecular for visible-light-driven activation of peroxymonosulfate towards efficient degradation of iohexol. <i>Chemical Engineering Journal</i> , 2023, 462, 142116.	6.6	6
15585	Exploring the Relationship between Reactivity and Electronic Structure in Isorhodanine Derivatives Using Computer Simulations. <i>Molecules</i> , 2023, 28, 2360.	1.7	1
15586	Theoretical insights into luminescence mechanism of Naphthyridine-based thermally activated delayed fluorescence emitter with aggregation-induced emission. <i>Chemical Physics Letters</i> , 2023, 817, 140407.	1.2	3
15587	Circumcoronenes. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	1
15588	<sc>3D</sc> molecular stars with covalent axial bonding. <i>Journal of Computational Chemistry</i> , 2023, 44, 1410-1417.	1.5	0
15589	Crystal and electronic structure of thiazolium pentaiodide: an experimental and theoretical study of covalent and non-covalent bonds. <i>Structural Chemistry</i> , 0, , .	1.0	0
15590	Superhydrophilic All-Carbon Adaptable Redox Conjugated Porous Polymers as Universal and Ultrarobust Ion Hosts for Diverse Energy Storage with Chemical Self-Chargeability. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	1
15591	Copper and Nickel Complexes of Oxamate-Phenol Containing Ligands: A Structural Dichotomy in Oxidized Species. <i>European Journal of Inorganic Chemistry</i> , 2023, 26, .	1.0	1
15592	Selective binding and periodic arrangement of magic boron clusters on monolayer borophene. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2023, 120, .	3.3	2
15593	Sulphur vs NH Group: Effects on the CO ₂ Electroreduction Capability of Phenylenediamine-Cp Cobalt Complexes. <i>Molecules</i> , 2023, 28, 2364.	1.7	1
15594	Virtual Screening, Structural Analysis, and Formation Thermodynamics of Carbamazepine Cocrystals. <i>Pharmaceutics</i> , 2023, 15, 836.	2.0	8
15595	Circumcoronenes. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	9

#	ARTICLE	IF	CITATIONS
15596	Microscopic Mechanism of Electrical Aging of PVDF Cable Insulation Material. <i>Polymers</i> , 2023, 15, 1286.	2.0	0
15597	Selektive Darstellung von Phosphormononitrid (Pâ%¸jN) aus Phosphinazid und Reversible Oxidation zu Phosphinnitren. <i>Angewandte Chemie, O, , .</i>	1.6	0
15598	Synthesis, characterization and exploration of photovoltaic behavior of hydrazide based scaffolds: a concise experimental and DFT study. <i>RSC Advances</i> , 2023, 13, 7237-7249.	1.7	1
15599	Tetrel bond involving -CH₃ group in H_nXCH₃ (Xâ€¸=â€¸F, Cl, and Br, nâ€¸=â€¸0;) Tj ETQq Physics, 2023, 121, .	0.8	1
15600	Catalystâ€Free Photochemical Activation of Peroxymonosulfate in Xantheneâ€Rich Systems for Fentonâ€Like Synergistic Decontamination: Efficacy of Proton Transfer Process. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	14
15601	Mechanism and origins of ligand-controlled regioselectivity of copper-catalyzed borocarbonylation of imines with B₂pin₂ and alkyl iodides: a computational study. <i>Organic Chemistry Frontiers</i> , 2023, 10, 2024-2032.	2.3	0
15602	Effects of Electron Donating Ability of Substituents and Molecular Conjugation on the Electronic Structures of Organic Radicals. <i>Chemical Research in Chinese Universities</i> , 2023, 39, 202-207.	1.3	1
15603	Synthesis of heterometallic binuclear cobalt(II) phthalocyanines and their catalytic activity in the oxidation of a mercaptan. <i>Journal of Porphyrins and Phthalocyanines</i> , 2023, 27, 694-701.	0.4	0
15604	Metal Atoms (Li, Na, and K) Tuning the Configuration of Pyrrole for the Selective Recognition of C₆₀. <i>Inorganic Chemistry</i> , 2023, 62, 4618-4624.	1.9	2
15605	Selective Preparation of Phosphorus Mononitride (Pâ%¸jN) from Phosphinoazide and Reversible Oxidation to Phosphinonitrene. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	4
15606	Study on Removal Mechanism for Copper Cyanide Complex Ions in Water: Ion Species Differences and Evolution Process. <i>International Journal of Molecular Sciences</i> , 2023, 24, 5066.	1.8	0
15607	Cold Oxidative Demetalation of Aryl Organometallics: A Novel Route to Demetalate Ullmann Intermediates without Heating. <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
15608	Sex-Specific Bioaccumulation, Maternal Transfer, and Tissue Distribution of Legacy and Emerging Per- and Polyfluoroalkyl Substances in Snakes (<i>Enhydri chinensis</i>) and the Impact of Pregnancy. <i>Environmental Science & Technology</i> , 2023, 57, 4481-4491.	4.6	2
15609	Bis(perfluoroaryl)chalcogenes Ar^F₂Ch (Ch = S, Se, Te) as ĩf/ĩ-Hole Donors for Supramolecular Applications Based on Noncovalent Bonding. <i>Crystal Growth and Design</i> , 2023, 23, 2593-2601.	1.4	3
15610	Antioxidant activity of Hibiscetin and Hibiscitrin: insight from DFT, NCI, and QTAIM. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	7
15611	Using a diphenyl-bi-(1,2,4-triazole) tricarbonylrhenium(<sc>i</sc>) complex with intramolecular ĩâ€ĩ stacking interaction for efficient solid-state luminescence enhancement. <i>Dalton Transactions</i> , 2023, 52, 5453-5465.	1.6	3
15612	Heteronuclear Dual Single-Atom Catalysts for Ambient Conversion of CO₂ from Air to Formate. <i>ACS Catalysis</i> , 2023, 13, 3915-3924.	5.5	12
15613	Development of Carbon Nanotube/Grapheneâ€Based Alginate Interpenetrating Hydrogels for Removal of Antibiotic Pollutants. <i>ChemPlusChem</i> , 2023, 88, .	1.3	4

#	ARTICLE	IF	CITATIONS
15614	Unraveling the charge transfer variation of tetrathiafulvalene-based organic crystals through fragment charge difference calculation. <i>APL Materials</i> , 2023, 11, 031104.	2.2	0
15615	Photovoltaic characteristics of organic heterocyclic 2,9-dimethyl quinacridone in different solvents using DFT approach. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 441, 114664.	2.0	9
15616	Heteroatom (B, N, P, and S)-Doped Cyclodextrin as a Hydroxyurea (HU) Drug Nanocarrier: A Computational Approach. <i>ACS Omega</i> , 2023, 8, 9861-9872.	1.6	14
15617	Theoretical framework for achieving high V_{oc} in non-fused non-fullerene terthiophene-based end-capped modified derivatives for potential applications in organic photovoltaics. <i>RSC Advances</i> , 2023, 13, 7535-7553.	1.7	26
15618	Odorant-Binding Protein 6 Contributes High Binding Affinity to Insecticides in a Parasitic Wasp <i>Meteorus pulchricornis</i> (Hymenoptera: Braconidae). <i>Journal of Agricultural and Food Chemistry</i> , 2023, 71, 4498-4509.	2.4	9
15619	Synthesis and a combined experimental/theoretical structural study of a comprehensive set of Pd/NHC complexes with o -, m -, and p -halogen-substituted aryl groups (X = F, Cl, Br). <i>TJ ETQq1 1 0.7843164 rgBT /Overlock</i>	1.6	0
15620	Theoretical Investigation of Ru(II) Complexes with Long Lifetime and a Large Two-Photon Absorption Cross-Section in Photodynamic Therapy. <i>Journal of Medicinal Chemistry</i> , 2023, 66, 4167-4178.	2.9	10
15621	Penta-coordinated or -valent: the nature of the chemical bond of some Ti-C-Al compounds. <i>Dalton Transactions</i> , 2023, 52, 4494-4500.	1.6	0
15622	New insights into the alkoxy effects on auxiliary adsorption and inhibiting charge recombination in dye-sensitized solar cells with high open circuit voltage: a theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8532-8543.	1.3	1
15623	Multiple stable redox states and tunable ground states via the marriage of viologens and Chichibabin's hydrocarbon. <i>Chemical Science</i> , 2023, 14, 3548-3553.	3.7	5
15624	Use the Functional Electrolyte Containing 2-Propynemethanesulfonate or 2-Propynebenzenesulfonate Additives to Improve the Long-Cycle Performance of $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ /Graphite Batteries. <i>Journal of the Electrochemical Society</i> , 2023, 170, 030526.	1.3	0
15626	Efficient synergistic degradation of tetracycline hydrochloride by protonated g-C ₃ N ₄ and <i>Chlorella pyrenoidosa</i> : Kinetics and mechanism. <i>Chemical Engineering Journal</i> , 2023, 462, 142331.	6.6	2
15627	Experimental and Computational Study on the Effects of High Pressure on the Crystal Structure of Boron Nitridetriacetate. <i>Crystal Growth and Design</i> , 2023, 23, 2745-2754.	1.4	1
15628	Synthesis, Structure, Hirshfeld Surface Analysis, Non-Covalent Interaction, and In Silico Studies of 4-Hydroxy-1-[(4-Nitrophenyl)Sulfonyl]Pyrrolidine-2-Carboxylic Acid. <i>Journal of Chemical Crystallography</i> , 2023, 53, 386-399.	0.5	2
15629	One-Component Artificial Gustatory System Based on Hydrogen-Bond Organic Framework for Discrimination of Versatile Analytes. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	10
15630	Quantum chemical analysis and spectroscopic characterization of Escitalopram. <i>Materials Today: Proceedings</i> , 2023, , .	0.9	1
15631	Supramolecular Organization in Salts of Riluzole with Dihydroxybenzoic Acids—The Key Role of the Mutual Arrangement of OH Groups. <i>Pharmaceutics</i> , 2023, 15, 878.	2.0	4
15632	Cu(II) removal from water by trimercapto-s-triazine trisodium salt modified alkaline lignin. <i>Environmental Science and Pollution Research</i> , 2023, 30, 55314-55325.	2.7	0

#	ARTICLE	IF	CITATIONS
15633	DFT calculations, spectroscopic investigations, and molecular docking study of Methylprednisolone with some selective cancer proteins. <i>Materials Today: Proceedings</i> , 2023, , .	0.9	1
15634	REDUCTION PROPERTIES OF GERMANIUM DICHLORIDE WITH RESPECT TO THE REDOX-ACTIVE MONOIMINOACENAPHTHENONE dpp-MIAN. <i>Journal of Structural Chemistry</i> , 2023, 64, 288-301.	0.3	0
15635	O,S-Acetals in a New Modification of oxo-Friedelâ€“Craftsâ€“Bradsher Cyclizationâ€“Synthesis of Fluorescent (Hetero)acenes and Mechanistic Considerations. <i>Molecules</i> , 2023, 28, 2474.	1.7	1
15636	Theoretical Insights into the Selectivity of Hydrophilic Sulfonated and Phosphorylated Ligands to Am(III) and Eu(III) Ions. <i>Inorganic Chemistry</i> , 2023, 62, 4581-4589.	1.9	5
15637	K ⁺ -Selectivity Due to Coordination with a D ₄ -Symmetric Homochiral Proline Octamer Verified by Mass Spectrometry and Infrared Photodissociation Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 2660-2664.	2.1	2
15638	Reactions of Zinc Hydride with Silylenes: From Oxidative Addition to Ligand Exchange Reactions. <i>Organometallics</i> , 2023, 42, 457-464.	1.1	0
15639	Extremely-Long-Lifespan and Ultrahigh-Rate Li-Ion Batteries Using Conjugated Porous Triazine Polymers. <i>ACS Applied Materials & Interfaces</i> , 0, , .	4.0	1
15640	Vanadium Pentafulvene Complexes: Synthons for Unprecedented Vanadocene ^{III} Derivatives. <i>Chemistry - A European Journal</i> , 2023, 29, , .	1.7	1
15641	Dynamic Disorder Drives Exciton Dynamics in Diketopyrrolopyrroleâ€“Thiophene-Containing Molecular Crystals. <i>Journal of Physical Chemistry C</i> , 2023, 127, 5519-5532.	1.5	0
15642	Assessment of the Capability and Potential of Pristine, Sc-, Ti-, and Ni-Doped C24 Nanocages to Delivery and Sensor Property of Prothionamide Drug: Insight of DFT, TD-DFT Computational Methods. <i>Journal of Computational Biophysics and Chemistry</i> , 2023, 22, 551-568.	1.0	0
15643	DFT study of efficient hydrogen storage on B ₁₂ @Ca ₁₄ cage. <i>Physica Scripta</i> , 2023, 98, 045409.	1.2	0
15644	Disturbance of intermolecular forces: eutectics as a new tool for the preparation of vapor-phase deposition precursors. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8336-8340.	1.3	2
15645	A BODIPY-based probe for amyloid- β^2 imaging <i>in vivo</i> . <i>Organic Chemistry Frontiers</i> , 2023, 10, 1903-1909.	2.3	4
15646	Bottom-Up Synthesis of Metalated Carbyne Ribbons via Elimination Reactions. <i>Journal of the American Chemical Society</i> , 2023, 145, 6203-6209.	6.6	0
15647	Density of States Engineering of nâ€“Doped Conjugated Polymers for High Charge Transport Performances. <i>Advanced Materials</i> , 2023, 35, , .	11.1	10
15648	Improving the stability of hydrazinium pentazolates through cocrystallization. <i>CrystEngComm</i> , 2023, 25, 2027-2031.	1.3	4
15649	Research on separation sulfides from fuel oil using sulfolane: Liquid-liquid equilibrium and mechanism exploration. <i>Journal of Chemical Thermodynamics</i> , 2023, 182, 107036.	1.0	5
15650	Ternary synergistic aggregation of chlorophyll/Soy protein isolate improves chlorophyll stability. <i>Food Hydrocolloids</i> , 2023, 140, 108662.	5.6	1

#	ARTICLE	IF	CITATIONS
15651	Tetrel-Bond Interactions Involving Metallylenes TH ₂ (T = Si, Ge, Sn, Pb): Dual Binding Behavior. <i>Molecules</i> , 2023, 28, 2577.	1.7	2
15652	Thermally Stable and Insensitive Energetic Cocrystals Comprising Nitrobarbituric Acid Cofomers. <i>Crystal Growth and Design</i> , 2023, 23, 2826-2836.	1.4	5
15653	Excited-State Polarizabilities: A Combined Density Functional Theory and Information-Theoretic Approach Study. <i>Molecules</i> , 2023, 28, 2576.	1.7	4
15654	Source preventing mechanism of florfenicol resistance risk in water by VUV/UV/sulfite advanced reduction pretreatment. <i>Water Research</i> , 2023, 235, 119876.	5.3	4
15655	Divalent organic cations as a novel protective layer for perovskite materials. <i>Journal of Materials Chemistry A</i> , 2023, 11, 11684-11695.	5.2	3
15656	Dynamic Approach to Synthetic Lectin for Glucose with Boosted Binding Affinity through C ⁺ H Hydrogen Bonds. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	3
15657	Modulating the Roaming Dynamics for the NO Release in <i>ortho</i> -Nitrobenzenes. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 2816-2822.	2.1	3
15658	Strong External Electric Fields Reduce Explosive Sensitivity: A Theoretical Investigation into the Reaction Selectivity in NH ₂ NO ₂ • TM • TM NH ₃ . <i>Molecules</i> , 2023, 28, 2586.	1.7	1
15659	Analysis of the Electron Density of a Water Molecule Encapsulated by Two Cholic Acid Residues. <i>International Journal of Molecular Sciences</i> , 2023, 24, 5359.	1.8	1
15660	Asymmetrically coordinated cobalt single atom on carbon nitride for highly selective photocatalytic oxidation of CH ₄ to CH ₃ OH. <i>CheM</i> , 2023, 9, 1017-1035.	5.8	25
15661	Smart Reversible Transformations between Chiral Superstructures of Copper Clusters for Optical and Chiroptical Switching. <i>Journal of the American Chemical Society</i> , 2023, 145, 6166-6176.	6.6	20
15662	Group IIIA Single-Metal Atoms Anchored on Hexagonal Boron Nitride for Selective Adsorption Desulfurization via S ⁺ M Bonds. <i>Inorganic Chemistry</i> , 2023, 62, 4883-4893.	1.9	12
15663	Searching for Systems with Planar Hexacoordinate Carbons. <i>Atoms</i> , 2023, 11, 56.	0.7	2
15664	Structural Analysis of Interactions between Epidermal Growth Factor Receptor (EGFR) Mutants and Their Inhibitors. <i>Biophysica</i> , 2023, 3, 203-213.	0.6	3
15665	Theoretical study on the solvent-free self-catalyzed coupling mechanism of a chiral vicinal diamine and isobutyraldehyde mediated by the outgrowth H ₂ O. <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
15666	A Novel Pyridine and Julolidine Based Chemosensor for Al ³⁺ Detection. <i>ChemistrySelect</i> , 2023, 8, .	0.7	2
15667	Target State Optimized Density Functional Theory for Electronic Excited and Diabatic States. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1777-1789.	2.3	3
15668	Two-photon fluorescence imaging and specifically biosensing of norepinephrine on a 100-ms timescale. <i>Nature Communications</i> , 2023, 14, .	5.8	10

#	ARTICLE	IF	CITATIONS
15669	A review on medicinally important heterocyclic compounds and importance of biophysical approach of underlying the insight mechanism in biological environment. Journal of Biomolecular Structure and Dynamics, 2023, 41, 14599-14619.	2.0	3
15670	Interpretable Machine Learning Model for Predicting Interaction Energies between Dimethyl Sulfide and Potential Absorbing Solvents. Industrial & Engineering Chemistry Research, 2023, 62, 5274-5285.	1.8	2
15671	Synthesis and Properties of a Through-Space Interacting Diradicaloid. , 2023, 1, 183-191.		3
15672	Influence of β -Cyclodextrin Methylation on Host-Guest Complex Stability: A Theoretical Study of Intra- and Intermolecular Interactions as Well as Host Dimer Formation. Molecules, 2023, 28, 2625.	1.7	3
15673	Amido-ene(amido) Ni(II)-Catalyzed Highly Enantioselective Transfer Hydrogenations of Ketone: Dual Functions of the Ene(amido) Group. ACS Catalysis, 2023, 13, 4261-4271.	5.5	9
15674	A Comprehensive Ab Initio Study of Halogenated A \cdot U and G \cdot C Base Pair Geometries and Energies. International Journal of Molecular Sciences, 2023, 24, 5530.	1.8	2
15675	A Comprehensive Investigation into the Crystallography, Molecule, and Quantum Chemistry Properties of Two New Hydrous Long-Chain Dibasic Ammonium Salts C _n H _{2n+8} N ₂ O ₆ (n = 35 and 37). International Journal of Molecular Sciences, 2023, 24, 5467.	1.8	0
15676	Quantifying the Contribution of London Dispersion Interaction and Adjacent Chain Packing on the Polymer Stiffness: A DFT Study. Crystal Growth and Design, 2023, 23, 2971-2979.	1.4	1
15677	Reciprocity of C \cdot O \cdot interactions with the dominant anion \cdot on fullerene (C ₆₀) \cdot amine-based organocatalysts: a mechanistic elucidation for addition vs. decarboxylation reaction. Physical Chemistry Chemical Physics, 2023, 25, 10647-10660.	1.3	1
15678	Tailoring Asymmetric Interface-Triggered Peroxymonosulfate Activation via Staircase-Shaped Edge-Rich-Defective Ti ₃ C ₂ T _x by Mechanochemical Treatment: Hydroxyl Capping or Subtraction Strategy?. ACS ES&T Engineering, 2023, 3, 544-556.	3.7	3
15679	Virtual screening and structure-activity relationship study of novel BTK inhibitors in Traditional Chinese Medicine for the treatment of rheumatoid arthritis. Journal of Biomolecular Structure and Dynamics, 0, , 1-15.	2.0	4
15680	Bubble wall confinement-driven molecular assembly toward sub-12 nm and beyond precision patterning. Science Advances, 2023, 9, .	4.7	3
15681	Boosted visible-light-driven degradation over stable ternary heterojunction as a plasmonic photocatalyst: Mechanism exploration, pathway and toxicity evaluation. Journal of Colloid and Interface Science, 2023, 641, 758-781.	5.0	2
15682	Toward Complete Transformation of Sodium Polysulfides by Regulating the Second-Shell Coordinating Environment of Atomically Dispersed Fe. Angewandte Chemie - International Edition, 2023, 62, .	7.2	8
15683	High-strength, ultra-thin anion exchange membranes with a branched structure toward alkaline membrane fuel cells. Journal of Materials Chemistry A, 2023, 11, 10738-10747.	5.2	20
15684	A {Cu ₂ I ₃ } ⁿ chain hybrid with two-step phase transition, switchable dielectrics, thermochromism and piezochromism. Dalton Transactions, 0, , .	1.6	1
15685	Thermodynamics, Kinetics, and Optical Properties of Rotaxane: A First-Principles Molecular Dynamics Study. Journal of Physical Chemistry A, 2023, 127, 2671-2687.	1.1	2
15686	Stable LiF-Rich Electrode-Electrolyte Interface toward High-Voltage and High-Energy-Density Lithium Metal Solid Batteries. Small, 2023, 19, .	5.2	8

#	ARTICLE	IF	CITATIONS
15687	Electronic Structure and Aromaticity of an Unusual Cyclo[18]carbon Precursor, C ₁₈ Br ₆ . Chemistry - A European Journal, 2023, 29, .	1.7	10
15688	Single-Crystal-Structure Directed Predesign of Cationic Covalent Organic Polymers for Rapidly Capturing ⁹⁹ TcO ₄ ⁻ . Chemistry of Materials, 2023, 35, 2531-2540.	3.2	6
15689	Regulating through space charge transfer in thermally activated delayed fluorescence molecules via donor architectures: theoretical perspective and molecular design. Physical Chemistry Chemical Physics, 2023, 25, 10977-10990.	1.3	3
15690	Syntheses, Structures, and Electronic Properties of Mono- and Bimetallic Thiolato Complexes Containing Unusual Coordination Modes of Thiolato Ligands. European Journal of Inorganic Chemistry, 2023, 26, .	1.0	0
15691	Oxidative cyclopalladation triggers the hydroalkylation of alkynes. Chinese Chemical Letters, 2023, 34, 108339.	4.8	2
15692	Toward Complete Transformation of Sodium Polysulfides by Regulating the Second-Shell Coordinating Environment of Atomically Dispersed Fe. Angewandte Chemie, 2023, 135, .	1.6	0
15693	Combination of Energetic Tetrazole and Triazole: Promising Materials with Exceptional Stability and Low Mechanical Sensitivity as Propellants and Gas Generators. ACS Applied Materials & Interfaces, 2023, 15, 15311-15320.	4.0	2
15694	Characterization of Two Novel Rumen-Derived Exo-Polygalacturonases: Catalysis and Molecular Simulations. Microorganisms, 2023, 11, 760.	1.6	1
15695	The Solute Polarization and Structural Effects on the Nonlinear Optical Response of Based Chromone Molecules. ChemPhysChem, 2023, 24, .	1.0	3
15696	Nature of photoexcited states in ZnO-embedded graphene quantum dots. Physical Chemistry Chemical Physics, 2023, 25, 10525-10535.	1.3	3
15697	Switching Monomer-to-Excimer Fluorescence by Noncovalent Interaction Competition Strategy. Advanced Functional Materials, 2023, 33, .	7.8	6
15698	NA ₄ X ₄ ⁺ (X = S, Se, Te): Clusters with a planar tetracoordinate nitrogen and significantly improved stability. Journal of Chemical Physics, 2023, 158, .	1.2	2
15699	Photophysical and electrochemical properties of alternating copolymers consisting of 3,4-ethylenedioxythiophene and 4,4'-diphenylamine/3,6-carbazole. Polymer-Plastics Technology and Materials, 2022, 61, 642-649.	0.6	0
15700	Molecular Structure, Spectral Analysis, Molecular Docking and Physicochemical Studies of 3-Bromo-2-hydroxypyridine Monomer and Dimer as Bromodomain Inhibitors. Molecules, 2023, 28, 2669.	1.7	2
15701	Deaminative radical reactions via relayed proton-coupled electron transfer. Organic Chemistry Frontiers, 2023, 10, 2155-2164.	2.3	6
15702	Amorphous Copper-Based Nanoparticles with Clusterization-Triggered Phosphorescence for Ultrasensing 2,4,6-trinitrotoluene. Advanced Materials, 2023, 35, .	11.1	11
15703	A Computational Insight on the Effect of Encapsulation and Li Functionalization on Si ₁₂ C ₁₂ Heterofullerene for H ₂ Adsorption: A Strategy for Effective Hydrogen Storage. ACS Applied Energy Materials, 2023, 6, 3374-3389.	2.5	8
15704	A high quantum yield xanthene-based fluorescent probe for the specific detection of tyrosinase and cell imaging. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 441, 114693.	2.0	4

#	ARTICLE	IF	CITATIONS
15705	Unified Picture of Interatomic Interactions, Structures, and Chemical Reactions by Means of Electrostatic and Kinetic Force Density Fields: Appelâ€™s Salt and Its Ion Pairs. <i>Crystal Growth and Design</i> , 2023, 23, 3002-3018.	1.4	7
15706	Room-Temperature One-Pot Synthesis of pH-Responsive Pyridine-Functionalized Carbon Surfaces. <i>ACS Omega</i> , 2023, 8, 10796-10805.	1.6	0
15707	Performance of Copper Corrosion Inhibitors on Pipecoridithiocarbamic Acid in 3 wt% NaCl Solution. <i>Electrochemistry</i> , 2023, , .	0.6	0
15708	Molecular dynamics simulation of polymorphic transformation between $\hat{\mu}$ -CL-20 and $\hat{\iota}^2$ -CL-20 by short range order and orientational order parameter. <i>Journal of Crystal Growth</i> , 2023, 610, 127179.	0.7	0
15709	Modulating Triplet Excited States of Organic Semiconductors via Tuning Molecular Conformation for Dualâ€™ratiometric Thermometers. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	11
15710	Sulfonamide derived Schiff base Mn (II), Co (II), and Ni (II) complexes: Crystal structures, density functional theory and Hirshfeld surface analysis. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	13
15711	Molecular Structure, Electronic Properties, Reactivity (ELF, LOL, and Fukui), and NCI-RDG Studies of the Binary Mixture of Water and Essential Oil of <i>Phlomis bruguieri</i> . <i>Molecules</i> , 2023, 28, 2684.	1.7	14
15712	The study of the PES and the reaction mechanism between ketene and Lithium Carbenoids and the formation of cyclopropanone. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	0
15713	Modulating Triplet Excited States of Organic Semiconductors via Tuning Molecular Conformation for Dualâ€™ratiometric Thermometers. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	0
15714	5-fluorouracil-caffeic acid cocrystal delivery agent with long-term and synergistic high-performance antitumor effects. <i>Nanomedicine</i> , 2022, 17, 2215-2229.	1.7	2
15715	Designing of Thiophene [3, 2-b] Pyrrole Ring-Based NFAs for High-Performance Electron Transport Materials: A DFT Study. <i>ACS Omega</i> , 2023, 8, 11118-11137.	1.6	2
15716	Tailoring fluorine-substituted cobalt phthalocyanine/activated carbon nanocomposites for stable and long-life Li/SOCl ₂ batteries. <i>Journal of Electroanalytical Chemistry</i> , 2023, 935, 117345.	1.9	0
15717	Promising insights in parallel gridâ€™based algorithms for quantum chemical topology. <i>Journal of Computational Chemistry</i> , 2023, 44, 1505-1516.	1.5	0
15718	How the coordination modes change the performance of Rh-PPh ₃ for complexes catalyst allyl alcohol hydroformylation: A theoretical study. <i>Catalysis Communications</i> , 2023, 177, 106647.	1.6	0
15719	Neglected but Efficient Electron Utilization Driven by Biochar-Coactivated Phenols and Peroxydisulfate: Polyphenol Accumulation Rather than Mineralization. <i>Environmental Science & Technology</i> , 2023, 57, 5703-5713.	4.6	24
15720	Stereochemistry of the Reactions between Palladacycle Complexes and Primary Alkyl Iodides. <i>Organometallics</i> , 2023, 42, 606-614.	1.1	0
15721	Planar $\hat{\iota}$ -Aromaticity in Ga-Doped Au Clusters. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2697-2704.	1.1	2
15722	Exciton States of Azobenzene Aggregates: A Firstâ€™Principles Study. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	2

#	ARTICLE	IF	CITATIONS
15723	Study on the Crystal Structure and Properties of a New Crystal Form: $\hat{\Gamma}$ -HMX. <i>Journal of Physical Chemistry C</i> , 2023, 127, 6101-6108.	1.5	0
15724	Tuning the Intermolecular Electrostatic Interaction toward High Efficiency and Low Cost Organic Solar Cells. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	10
15725	A Self-regulatory organosulfur copolymer cathode towards high performance lithium-sulfur batteries. <i>Energy Storage Materials</i> , 2023, 58, 222-231.	9.5	5
15726	Reducing Efficiency Roll-off in Multi-Resonant Thermally Activated Delayed Fluorescent OLEDs through Modulation of the Energy of the $T_{2\text{State}}$. <i>Advanced Optical Materials</i> , 2023, 11, .	3.6	6
15727	The Electronic Nature of Cationic Group 10 Ylidyne Complexes. <i>Inorganics</i> , 2023, 11, 129.	1.2	5
15728	Cooperative Ternary Assemblies Involving Anion- π/π -Anion- π Assemblies and Unconventional Cl π -Cl Interactions in Cu(II) Coordination Compounds: Experimental and Theoretical Studies. <i>Crystals</i> , 2023, 13, 517.	1.0	3
15729	Investigation of the N π C Ligand Effects on Emission Characteristics in a Series of Bis-Metalated [Ir(N π C)2(N π N)] $^+$ Complexes. <i>Molecules</i> , 2023, 28, 2740.	1.7	2
15730	Enhancing the Photovoltaic Properties via Incorporation of Selenophene Units in Organic Chromophores with A2- π 2-A1- π 1-A2 Configuration: A DFT-Based Exploration. <i>Polymers</i> , 2023, 15, 1508.	2.0	4
15731	Polypyridyl Coordinated Re(I) complexes for human tenascin-C (TNC) as an Antibreast Cancer Agent: An Intuition from Molecular Modeling and Simulations. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-17.	1.4	7
15732	Manipulation of the through-space interactions in diphenylmethane. , 2023, 1, .		4
15733	Cooperative Bond Activation and Catalytic CO $_{2\text{Functionalization}}$ with a Geometrically Constrained Bis(silylene)-Stabilized Borylene. <i>Journal of the American Chemical Society</i> , 2023, 145, 7011-7020.	6.6	11
15734	Homoleptic Alkynylphosphonium Au(I) Complexes as Push-Pull Phosphorescent Emitters. <i>Inorganic Chemistry</i> , 2023, 62, 5123-5133.	1.9	3
15735	The selective and sustainable separation of Cd(II) using C6MImT/[C6MIm]PF6 extractant. <i>Ecotoxicology and Environmental Safety</i> , 2023, 255, 114792.	2.9	1
15736	Highly stable lithium-ion wide-temperature storage performance achieved via anion-dominated solvation structure and electric double-layer engineering. <i>Journal of Power Sources</i> , 2023, 567, 232975.	4.0	1
15737	An Ultra-Thin, Ultra-High Capacitance Density Tantalum Capacitor for 3D Packaging. <i>Advanced Materials Technologies</i> , 2023, 8, .	3.0	1
15738	Adsorption and dissociation of H $_{2\text{molecule}}$ over first-row transition metal doped C $_{24\text{nanocage}}$ as remarkable SACs: A comparative study. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 20633-20645.	3.8	9
15739	Effects of chain length and anions on ion transport in PEO-lithium salt systems. <i>Molecular Simulation</i> , 2023, 49, 720-728.	0.9	1
15740	Charge-Shifted Weak Noncovalent Interactions in the Atmospherically Important OCS Microhydrates. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3293-3304.	1.1	2

#	ARTICLE	IF	CITATIONS
15741	Deep transfer learning for predicting frontier orbital energies of organic materials using small data and its application to porphyrin photocatalysts. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10536-10549.	1.3	4
15742	First-principles study of square chalcogen bond interactions and its adsorption behavior on silver surface. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10836-10844.	1.3	0
15743	A Protophilic MOF Enables Ni-Rich Lithium-Battery Stable Cycling in a High Water/Acid Content. <i>Advanced Materials</i> , 2023, 35, .	11.1	8
15744	On the energetic and magnetic stability of neutral and charged lithium clusters doped with one and two yttrium atoms. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 9656-9668.	1.3	0
15745	Vinylene-linked covalent organic frameworks with manipulated electronic structures for efficient solar-driven photocatalytic hydrogen production. <i>Chinese Journal of Catalysis</i> , 2023, 47, 171-180.	6.9	34
15746	Selective Detection of Copper Ions and Biological Activities of Isoniazid Schiff Bases. <i>ChemistrySelect</i> , 2023, 8, .	0.7	1
15747	New Insights into the Nature of Ti(II) and Ti(III) Active Sites in the Heterogeneous Ziegler-Natta Catalyst. <i>Journal of Physical Chemistry C</i> , 2023, 127, 5720-5730.	1.5	3
15748	Roles of Molecular Spatial Arrangement in Exciton Energy Transfer in Organic Light-Emitting Diodes: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2023, 127, 5950-5957.	1.5	0
15749	Hirshfeld Atom Refinement of Metal-Organic Complexes: Treatment of Hydrogen Atoms Bonded to Transition Metals. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3020-3035.	1.1	5
15750	Enantioselective Photochemical Carbene Insertion into C-C and C-H Bonds of 1,3-Diketones by a Guanidine-Amide Organocatalyst. <i>ACS Catalysis</i> , 2023, 13, 4656-4666.	5.5	10
15751	Mechanistic insight into the carboxylic derivatives formation from CO ₂ and ethylene over iron(0)-based catalyst. <i>Molecular Catalysis</i> , 2023, 541, 113084.	1.0	0
15752	Investigations of <i>p</i> -toloxy-1,3,4-oxadiazole propionamides as soybean 15-lipoxygenase inhibitors in comforting with <i>in vitro</i> and <i>in silico</i> studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 15549-15568.	2.0	1
15753	Path separation of dissipation-corrected targeted molecular dynamics simulations of protein-ligand unbinding. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	5
15754	Improving a Methane C-H Activation Complex by Metal and Ligand Alterations from Computational Results. <i>Inorganic Chemistry</i> , 2023, 62, 5058-5066.	1.9	0
15755	Comparative analysis and structure identification of oxidative metabolites and hydrogenation metabolite enantiomers for 2-fluorodeschloroketamine. <i>Journal of Analytical Toxicology</i> , 0, , .	1.7	0
15756	Interactions between Paracetamol and Formaldehyde: Theoretical Investigation and Topological Analysis. <i>ACS Omega</i> , 2023, 8, 11725-11735.	1.6	1
15757	Hollow polyhedral structures and properties of Ag _{2n-1} Sn ⁿ⁺ (n=1-11) clusters: A theoretical study. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	1
15758	Two Calix[3]Phenothiazine-Based Amorphous Pure Organic Room-Temperature Phosphorescent Supramolecules Mediated by Guest. <i>Advanced Optical Materials</i> , 2023, 11, .	3.6	4

#	ARTICLE	IF	CITATIONS
15760	Influence of Î€-linker on pyrone-based hole transporting materials in perovskite solar cells. <i>Molecular Simulation</i> , 2023, 49, 701-710.	0.9	0
15761	A Template-free Pd ₂ L ₄ Cage with up to Nanomolar Affinity for Chloride in Aqueous Solutions**. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	2
15762	Revealing the Interfacial Chemistry of Fluoride Alkyl Magnesium Salts in Magnesium Metal Batteries. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	11
15763	Revealing the Interfacial Chemistry of Fluoride Alkyl Magnesium Salts in Magnesium Metal Batteries. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	1
15764	Tuning Fe ₃ O ₄ for sustainable cathodic heterogeneous electro-Fenton catalysis by acetylated chitosan. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2023, 120, .	3.3	2
15765	First-Principles Study of Two-Dimensional Layered MoSi ₂ N ₄ and WSi ₂ N ₄ for Photocatalytic Water Splitting. <i>Russian Journal of Physical Chemistry A</i> , 2022, 96, 3283-3289.	0.1	0
15766	Heteronuclear Trimetallic MFe ₂ and M ₂ Fe (M=V, Nb, and Ta) Clusters for Dinitrogen Activation. <i>ChemPhysChem</i> , 2023, 24, .	1.0	2
15767	Multifunctional IL-Based Hydrogel Modulator for the Synergistic Acceleration of Wound Healing: Optimizing Drug Solubility, Antioxidant, and Anti-Inflammatory Effects. <i>ACS Sustainable Chemistry and Engineering</i> , 2023, 11, 5122-5134.	3.2	0
15768	Molecular Assembly of Rhodanine with Torus-shaped Cyclodextrins and Their Innovative Applications by Physicochemical Contrivance Simultaneously Optimized by Computational Study. <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
15769	Non-covalent interaction, adsorption characteristics and solvent effect of procainamide anti-arrhythmias drug on silver and gold loaded silica surfaces: SERS spectroscopy, density functional theory and molecular docking investigations. <i>RSC Advances</i> , 2023, 13, 9539-9554.	1.7	6
15770	Benzothieniodolium Cations Doubly Bonded to Anions via Halogen-Chalcogen and Halogen-Hydrogen Supramolecular Synthons. <i>Crystal Growth and Design</i> , 2023, 23, 2661-2674.	1.4	4
15771	Autonomous Healable Elastomers with High Elongation, Stiffness, and Fatigue Resistance. <i>Langmuir</i> , 2023, 39, 4720-4729.	1.6	0
15772	Experimental study combined with density functional theory and molecular dynamics simulation on the mechanism of glucose alcoholysis reaction. <i>Asia-Pacific Journal of Chemical Engineering</i> , 2023, 18, .	0.8	2
15773	Structural, Spectroscopic, and Bonding Analyses of La(III)/Ce(III)-Tetrel Ate-Complexes. <i>Inorganic Chemistry</i> , 2023, 62, 5660-5668.	1.9	2
15774	Insights into the Three-Component Coupling Reactions of Aldehydes, Alkynes, and Amines Catalyzed by N-heterocyclic Carbene Silver: A DFT Study. <i>Catalysts</i> , 2023, 13, 646.	1.6	0
15775	Stable Immobilization of Nickel Ions on Covalent Organic Frameworks for Panchromatic Photocatalytic Hydrogen Evolution. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	3
15776	Role of Non-Covalent Interactions in Carbonic Anhydrase Î€-Topiramate Complex Based on QM/MM Approach. <i>Pharmaceuticals</i> , 2023, 16, 479.	1.7	0
15777	Screening Physical Solvents for Methyl Mercaptan Absorption Using Quantum Chemical Calculation Coupled with Experiments. <i>ACS Omega</i> , 2023, 8, 11790-11800.	1.6	0

#	ARTICLE	IF	CITATIONS
15778	Elucidating the N ⁺ -N and C ⁺ -N Bond-Breaking Mechanism in the Photoinduced Formation of Nitrile Imine. <i>ChemPhysChem</i> , 0, , .	1.0	1
15779	Separation of azeotrope acetone-methanol mixture at high-concentration conditions: Experimental and theoretical perspective of the molecular packing effects in mesopores. <i>Applied Surface Science</i> , 2023, 624, 157113.	3.1	1
15780	Stable Immobilization of Nickel Ions on Covalent Organic Frameworks for Panchromatic Photocatalytic Hydrogen Evolution. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	23
15781	A DFT study on structural evolution, electronic property and spectral analysis of yttrium-doped germanium clusters. <i>Molecular Physics</i> , 2023, 121, .	0.8	6
15782	Mechano-/seeding-triggered crystal-to-crystal phase transition in luminescent switching cocrystals. <i>Dyes and Pigments</i> , 2023, 215, 111275.	2.0	0
15783	Exploration of Diverse Interactions of L-Methionine in Aqueous Ionic Liquid Solutions: Insights from Experimental and Theoretical Studies. <i>ACS Omega</i> , 2023, 8, 12098-12123.	1.6	3
15784	External Electric Field Effects on AFM-like Magnetism in Nitroxide-Functionalized C ₆₀ :C Base Pair. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 2037-2046.	2.5	2
15785	Understanding of Cumene Oxidation Catalyzed by Metal-Nitrogen-Carbon through Theoretical Simulations and Kinetic Validation. <i>ACS Sustainable Chemistry and Engineering</i> , 2023, 11, 5773-5781.	3.2	3
15786	Controlling Morphological Dimensions of Organic Charge-Transfer Cocrystal by Manipulating the Growth Kinetics for Optical Waveguide Applications. <i>Advanced Optical Materials</i> , 2023, 11, .	3.6	2
15787	Pseudorotaxane Ligand-Induced Formation of Copper(I) Iodide Cluster Based Assembly Materials: From Zero to Three Dimensional. <i>Chinese Journal of Chemistry</i> , 2023, 41, 1943-1949.	2.6	4
15788	Theoretical studies on spiro[acridine-fluorene]-based emitters with efficient thermally activated delayed fluorescence. <i>Journal of Molecular Structure</i> , 2023, 1284, 135431.	1.8	0
15789	Binary Organic Solar Cells with 19.2% Efficiency Enabled by Solid Additive. <i>Advanced Materials</i> , 2023, 35, .	11.1	116
15790	Ibuprofen and Paracetamol when They Meet: Quantum Theory of Atoms in Molecules Perspective. <i>Cumhuriyet Science Journal</i> , 2023, 44, 188-196.	0.1	1
15791	Novel Bis-1,3,4-Thiadiazoles Derivatives: Synthesis, Spectroscopic Characterization, DFT Calculations and Evaluation of their Antimicrobial and Antioxidant Activities. <i>Cumhuriyet Science Journal</i> , 2023, 44, 81-89.	0.1	0
15792	Complexation behaviour of piceatannol ligand with Ti(IV) and Zr(IV) metal ions: a combined DFT and deep learning investigation. <i>Structural Chemistry</i> , 2023, 34, 2139-2152.	1.0	3
15793	Chiral discrimination of cyclodecapeptide to anti-COVID-19 clinical candidates: a theoretical study. <i>Structural Chemistry</i> , 0, , .	1.0	0
15794	Precise synthesis of schwarzite carbon: hypothesis or reality?. <i>Organic Chemistry Frontiers</i> , 2023, 10, 2808-2812.	2.3	5
15795	A coumarin-based fluorescent chemosensor as a Sn indicator and a fluorescent cellular imaging agent. <i>RSC Advances</i> , 2023, 13, 9811-9823.	1.7	0

#	ARTICLE	IF	CITATIONS
15796	Comparative <i>in silico</i> and <i>in vitro</i> study of the stability and biological activity of an octapeptide from microalgae <i>Isochrysis zhanjiangensis</i> and its truncated short peptide. <i>Food and Function</i> , 2023, 14, 3659-3672.	2.1	4
15797	Engineering the BASHY Dye Platform toward Architectures with Responsive Fluorescence. <i>Chemistry - A European Journal</i> , 0, , .	1.7	1
15798	Histidine-Mediated Synthesis of Chiral Cobalt Oxide Nanoparticles for Enantiomeric Discrimination and Quantification. <i>Small</i> , 2023, 19, .	5.2	3
15799	Propane Oxidative Dehydrogenation on Nanosized Boron Carbide: Effect of Boron Content and Its Oxidation Implicated by DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2023, 127, 6280-6293.	1.5	0
15800	Quantitative analysis of the interplay of hydrogen bonds in M(II)-hexaaqua complexes with HMTA [M(II)=Co(II), Mg(II); HMTA=hexamethylenetetramine]. <i>Journal of Molecular Structure</i> , 2023, 1284, 135448.	1.8	7
15801	Dehydration-Triggered Afterglow Transition in a Mellitate-Based Coordination Polymer. <i>Chemistry of Materials</i> , 2023, 35, 3015-3023.	3.2	3
15802	Mechanistic Insights Into the Rhodium-Catalyzed C-H Alkenylation/Directing Group Migration and [3+2] Annulation: A DFT Study. <i>Journal of Organic Chemistry</i> , 2023, 88, 4494-4503.	1.7	0
15803	Low-cost organic photovoltaic materials with great application potentials enabled by developing isomerized non-fused ring acceptors. <i>Science China Chemistry</i> , 2023, 66, 1101-1110.	4.2	20
15804	Stability of gold-polysulphide species: a DFT insight. <i>Bulletin of Materials Science</i> , 2023, 46, .	0.8	0
15805	A class of non-aromatic 1,3-disilapyrroles acting as stable organosilicon-based triplet diradicals. , 2023, 2, 678-687.		3
15806	Substituent and redox effects on the second-order NLO response of Ru(II) complexes with polypyridine ligands: a theoretical study. <i>New Journal of Chemistry</i> , 2023, 47, 7326-7334.	1.4	1
15807	Riboflavin kinase and pyridoxine 5-phosphate oxidase complex formation envisages transient interactions for FMN cofactor delivery. <i>Frontiers in Molecular Biosciences</i> , 0, 10, .	1.6	4
15808	Planar Four-Membered Diboron Actinide Compound with Double Ambis Aromaticity. <i>Journal of the American Chemical Society</i> , 2023, 145, 8107-8113.	6.6	2
15809	Roles of the Zinc Ion and Water Molecule in the Active Site of the Copper-Zinc SOD Catalyst. <i>Izvestiya of Altai State University</i> , 2023, , 55-59.	0.1	0
15810	Density functional theory computation of the intermolecular interactions of Al ₂ @C ₂₄ and Al ₂ @Mg ₁₂ O ₁₂ semiconducting quantum dots conjugated with the glycine tripeptide. <i>RSC Advances</i> , 2023, 13, 9824-9837.	1.7	2
15811	Engineering supramolecular helical assemblies <i>via</i> interplay between carbon(sp) tetrel and halogen bonding interactions. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
15812	Multistimuli-responsive behavior of a phosphorescent Cu ₃ pyrazolate ₃ complex for luminescent logic gates and encrypted information transformation. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 2594-2606.	3.0	6
15813	Enhanced Stability of Rhombic Dodecahedron Nb ₁₅ with Well-Organized Superatomic States. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2912-2920.	1.1	0

#	ARTICLE	IF	CITATIONS
15814	Influence of the Solvent on the Stability of Aminopurine Tautomers and Properties of the Amino Group. <i>Molecules</i> , 2023, 28, 2993.	1.7	0
15815	A density functional theory insight into the extraction mechanism of lithium recovery from alkaline brine by β -diketones. <i>AIChE Journal</i> , 2023, 69, .	1.8	2
15816	Quantum computational investigation into structural, spectroscopic, topological and electronic properties of L-histidinium-L-tartrate hemihydrate: Nonlinear optical organic single crystal. <i>Heliyon</i> , 2023, 9, e14879.	1.4	3
15817	Photooxidation Chemistry of Hydrofluoroolefins: Assessing the Impact of Substituents on the Greenhouse Gas Replacements. <i>ACS Earth and Space Chemistry</i> , 2023, 7, 876-884.	1.2	0
15818	Fluorescence enhancement of organic aggregates induced by bromine substituents: Heavy-atom effect and vibronic coupling. <i>Dyes and Pigments</i> , 2023, 215, 111269.	2.0	3
15819	CA ₁₁ ⁺ : a molecular rotor with a quasi-planar tetracoordinate carbon. <i>Chemical Communications</i> , 2023, 59, 4966-4969.	2.2	6
15820	Toward a Combined Molecular Dynamics and Quantum Mechanical Approach to Understanding Solvent Effects on Chemical Processes in the Pharmaceutical Industry: The Case of a Lewis Acid-Mediated S _N Ar Reaction. <i>Organic Process Research and Development</i> , 2023, 27, 742-754.	1.3	0
15821	DNA Binding and Cleavage, Stopped-Flow Kinetic, Mechanistic, and Molecular Docking Studies of Cationic Ruthenium(II) Nitrosyl Complexes Containing ϵ -NS ₄ -Core. <i>Molecules</i> , 2023, 28, 3028.	1.7	1
15822	New Insights into the Solubilization of Multicomponent Crystals: A Case Study of Pipemidic Acid. <i>Crystal Growth and Design</i> , 2023, 23, 3367-3383.	1.4	3
15823	Tetralactam macrocycle based indicator displacement assay for colorimetric and fluorometric dual-mode detection of urinary uric acid. <i>Chemical Communications</i> , 2023, 59, 5411-5414.	2.2	16
15824	Photo-Response with Radical Afterglow by Regulation of Spin Populations and Hole-Electron Distributions. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	7
15825	Computational investigation of dimethoate and β -cyclodextrin inclusion complex: molecular structures, intermolecular interactions, and electronic analysis. <i>Structural Chemistry</i> , 2023, 34, 1189-1204.	1.0	2
15826	Photo-Response with Radical Afterglow by Regulation of Spin Populations and Hole-Electron Distributions. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	0
15827	Tuning Fluorination of Carbonates for Lithium-Ion Batteries: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2023, 127, 3026-3040.	1.2	1
15828	New insights into the mechanism of synergetic photoredox/copper(<i>i</i>)-catalyzed carbocyanation of 1,3-dienes: a DFT study. <i>Chemical Science</i> , 2023, 14, 4580-4588.	3.7	3
15829	<i>meso</i> -Carbazole decorated BODIPYs as an electron donor-acceptor system with excellent fluorosolvato/vapochromic behavior, aggregation-induced emission, and antileishmanial activity. <i>New Journal of Chemistry</i> , 2023, 47, 8277-8290.	1.4	2
15830	Structure of choline chloride-carboxylic acid deep eutectic solvents by wide-angle X-ray scattering and DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10481-10494.	1.3	4
15831	Comparative study on the unimolecular decompositions of energetic regioisomers: BFTF-1 and BFTF-2. <i>FirePhysChem</i> , 2023, , .	1.5	1

#	ARTICLE	IF	CITATIONS
15832	Design of Intramolecular Dihedral Angle between Electronic Donor and Acceptor in Thermally Activated Delayed Fluorescence Molecules. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 3335-3342.	2.1	1
15833	Theoretical design of a new hydrogen storage based on the decorated phosphorene nanosheet by alkali metals. <i>Journal of Physics and Chemistry of Solids</i> , 2023, 178, 111354.	1.9	2
15834	Effect of Organic Molecular Volume on Organic Photodiodes. <i>Advanced Optical Materials</i> , 0, , .	3.6	0
15835	Copperâ€“Supramolecular Pair Catalyst Promoting C₂+</sub>Product Formation in Electrochemical CO₂Reduction. <i>ACS Catalysis</i> , 2023, 13, 5114-5121.	5.5	8
15836	Arylsulfonamide chalcones as alternatives for fuel additives: antioxidant activity and machine learning protocol studies. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
15837	Structure property relationship in two thiazole derivatives: Insights of crystal structure, Hirshfeld surface, DFT, QTAIM, NBO and molecular docking studies. <i>Molecular Crystals and Liquid Crystals</i> , 2023, 763, 54-72.	0.4	1
15838	Unveiling the mechanism, selectivity, solvent and temperature effects on the [3+2] cycloaddition reaction of N-methyl-C-(2-furyl) nitron with maleimide derivatives from the molecular electron density theory perspective. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	1
15839	Triphenylamineâ€“Derived Solidâ€“State Emissive Carbon Dots for Multicolor Highâ€“Efficiency Electroluminescent Lightâ€“Emitting Diodes. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	19
15840	New insight into atomic-level interpretation of interactions in molecules and reacting systems. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 11398-11409.	1.3	4
15841	Mechanistic Insights into the Binding of Different Positron Emission Tomography Tracers to Chronic Traumatic Encephalopathy Tau Protofibrils. <i>ACS Chemical Neuroscience</i> , 0, , .	1.7	2
15842	An umpolung mechanism of B(pin)-mediated Cu/B rearrangement and origin of regioselectivity for NHC-Cu-catalyzed allylation of imines. <i>Organic Chemistry Frontiers</i> , 0, , .	2.3	0
15843	Acceleration of Stepwise Carbon-Polygold Bonding Cleavage in Hypercoordinated Carbon-Centered Gold(I) Clusters. <i>Inorganic Chemistry</i> , 2023, 62, 6147-6154.	1.9	0
15844	Hydrogen Dissociation Reaction on First-Row Transition Metal Doped Nanobelts. <i>Materials</i> , 2023, 16, 2792.	1.3	5
15845	Exceptional alkaline hydrogen evolution by molybdenum-oxide-nitride-based electrocatalysts with fast water-dissociation and hydrogen-adsorption kinetics. <i>Materials Chemistry Frontiers</i> , 2023, 7, 2683-2692.	3.2	6
15846	Sensitivity of KÎ² mainline X-ray emission to structural dynamics in iron photosensitizer. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10447-10459.	1.3	2
15847	Triphenylamineâ€“Derived Solidâ€“State Emissive Carbon Dots for Multicolor Highâ€“Efficiency Electroluminescent Lightâ€“Emitting Diodes. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	3
15848	C-P/C=O bonds assisted desolvation effect in ultra-micropores carbon for boosting Zn-ion storage capability. <i>Energy Storage Materials</i> , 2023, 58, 332-343.	9.5	10
15849	Assessing the recyclability of superbase-derived ionic liquids in cellulose processing: An insight from degradation mechanisms. <i>Chemical Engineering Journal</i> , 2023, 465, 142718.	6.6	3

#	ARTICLE	IF	CITATIONS
15850	A new look at the chalcogen bond: σ -hole-based chalcogen (Se, Te) bonding which does not include a π -hole interaction. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 3065-3081.	3.0	6
15851	Research on excited states of PPV-COF spectra based on first principles. <i>AIP Advances</i> , 2023, 13, .	0.6	1
15852	The Tetrel Bond and Tetrel Halide Perovskite Semiconductors. <i>International Journal of Molecular Sciences</i> , 2023, 24, 6659.	1.8	1
15853	A Fused [5]Helicene Dimer with a Figureâ€Eight Topology: Synthesis, Chiral Resolution, and Electronic Properties. <i>Angewandte Chemie</i> , 0, , .	1.6	0
15854	Diversity of Chemical Bonding in Zintl Clusters. , 2024, , 452-470.		0
15855	Structure and stability of a new set of noble gas insertion compounds, $XNgOPO(OH)_2$ ($X = F, Cl, Br, Ng$) <i>Tj ETQq1 1 0.784314 rgBT /Ove</i>	0.5	0
15856	Enhanced adsorption capacity of tetracycline on porous graphitic biochar with an ultra-large surface area. <i>RSC Advances</i> , 2023, 13, 10397-10407.	1.7	7
15857	A Fused [5]Helicene Dimer with a Figureâ€Eight Topology: Synthesis, Chiral Resolution, and Electronic Properties. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	16
15858	Polymorphism of Butyl Ester of Oleanolic Acidâ€”The Dominance of Dispersive Interactions over Electrostatic. <i>International Journal of Molecular Sciences</i> , 2023, 24, 6572.	1.8	0
15859	Importance of spin-triplet excited-state character in the reverse intersystem crossing process of spiro-based TADF emitters. <i>Journal of Materials Chemistry C</i> , 2023, 11, 6119-6129.	2.7	1
15860	Probing the Structural Evolution, Stabilities and Properties of $LiBn$ ($n = 2-12$) Clusters. <i>Journal of Cluster Science</i> , 0, , .	1.7	0
15861	Co-catalysis of rhodium/phosphoramidite catalyst and ZSM-35(10) for the tandem hydroformylationâ€acetalization of olefins. <i>Chemical Communications</i> , 2023, 59, 5237-5240.	2.2	2
15862	Iminium substituent directs cyanide and hydride additions to triiron vinyliminium complexes. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
15863	Genuine quadruple bonds between two main-group atoms. <i>Chemical bonding in AeF_4 ($Ae = Tj ETQq1 1 0.784314 rgBT /Ove$)</i> of heavier alkaline-earth atoms. <i>Chemical Science</i> , 2023, 14, 4872-4887.	3.7	8
15864	Discovery of Flexible Bonds Based on an Extremely Elongated Câ€C Single Bond. <i>Springer Theses</i> , 2023, , 41-78.	0.0	0
15865	Regulating the photophysical properties of ESIPT-based fluorescent probes by functional group substitution: a DFT/TDDFT study. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	1
15866	Deciphering the Differences in Ambident Reactivity between the Cyanate, Thiocyanate Ions, and their Pâ€ and Asâ€Containing Analogues. <i>Chemistry - A European Journal</i> , 0, , .	1.7	0
15867	Two Carbon Dioxide Molecules Consecutively Reduced by Metal-Free B_{2O_2} Anions. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3082-3087.	1.1	0

#	ARTICLE	IF	CITATIONS
15868	Synthesis, Antifungal Activity, and DFT Calculation Study of Novel 1- <i>N</i> -Acyl-5-amino-1,2,4-triazole- <i>N</i> -thioether Derivatives Containing Natural <i>gem</i> -Dimethylcyclopropane Ring Structure. <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
15869	Solvent Effect on the Nonlinear Optical Property in Cr(CO) ₃ L Complexes (L = 1,6-Benzene and) <i>J. Phys. Chem. B</i> , 2023, 127, 10711-10717.	0.2	0
15870	Synergistic inhibition of azoles compounds on chloride-induced atmospheric corrosion of copper: Experimental and theoretical characterization. <i>Corrosion Science</i> , 2023, 218, 111161.	3.0	5
15871	Creation and Demonstration of the Longest C-C Single Bond with a Bond Length Beyond 1.8 Å... <i>Springer Theses</i> , 2023, , 9-40.	0.0	0
15872	Twisted intramolecular charge-transfer state of <i>trans</i> - <i>N,N'</i> -bis(2-quinolinecarboxyl)ethane-1,2-diamine. <i>J. Phys. Chem. A</i> , 2023, 127, 10711-10717.	0.8	0
15873	Role of functionalization in the fluorescence quantum yield of graphene quantum dots. <i>Applied Physics Letters</i> , 2023, 122, .	1.5	2
15874	Mechanism Research on Excited-State Photoinduced Electron Transfer in a Pyrazine Derivative under an External Electric Field. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3356-3361.	1.1	1
15875	Insights into the Fluxional Processes of Monomethylcyclohexenyl Manganese Tricarbonyl. <i>Molecules</i> , 2023, 28, 3232.	1.7	1
15876	Fluorescent Molecular Rotors Based on Hinged Anthracene Carboxyimides. <i>Molecules</i> , 2023, 28, 3217.	1.7	1
15877	Computational evaluation on molecular stability and binding affinity of methyl dopa against Lysine-specific demethylase 4D Enzyme through quantum chemical computations and molecular docking analysis. <i>Journal of Molecular Structure</i> , 2023, 1286, 135518.	1.8	6
15878	Novel Strategy of Machine Learning for Predicting Henry's Law Constants of CO ₂ in Ionic Liquids. <i>ACS Sustainable Chemistry and Engineering</i> , 2023, 11, 6090-6099.	3.2	1
15879	Anomalous deep-red luminescence of perylene black analogues with strong π - π interactions. <i>Nature Communications</i> , 2023, 14, .	5.8	19
15880	Competing and directing interactions in new phosphoramidate/thiophosphoramidate structures: energy considerations and evidence for CH \cdots HC contacts and aliphatic \cdots aromatic stacking. <i>CrystEngComm</i> , 0, , .	1.3	0
15881	Two Quasi-Degenerate Isomers of Mo ₁₃ . <i>Journal of Cluster Science</i> , 0, , .	1.7	1
15882	Solution-Processable Small-Molecule Hole Transport Material for High-Performance QLED via Manipulating Dipole Moments. <i>Advanced Materials Technologies</i> , 2023, 8, .	3.0	4
15883	An overview of corrosion. , 2023, , 3-17.		0
15884	Identification of high oxygen-consuming substances in stormwater drainage systems illicitly connected with sewage system. <i>Journal of Environmental Sciences</i> , 2024, 138, 132-140.	3.2	2
15885	Conversion of Dinitrogen and Oxygen to Nitric Oxide Mediated by Triatomic Yttrium Cations: Reversible N-N Bond Switching. <i>Inorganic Chemistry</i> , 2023, 62, 6102-6108.	1.9	3

#	ARTICLE	IF	CITATIONS
15886	Hypothetical confirmation for the anti-bacterial compound potassium succinate-succinic acid in comparison with certain succinate derivatives. <i>Journal of Biomolecular Structure and Dynamics</i> , 2024, 42, 1237-1248.	2.0	1
15887	Searching for the analogues of 1,1-dinitro-2,2-diamino ethylene (FOX-7) by high-throughput computation and machine learning. <i>FirePhysChem</i> , 2023, , .	1.5	2
15888	Properties of Naked Silver Clusters with Up to 100 Atoms as Found with Embedded-Atom and Density-Functional Calculations. <i>Molecules</i> , 2023, 28, 3266.	1.7	2
15889	Electrophilic substitution reactivity prediction of crown ether derivatives. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	0
15890	On the Nature of the Partial Covalent Bond between Noble Gas Elements and Noble Metal Atoms. <i>Molecules</i> , 2023, 28, 3253.	1.7	0
15891	Effect of Hydrogen Bonds on CO ₂ Capture by Functionalized Deep Eutectic Solvents Derived from 4-Fluorophenol. <i>ACS Sustainable Chemistry and Engineering</i> , 2023, 11, 6272-6279.	3.2	4
15892	DFT Investigations on the Interactions Between Pyrimidine Derivatives and Ag/Au/Cu Metal Clusters: Solvation Effects and Reactivity Analysis. <i>Journal of Cluster Science</i> , 2023, 34, 2847-2858.	1.7	3
15893	Separation of phenolic compounds from water by using monoterpenoid and fatty acid based hydrophobic deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2023, 381, 121806.	2.3	1
15894	Geometric structures and hydrogen storage properties of M ₂ B ₇ (M=Be, Mg, Ca) clusters. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 25821-25829.	3.8	0
15895	High-Valent Iridium Complexes Containing a Tripodal Bis-Cyclometalated C ^N C Ligand. <i>Organometallics</i> , 0, , .	1.1	0
15896	Pyridone- δ -Doped Acenes with Improved Stability. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	0
15897	Small Energetic Disorder Enables Ultralow Energy Losses in Non-Fullerene Organic Solar Cells. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	12
15898	Half-Planar-Half-Twisted Small Molecule Acceptors for Efficient Polymer Solar Cells. <i>ACS Applied Energy Materials</i> , 0, , .	2.5	0
15899	Half-Sandwich Manganese Complex Bearing Fused Oxazoline-NHC Ligand: Conformational Analysis and Evaluation in Asymmetric Ketone Hydrosilylation. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	0
15900	The relationships between direct substituents, aromaticity and kinetic stability of pentazole ring. <i>FirePhysChem</i> , 2023, 3, 350-355.	1.5	1
15901	CA ₄ X ₄ (X = Te, Po): Double Aromatic Molecular Stars Containing Planar Tetracoordinate Carbon Atoms. <i>Molecules</i> , 2023, 28, 3280.	1.7	3
15902	Conductive Li ⁺ Moieties-Rich Cathode Electrolyte Interphase with Electrolyte Additive for 4.6 V Well-Cycled Li LiCoO ₂ Batteries. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	12
15903	Thermal hazard and pyrolysis mechanism investigation using thermal analysis coupled with quantum-chemical DFT simulation for 1-hydroxy-7-azabenzotriazole. <i>Journal of Thermal Analysis and Calorimetry</i> , 0, , .	2.0	1

#	ARTICLE	IF	CITATIONS
15904	Reaction mechanism between Ge Ge_n ($n=2-5$) clusters and single water molecule based on density functional theory. <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	0
15905	On using non-Kekulé triangular graphene quantum dots for scavenging hazardous sulfur hexafluoride components. <i>Heliyon</i> , 2023, 9, e15388.	1.4	3
15906	Experimental, theoretical, computational and spectroscopic analysis in binary liquid mixtures containing 1-propanol and C-1 to C-4 alkyl acetates ($T_A=298.15-318.15\text{K}$): Physicochemical properties and molecular interaction studies. <i>Journal of Molecular Liquids</i> , 2023, 381, 121829.	2.3	4
15907	Rational design of high-performance soluble intrinsic black polyimide with full absorption of visible light. <i>European Polymer Journal</i> , 2023, 192, 112062.	2.6	1
15908	Vitamin B1-catalyzed one-pot ultrasound-assisted synthesis of 1,2-disubstituted benzimidazole and its selective recognition of metal ions. <i>Research on Chemical Intermediates</i> , 0, , .	1.3	0
15909	Modulation of electronic density states of carbon atom via multifaceted Cu doped Co2P particle for robust and efficient electrocatalytic hydrogen evolution reaction in aqueous acidic medium. <i>Electrochimica Acta</i> , 2023, 455, 142378.	2.6	3
15910	Enhanced efficiency of DSSCs by co-sensitizing dyes with complementary absorption spectra. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 442, 114758.	2.0	3
15911	A combined spectroscopic and quantum chemical approach to study the molecular interaction between anti-inflammatory drug Hydrocortisone and amino acid L-Phenylalanine. <i>Journal of Molecular Structure</i> , 2023, 1286, 135546.	1.8	3
15912	High-density frustrated Lewis pairs based on Lamellar Nb2O5 for photocatalytic non-oxidative methane coupling. <i>Nature Communications</i> , 2023, 14, .	5.8	16
15913	Effect of Substituents on the Intramolecular $n\pi^*$ Interaction in 3-[2-(Dimethylamino) phenyl] propanal: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3339-3346.	1.1	2
15914	Realizing efficient blue and deep-blue delayed fluorescence materials with record-beating electroluminescence efficiencies of 43.4%. <i>Nature Communications</i> , 2023, 14, .	5.8	35
15915	Role of the Polar Proportion of Compound Collectors in Low-Rank Coal Flotation Upgrading: Insights from the Molecular Scale. <i>Minerals (Basel, Switzerland)</i> , 2023, 13, 524.	0.8	0
15916	Hydrogen-bond-bridged intermediate for perovskite solar cells with enhanced efficiency and stability. <i>Nature Photonics</i> , 2023, 17, 478-484.	15.6	62
15917	Self-healing of electrical damage in insulating robust epoxy containing dynamic fluorine-substituted carbamate bonds for green dielectrics. <i>Materials Horizons</i> , 2023, 10, 2542-2553.	6.4	1
15918	Two triplet emitting states in one emitter: Near-infrared dual-phosphorescent Au Au_{20} nanocluster. <i>Science Advances</i> , 2023, 9, .	4.7	22
15919	Synthesis and characterization of Y-shaped optical nonlinear chromophores with strong acceptors. <i>New Journal of Chemistry</i> , 2023, 47, 9203-9211.	1.4	1
15920	Sensitive photodetection below silicon bandgap using quinoid-capped organic semiconductors. <i>Science Advances</i> , 2023, 9, .	4.7	16
15921	Monitoring the melting behavior of boron nanoparticles using a neural network potential. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 12841-12853.	1.3	3

#	ARTICLE	IF	CITATIONS
15922	Regulating Intramolecular Charge Transfer and Resonance Effects to Realize Ultrawide Bandgap Conjugated Polymer for High-Performance All-Polymer Solar Cells. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	17
15923	Ï-Extended Octupolar Cyclized Indole Tetramer and Trimer Derivatives with Second- and Third-Order Nonlinear Optical Properties. <i>Journal of Organic Chemistry</i> , 2023, 88, 5520-5529.	1.7	3
15924	Luminescent [CO ₂ @Ag ₂₀ (SAdm) ₁₀ (CF ₃ COO) ₁₀ (DMA) ₂] ₃ nanocluster: synthetic strategy and its implication towards white light emission. <i>Nanoscale</i> , 2023, 15, 8377-8386.	2.8	3
15925	Insights on adsorption properties of a DNA base, guanine on nano metal cages (Ag ₂₄ /Au ₂₄ /Cu ₂₄): DFT, SERS, NCI and solvent effects. <i>Journal of Molecular Structure</i> , 2023, 1285, 135541.	1.8	4
15926	Regiodivergent catalytic asymmetric dearomative cycloaddition of bicyclic heteroaromatics. <i>Science Advances</i> , 2023, 9, .	4.7	5
15927	Synthesis, crystal structure and DFT study of tert-butyl 6-chloro-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1 <i>H</i> -indole-1-carboxylate. <i>Molecular Crystals and Liquid Crystals</i> , 0, , 1-16.	0.4	0
15928	Versatile Solid Modifications of Multicomponent Pharmaceutical Salts: Novel Metformin-Rhein Salts Based on Advantage Complementary Strategy Design. <i>Pharmaceutics</i> , 2023, 15, 1196.	2.0	4
15929	Design, Synthesis and Aromaticity of an Alternating Cyclo[4]Thiophene[4]Furan. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	1
15930	Mechanism of fluorescence enhancement of HClO detected by HBT-OMe molecule based on ESIPT. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2023, .	0.2	0
15931	Nucleophile Effects on the E ₂ /S _N ² Competition for the X ⁺ + CH ₃ CH ₂ Cl Reactions: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3381-3389.	1.1	3
15932	Realizing <i>p</i> -Type and <i>n</i> -Type Doping of a Single Conjugated Polymer via Incorporation of a Thienoisatin-Terminated Quinoidal Unit. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	9
15933	Mechanism of pH influence on aptamer binding with Cd ²⁺ revealed by molecular dynamics simulation. <i>New Journal of Chemistry</i> , 2023, 47, 9239-9249.	1.4	2
15934	Constructing 1-Ethoxyphenanthro[9,10- <i>bc</i>]acephenanthrylene for the Synthesis of a Polyaromatic Hydrocarbon Containing a Formal Azulene Unit. <i>Journal of Organic Chemistry</i> , 2023, 88, 5473-5482.	1.7	1
15935	Theoretical investigation of electrochromic mechanism in D-A conjugated polymers in visible and infrared bands. <i>RSC Advances</i> , 2023, 13, 11337-11345.	1.7	2
15936	Ammonia versus Water Elimination in the Reaction of Diols with Urea under Metal Oxide Catalysis. <i>ACS Catalysis</i> , 2023, 13, 5643-5655.	5.5	1
15937	MOF-derived Co/Fe@NPC-500 with large amounts of low-valent metals as an electro-Fenton cathode for efficient degradation of ceftazidime. <i>Applied Catalysis B: Environmental</i> , 2023, 333, 122755.	10.8	21
15938	Oriented Self-Assembly of Hierarchical Branch Organic Crystals for Asymmetric Photonics. <i>Journal of the American Chemical Society</i> , 2023, 145, 9285-9291.	6.6	13
15939	Infrared Photodissociation Spectroscopy of Mass-Selected [TaO ₃ (CO ₂) _n] ⁺ (n = 2-5) Complexes in the Gas Phase. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	2

#	ARTICLE	IF	CITATIONS
15940	Iron(II) Complexes with Porphyrin and Tetrabenzoporphyrin: CASSCF/MCQDPT2 Study of the Electronic Structures and UV-Vis Spectra by sTD-DFT. <i>International Journal of Molecular Sciences</i> , 2023, 24, 7070.	1.8	2
15941	Whose Oxygen Atom Is Transferred to the Products? A Case Study of Peracetic Acid Activation via Complexed Mn ^{II} for Organic Contaminant Degradation. <i>Environmental Science & Technology</i> , 2023, 57, 6723-6732.	4.6	9
15942	Insights into the excited state hydrogen bond and proton transfer behaviors associated with solvent polarity for NHBQ fluorophore: a theoretical study. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	3
15943	Complex with Linear B ₂ Skeleton Trapped in Dinitrogen Matrix: Matrix Infrared Spectra and Quantum Chemical Calculations. <i>Inorganic Chemistry</i> , 2023, 62, 6314-6322.	1.9	1
15944	Reactivity Factors in Catalytic Methanogenesis and Their Tuning upon Coenzyme F430 Biosynthesis. <i>Journal of the American Chemical Society</i> , 2023, 145, 9039-9051.	6.6	1
15945	Highly Hydrophilic ZIF-8 as a Carbonic Anhydrase Mimetic Catalyst for Promoting CO ₂ Absorption. <i>Journal of Physical Chemistry C</i> , 2023, 127, 7184-7196.	1.5	8
15946	Investigation on the growth, structure and physical properties of pyridin-1-ium-2-carboxylate benzimidazole (1:1) hydrate single crystal. <i>Journal of Materials Science: Materials in Electronics</i> , 2023, 34, .	1.1	2
15947	Interaction between escitalopram and ibuprofen or paracetamol: DFT and molecular docking on the drug-drug interactions. <i>Journal of Biomolecular Structure and Dynamics</i> , 2024, 42, 672-686.	2.0	2
15948	Exploring potential SARS-CoV-2 Mpro non-covalent inhibitors through docking, pharmacophore profile matching, molecular dynamic simulation, and MM-GBSA. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	0
15949	Design and facile synthesis of quinazolinone-based full color-tunable boron difluoride dyes: Efficient solvent/solid-state emission and bioimaging application. <i>Dyes and Pigments</i> , 2023, 216, 111321.	2.0	3
15950	Supramolecular Gel-to-Gel Transition Induced by Nanoscale Structural Perturbation via the Rotary Motion of Feringa's Motor. <i>Small</i> , 2023, 19, .	5.2	3
15951	Removal of oxygen-containing functional groups during hydrothermal carbonization of biomass: Experimental and DFT study. <i>Energy</i> , 2023, 276, 127436.	4.5	4
15952	Impact of organic-inorganic wavefunction delocalization on the electronic and optical properties of one-dimensional hybrid perovskites. <i>Journal of Materials Chemistry C</i> , 0, .	2.7	0
15953	A novel surface molecularly imprinted polymer electrochemical sensor based on porous magnetic TiO ₂ for highly sensitive and selective detection of tetracycline. <i>Environmental Science: Nano</i> , 2023, 10, 1614-1628.	2.2	1
15954	Synthesis, characterization, and comparison of explosive hexaammincobalt(III) and nitropentammincobalt(III) cyclopentazolate (cyclo-N ₅) salts. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2023, 649, .	0.6	0
15955	Designing of anthracene-arylamine hole transporting materials for organic and perovskite solar cells. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 122, 108464.	1.3	3
15956	Interfacial engineered superelastic metal-organic framework aerogels with van-der-Waals barrier channels for nerve agents decomposition. <i>Nature Communications</i> , 2023, 14, .	5.8	11
15957	Aromaticity of Cope and Claisen rearrangements. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	3

#	ARTICLE	IF	CITATIONS
15958	Probing the Interaction of NO with C ₆₀ : Comparison between Endohedral and Exohedral Complexes. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3598-3607.	1.1	4
15959	Experimental and Theoretical Study on Crown Ether-Appended-Fe(III) Porphyrin Complexes and Catalytic Oxidation Cyclohexene with O ₂ . <i>Molecules</i> , 2023, 28, 3452.	1.7	0
15960	Revealing the Role of Donor/Acceptor Interfaces in Nonfullerene-Acceptor Based Organic Solar Cells: Charge Separation versus Recombination. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 3811-3817.	2.1	1
15961	Electronic Density Changes for Non-Equilibrium Molecular Geometries: A Charge " Charge Transfer " Dipolar Polarization Model. , 2024, , 152-174.		0
15962	Theoretical study on the interaction between cis-2 bis(benzofuro)[60]fullerene derivative and NO dominated double gas molecule. <i>FirePhysChem</i> , 2023, 3, 356-364.	1.5	1
15963	Mechanism of metalated pyrrole-singlet oxygen chemiluminescent reaction. <i>Polyhedron</i> , 2023, 238, 116421.	1.0	0
15964	An Aromaticity Study of Localized and Non-Localized Orbitals in B_{3n+0} , B_{4n+0} , B_{5n+0} , B_{6n+0} , and B_{7n+0} ($n = 0, 1, 2$) Rings. <i>Russian Journal of Physical Chemistry A</i> , 2023, 97, 151-167.	0.1	0
15965	Theoretical investigation of Aryl/Alkyl halide reduction with hydrated electrons from energy and AIMD aspects. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	1
15966	Electrostatic Potential as Solvent Descriptor to Enable Rational Electrolyte Design for Lithium Batteries. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	14
15967	Imaging Solvent-Triggered Gaseous Iodine Uptake on Single Covalent Organic Frameworks. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	6
15968	Anchoring and boosting: Ferrocene-based separators used to eliminate the polysulfide shuttle effect for Li-S batteries. <i>Journal of Membrane Science</i> , 2023, 678, 121660.	4.1	3
15969	Oxidization enhances type I ROS generation of AlE-active zwitterionic photosensitizers for photodynamic killing of drug-resistant bacteria. <i>Chemical Science</i> , 2023, 14, 4863-4871.	3.7	11
15970	A 1D/2D Bi ₂ O ₃ /g-C ₃ N ₄ step-scheme photocatalyst to activate peroxymonosulfate for the removal of tetracycline hydrochloride: insight into the mechanism, reactive sites, degradation pathway and ecotoxicity. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 12231-12244.	1.3	2
15971	Prediction, Application, and Mechanism Exploration of Liquid "Liquid Equilibrium Data in the Extraction of Aromatics Using Sulfolane. <i>Processes</i> , 2023, 11, 1228.	1.3	1
15972	High-rate, high-capacity electrochemical energy storage in hydrogen-bonded fused aromatics. <i>Joule</i> , 2023, 7, 986-1002.	11.7	8
15973	Building cross-phase ion transport channels between ceramic and polymer for highly conductive composite solid-state electrolyte. <i>Cell Reports Physical Science</i> , 2023, 4, 101382.	2.8	1
15974	Application of Newly Designed Y-Series Nonfullerene Acceptors for High-Efficient Organic Solar Cells. <i>Advanced Theory and Simulations</i> , 0, , .	1.3	0
15975	Effect of confinement and external mechanical force on the cleavage of the bond in a diatomic molecule. <i>Molecular Physics</i> , 0, , .	0.8	0

#	ARTICLE	IF	CITATIONS
15976	A DFT Study on the Conformation, Properties of the Excited States, and Excimer's Formation of Tetraphenylcyclotetrasiloxane. <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
15977	A novel electrochemical sensor based on mesoporous carbon hollow spheres/ZIF-67-derived Co-embedded N-doped carbon nanotubes composite for simultaneous determination of dihydroxybenzene isomers in environmental water samples. <i>Microchemical Journal</i> , 2023, 191, 108754.	2.3	5
15978	Novel phenolic modified acrylates: Synthesis, characterization and application in 3D printing. <i>European Polymer Journal</i> , 2023, 192, 112075.	2.6	0
15979	Kinetic and mechanistic study of the atmospheric degradation of C3F7OCHF2SCH2CH2OH with OH radical. <i>Chemical Physics Letters</i> , 2023, , 140516.	1.2	0
15980	DFT insight of hydroxide degradation pathways for heterocyclic quaternary ammonium cations in anion exchange membranes. <i>Journal of Membrane Science</i> , 2023, 678, 121672.	4.1	6
15981	Fabrication of amorphous metal-organic framework in deep eutectic solvent for boosted organophosphorus pesticide adsorption. <i>Journal of Environmental Chemical Engineering</i> , 2023, 11, 109963.	3.3	2
15982	Study on structural detailing of gossypetin and its medicinal application in UV filtering, radical scavenging, and metal chelation open up through NCI, TD-DFT, QTAIM, ELF, and LOL analysis. <i>Computational and Theoretical Chemistry</i> , 2023, 1225, 114126.	1.1	3
15983	Reinvestigation of the Room Temperature Photochemical Reaction between N-Methyl-1,2,4-triazoline-3,5-dione (MeTAD) and Benzene. <i>Organics</i> , 2023, 4, 164-172.	0.6	0
15984	Computational Characterization of the Inhibition Mechanism of Xanthine Oxidoreductase by Topiroxostat. <i>ACS Catalysis</i> , 2023, 13, 6023-6043.	5.5	5
15985	Effect of group electronegativity on spectroscopic, biological, chromogenic sensing and optical properties of 2-formyl-benzene sulfonic acid sodium salt-based Schiff bases. <i>Journal of Molecular Structure</i> , 2023, 1286, 135611.	1.8	2
15986	Green hydrophobic deep eutectic solvents as low-viscosity and efficient lubricants. <i>Tribology International</i> , 2023, 185, 108531.	3.0	3
15987	Fluorosumanenes as building blocks for organic crystalline dielectrics. <i>Pure and Applied Chemistry</i> , 2023, 95, 421-430.	0.9	3
15988	High-efficiency Narrowband Multi-resonance Emitter Fusing Indolocarbazole Donors for BT. 2020 Red Electroluminescence and Ultralong Operation Lifetime. <i>Advanced Materials</i> , 2023, 35, .	11.1	37
15989	Control and regulation of the performance of fullerene-based dye-sensitized solar cells with D-D-A structure by external electric fields. <i>Nanoscale Advances</i> , 0, , .	2.2	1
15990	High photovoltaic performance (23.75) of triazatruxene-based dye-sensitized solar cells containing different π bridges: computational investigation. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
15991	Bending Effect on the Electronic Properties and Nonlinear Optical Responses of Linear Porphyrin Oligomer. <i>Advanced Theory and Simulations</i> , 0, , .	1.3	0
15992	High-power and Ultrastable Aqueous Calcium-ion Batteries Enabled by Small Organic Molecular Crystal Anodes. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	10
15993	Terpolymerization and Regioisomerization Strategy to Construct Efficient Terpolymer Donors Enabling High-performance Organic Solar Cells. <i>Advanced Materials</i> , 2023, 35, .	11.1	23

#	ARTICLE	IF	CITATIONS
15994	Cooperative multiple interactions of donor-acceptor dyes enhance the efficiency and stability of perovskite solar cells. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
15995	The critical role of the donor polymer in the stability of high-performance non-fullerene acceptor organic solar cells. <i>Joule</i> , 2023, 7, 810-829.	11.7	17
15996	Highly Boosting Circularly Polarized Luminescence of Chiral Metal-Imidazolate Frameworks. <i>Advanced Science</i> , 2023, 10, .	5.6	7
15997	Synthesis and characterization of Pd(0) complexes with electronically differentiated ferrocene diphosphane ligands. <i>European Journal of Inorganic Chemistry</i> , 0, , .	1.0	0
15998	A novel CO ₂ -sensitive in situ deep eutectic solvent system: Efficient extraction of polyphenol phytochemicals. <i>Chemical Engineering Research and Design</i> , 2023, 194, 179-191.	2.7	0
15999	Transition metals based metalides TM-Janus-TM (where TM=Sc-Zn and Janus=F6C6H6); A theoretical study of nonconventional metalides with excellent static and dynamic nonlinear optical properties. <i>Materials Science in Semiconductor Processing</i> , 2023, 162, 107506.	1.9	6
16000	Designed Construction of 2D Honeycomb Cationic MOF Materials for Selective Removal of Sulfonic Anionic Dyes. <i>Langmuir</i> , 0, , .	1.6	0
16001	Stabilization of 2-Pyridyltellurium(II) Derivatives by Oxidorhenium(V) Complexes. <i>Chemistry</i> , 2023, 5, 934-947.	0.9	0
16002	Kinetic, Thermodynamic, and Dynamic Control in Normal vs. Cross [2 + 2] Cycloadditions of Ene-Keteniminium Ions: Computational Understanding, Prediction, and Experimental Verification. <i>Journal of the American Chemical Society</i> , 0, , .	6.6	1
16003	Solvent effect on molecular, electronic parameters, topological analysis and Fukui function evaluation with biological studies of imidazo [1, 2-a] pyridine-8-carboxylic acid. <i>Journal of Molecular Liquids</i> , 2023, 382, 121863.	2.3	10
16004	Enhanced removal of organophosphate esters by iron-modified biochar with developed mesoporous: Performance and mechanism based on site energy distribution theory. <i>Chemosphere</i> , 2023, 330, 138722.	4.2	1
16005	Environmental theoretical calculation for non-periodic systems. <i>Trends in Chemistry</i> , 2023, 5, 410-414.	4.4	11
16006	2D silicene nanosheets for the detection of DNA nucleobases for genetic biomarker: a DFT study. <i>Structural Chemistry</i> , 2024, 35, 25-37.	1.0	1
16007	Synthesis, crystallographic and spectroscopic investigation, chemical reactivity, hyperpolarizabilities and in silico molecular docking study of (Z)-2N-(tert-butylimino)-3N TM -(4-methoxyphenyl) thiazolidin-4-one. <i>Journal of Molecular Structure</i> , 2023, 1287, 135620.	1.8	6
16008	Synthesis, non-covalent interactions and chemical reactivity of 1-pentyl-3-phenylquinoxalin-2(1H)-one - Structural and computational studies. <i>Journal of Molecular Structure</i> , 2023, 1286, 135622.	1.8	4
16009	DFT study of molecular interaction between Menthol and Myristic Acid. <i>Materials Today: Proceedings</i> , 2023, , .	0.9	1
16010	New organotin(IV) complexes derived from 1-adamantanethiol: synthesis, crystal structure, DFT calculation, and in vitro antifungal activity and cytotoxicity. <i>Transition Metal Chemistry</i> , 2023, 48, 113-124.	0.7	0
16011	Manipulating the antioxidative capacity of melanin-like nanoparticles by involving condensation polymerization. <i>Science China Chemistry</i> , 2023, 66, 1520-1528.	4.2	15

#	ARTICLE	IF	CITATIONS
16012	Pnictogen Bonding Enabled Photosynthesis of Chiral Selenium-Containing Pyridines from Pyridylphosphonium Salts. <i>Fundamental Research</i> , 2023, , .	1.6	2
16013	Decolorization Performance of a Methyl Benzyl Diallyl Quaternary Ammonium Salt Copolymer in a Simulated Reactive Dyeing Wastewater. <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
16014	Molecular hybrid of 1,2,3-triazole and schiff base as potential antibacterial agents: DFT, molecular docking and ADME studies. <i>Journal of Molecular Structure</i> , 2023, 1286, 135617.	1.8	6
16015	Physical mechanisms of contact-electrification induced photon emission spectroscopy from interfaces. <i>Nano Research</i> , 2023, 16, 11545-11555.	5.8	2
16016	Synthesis, virtual screening, and computational approach of 6-(4-methoxyphenyl)-4-phenyl-1,2-dihydropyrimidin-2-one as a potential target for thioredoxin glutathione reductase (TGR). <i>Journal of Molecular Structure</i> , 2023, 1286, 135623.	1.8	4
16017	Design of C1-symmetric tridentate ligands for enantioselective dearomative [3+2] annulation of indoles with aminocyclopropanes. <i>Nature Communications</i> , 2023, 14, .	5.8	12
16018	Unveiling the exclusive stereo and site selectivity in [3+2] cycloaddition reactions of a tricyclic strained alkene with nitrile oxides from the molecular electron density theory perspective. <i>Chemistry of Heterocyclic Compounds</i> , 0, , .	0.6	2
16019	Deepening Insights into Aggregation Effect of Intermolecular Charge-Transfer Aggregates for Highly Efficient Near-Infrared Non-Doped Organic Light-Emitting Diodes over 780Ånm. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	6
16020	Exploiting nonaqueous self-stratified electrolyte systems toward large-scale energy storage. <i>Nature Communications</i> , 2023, 14, .	5.8	1
16021	Exploring the Influence of Engineering the Linker between the Donor and Acceptor Fragments on Thermally Activated Delayed Fluorescence Characteristics. <i>ACS Omega</i> , 2023, 8, 15638-15649.	1.6	2
16022	Design and computational studies on energetic compounds composing bridged bis triazolo-triazine framework. <i>Chemical Physics</i> , 2023, 571, 111939.	0.9	2
16023	Understanding the Origins of Site Selectivity in Hydrogen Atom Transfer Reactions from Carbohydrates to the Quinuclidinium Radical Cation: A Computational Study. <i>Journal of Organic Chemistry</i> , 2023, 88, 5713-5730.	1.7	8
16024	Redox-switchable bistable nickel corrole. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 3037-3046.	3.0	1
16025	Crystal Structures of 3,3,5,5-Tetrabromo-4,4-bipyridine and Co(II) Coordination Polymer Based Thereon. <i>Crystals</i> , 2023, 13, 704.	1.0	1
16026	Flexible Molecular Electrochromic Devices Run by Low-Cost Commercial Cells. <i>Advanced Optical Materials</i> , 2023, 11, .	3.6	9
16027	$\langle \text{Cr}_2 \text{Ge} \rangle$ ($n=15-20$) clusters with two Cr atoms exhibited antiferromagnetic coupling. <i>Journal of Computational Chemistry</i> , 2023, 44, 1667-1672.	1.5	6
16028	Designing Electron-Deficient Diketone Unit Based Non-Fused Ring Acceptors with Amplified Optoelectronic Features for Highly Efficient Organic Solar Cells: A DFT Study. <i>Molecules</i> , 2023, 28, 3625.	1.7	10
16029	Synthesis, crystal structure, biological evaluation, docking study and DFT calculation of novel strobilurins containing oxime ether phenyl ring or dihydrobenzofuran moiety. <i>Journal of Molecular Structure</i> , 2023, 1286, 135636.	1.8	2

#	ARTICLE	IF	CITATIONS
16030	Regiumâ€™ Bonds Involving Nucleobases: Theoretical Study and Biological Implications. <i>Inorganic Chemistry</i> , 2023, 62, 6740-6750.	1.9	4
16031	Molecular design and experimental study of deep eutectic solvent extraction of keratin derived from feathers. <i>International Journal of Biological Macromolecules</i> , 2023, 241, 124512.	3.6	4
16032	Ultra-sensitive Baicalin electrochemical sensor based on Î³-cyclodextrin supramole derived N,Zn double-doped carbon nanosphere. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 669, 131484.	2.3	2
16033	Efficient detection of L-aspartic acid and L-glutamic acid by self-assembled fluorescent microparticles with AIE and FRET activities. <i>Organic and Biomolecular Chemistry</i> , 2023, 21, 4022-4027.	1.5	6
16034	A sulfur monoxide complex of platinum fluoride with a positively charged ligand. <i>RSC Advances</i> , 2023, 13, 12495-12501.	1.7	0
16035	Giant NLO response and ultraviolet transparency of superalakis decorated C ₆ O ₆ Li ₆ complexes; a DFT perspective. <i>Physica Scripta</i> , 2023, 98, 065909.	1.2	4
16036	Polyfluorinated crosslinker-based solid polymer electrolytes for long-cycling 4.5â€‰V lithium metal batteries. <i>Nature Communications</i> , 2023, 14, .	5.8	39
16037	Designing Y-shaped two-dimensional (2D) polymer-based donor materials with addition of end group acceptors for organic and perovskite solar cells. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	6
16038	Inhibition mechanisms of HAIB on Q235 rebar in the simulated concrete pore solution. <i>Journal of Building Engineering</i> , 2023, 72, 106565.	1.6	0
16039	Light and nitrogen vacancy-intensified nonradical oxidation of organic contaminant with Mn (III) doped carbon nitride in peroxymonosulfate activation. <i>Journal of Hazardous Materials</i> , 2023, 454, 131463.	6.5	6
16040	Enhancement of Atmospheric Nucleation Precursors on Iodic Acid-Induced Nucleation: Predictive Model and Mechanism. <i>Environmental Science & Technology</i> , 2023, 57, 6944-6954.	4.6	6
16041	Effect of maleylation and denaturation of human serum albumin on its interaction with scavenger receptors. <i>Proteins: Structure, Function and Bioinformatics</i> , 2023, 91, 1140-1151.	1.5	1
16042	Engineering highly permeable thin-film composite nanofiltration membranes by strengthening the diffusion control of amine monomer via deep eutectic solvent. <i>Journal of Membrane Science</i> , 2023, 678, 121689.	4.1	4
16043	Ultrathin Carbon Coating and Defect Engineering Promote RuO ₂ as an Efficient Catalyst for Acidic Oxygen Evolution Reaction with Superâ€™High Durability. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	15
16044	Synergistically Improving the Stability and Operating Potential of Organic Cathodes for Sodiumâ€™ion Battery. <i>Batteries and Supercaps</i> , 2023, 6, .	2.4	5
16045	A molecular electron density theory study of mechanism and selectivity of the intramolecular [3+2] cycloaddition reaction of a nitronâ€™vinylphosphonate adduct. <i>Chemistry of Heterocyclic Compounds</i> , 0, , .	0.6	0
16046	Thio/carbohydrazone derivatives from iso(thio)/cyanates: preparation, structure elucidation, DFT studies, antimicrobial activity and DNA interactions. <i>Research on Chemical Intermediates</i> , 2023, 49, 2639-2667.	1.3	2
16047	Boronâ€™Doped Electrolytes as Interfacial Modifiers for Highâ€™Rate Stable Lithium Metal Batteries. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	2

#	ARTICLE	IF	CITATIONS
16048	Influence pathways of nanocrystalline cellulose on the digestibility of corn starch: Gelatinization, structural properties, and α -amylase activity perspective. <i>Carbohydrate Polymers</i> , 2023, 314, 120940.	5.1	7
16049	An efficient biochar adsorbent for CO ₂ capture: Combined experimental and theoretical study on the promotion mechanism of N-doping. <i>Chemical Engineering Journal</i> , 2023, 466, 143095.	6.6	2
16050	Activation persulfate for efficient tetrabromobisphenol A degradation via carbon-based materials: Synergistic mechanism of doped N and Fe. <i>Journal of Hazardous Materials</i> , 2023, 455, 131471.	6.5	5
16051	Investigation of the cyclo[12]carbon nanoring and respective analogues (Al ₆ N ₆ and B ₆ N ₆) as support for the single atom catalysis of the hydrogen evolution reaction. <i>Materials Science in Semiconductor Processing</i> , 2023, 162, 107544.	1.9	6
16052	Ultrasonic-assisted binding of canistel (<i>Lucuma nervosa</i> A.DC) seed starch with quercetin. <i>Ultrasonics Sonochemistry</i> , 2023, 96, 106417.	3.8	5
16235	Enzyme-Mimetic Photo-decarboxylation Based on Geometry-Dependent Supramolecular Association. <i>ACS Catalysis</i> , 2023, 13, 6763-6772.	5.5	3
16255	Toward High-Energy and Low-Sensitivity Energetic Materials Based on a Fused [5,5,5,6]-Tetracyclic Backbone. <i>Organic Letters</i> , 2023, 25, 3487-3491.	2.4	4
16293	Stereoselective Synthesis of <i>trans</i> -Stilbenes through Silver-Catalyzed Self-Coupling of <i>N</i> -Triflylhydrazones: An Experimental and Theoretical Study. <i>Organic Letters</i> , 2023, 25, 3461-3465.	2.4	3
16388	New insights from a bonding evolution theory based on the topological analysis of the electron localization function. , 2023, , 465-481.		1
16391	On the analysis of the Fukui function. , 2023, , 421-432.		0
16392	Structure prediction using reactivity descriptors. , 2023, , 449-462.		0
16393	Quantum chemical descriptors as a modeling framework for large biological structures. , 2023, , 59-88.		0
16407	Predicting reactivity with a general-purpose reactivity indicator. , 2023, , 159-180.		1
16450	Hydrogen Bond Binding of Water to Two Cholic Acid Residues. , 0, , .		0
16570	Asymmetric [3+2]-cyclization of α -imino amide surrogates to construct 3,4-diaminopyrrolidine-2,5-diones. <i>Chemical Communications</i> , 2023, 59, 8250-8253.	2.2	0
16633	Interfullerene Electronic Interactions and Excited-State Dynamics in Fullerene Dumbbell Conjugates. <i>Journal of the American Chemical Society</i> , 2023, 145, 14190-14195.	6.6	2
16880	Modification of QuinoxP*-Type Bisphosphine Ligands for High-Performance Asymmetric Boryl Substitution of Racemic Allyl Electrophiles. <i>Springer Theses</i> , 2023, , 19-112.	0.0	0
16892	Computational Investigation on Copper(I)-Catalyzed Enantioselective Radical Borylation of Benzyl Halides. <i>Springer Theses</i> , 2023, , 213-223.	0.0	0

#	ARTICLE	IF	CITATIONS
17057	Thiazole Functionalized Hole Transport Material Featuring Defect Passivation Effects for High-Performance Perovskite Solar Cells. , 2023, 5, 1772-1780.		5
17084	Design and synthesis of anisotropic crystals with <i>π</i> -conjugated rings toward giant birefringence. <i>Materials Chemistry Frontiers</i> , 2023, 7, 3986-3993.	3.2	4
17137	Linear <i>π</i> -conjugated units of the <i>D_{2h}</i> point group as superior ultraviolet birefringent units. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 18646-18651.	1.3	0
17185	Application of Molecular Simulation Methods in Treating Intrinsic Structures of Energetic Materials. , 2023, , 41-113.		1
17193	Energetic Ionic Crystals. , 2023, , 203-234.		0
17197	Multi-spiro junctions enable efficient thermally activated delayed fluorescent emitter. <i>Chemical Communications</i> , 2023, 59, 9255-9258.	2.2	1
17209	Photoluminescent Humidity Sensors Based on Droplet-Enabled Porous Composite Gels. , 0, , 2074-2083.		0
17223	Current status of deMon2k for the investigation of the early stages of matter irradiation by time-dependent DFT approaches. <i>European Physical Journal: Special Topics</i> , 2023, 232, 2167-2193.	1.2	3
17270	Design and Synthesis of High-Performance Planar Explosives and Solid Propellants with Tetrazole Moieties. <i>Organic Letters</i> , 2023, 25, 5100-5104.	2.4	2
17306	Switching Singlet Exciton to Triplet for Efficient Pure Organic Room-Temperature Phosphorescence by Rational Molecular Design. <i>Jacs Au</i> , 2023, 3, 1835-1842.	3.6	3
17359	A multi-fused heat-resistant energetic compound constructed by hydrogen bonds. <i>Chemical Communications</i> , 2023, 59, 9864-9867.	2.2	2
17461	Interaction of Germanium Analogue of Organic Isonitrile with Cu(I) imide in Side-on Mode. <i>Dalton Transactions</i> , 0, , .	1.6	0
17626	Solvent-regulated fluorimetric differentiation of Al ³⁺ and Zn ²⁺ using a dual functional sensor based on the photo-induced electron transfer and intramolecular proton transfer mechanism. <i>MRS Communications</i> , 2023, 13, 634-640.	0.8	0
17684	Selective confinement of potassium, rubidium, or caesium ions in a non-covalent hydroxyproline octamer cage stabilized by <i>cis</i> -hydroxyl locks. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 22614-22618.	1.3	0
17914	Energetic performance of trinitromethyl nitrotriazole (TNMNT) and its energetic salts. <i>Chemical Communications</i> , 2023, 59, 11276-11279.	2.2	5
17955	Comment on "Be bonds in double-aromatic bridged Be ₂ ($\frac{1}{4}$ -SO) molecules" by F. Rezaie and S. Noorizadeh, <i>Dalton Transactions</i> , 2022, 51, 12596. <i>Dalton Transactions</i> , 0, , .	1.6	0
17983	Stereochemical modulation of ketyl radical cyclization enabled by pyridine-boryl radicals: catalytic diastereoselective synthesis of <i>trans</i> -2-alkyl-1-indanols. <i>Chemical Communications</i> , 2023, 59, 11983-11986.	2.2	0
18051	Hydrogen-bonding enables two-dimensional metal/semiconductor tunable contacts approaching the quantum limit and the modified Schottky-Mott limit simultaneously. <i>Materials Horizons</i> , 0, , .	6.4	0

#	ARTICLE	IF	CITATIONS
18246	Small Gold Clusters: Structure, Energetics and Biomedical Applications. , 2024, , 523-567.		0
18443	Assembly of three oxadiazole isomers toward versatile energetics. Journal of Materials Chemistry A, 0, , .	5.2	0
18830	Electronic delocalization in charged macrocycles is associated with global aromaticity. Chemical Communications, 0, , .	2.2	0
18968	Wellbore Surface Conditioning for Inhibition of Asphaltene Adsorption. , 2023, , .		0
18987	Cyclo[n]carbons and catenanes from different perspective. Disentangling molecular thread. Physical Chemistry Chemical Physics, 0, , .	1.3	0
19535	Pnictogen bonding at the service of gold catalysis: the case of a phosphinostiborane gold complex. Chemical Communications, 2023, 60, 192-195.	2.2	1
19550	External electric field, a potential catalyst for C=C-N cross-coupling reaction. Physical Chemistry Chemical Physics, 0, , .	1.3	0
19680	Strategic design of an NIR probe for viscosity imaging in inflammatory and non-alcoholic steatohepatitis mice. Chemical Communications, 2023, 59, 14025-14028.	2.2	0
19738	Tailoring hydroxyl groups of organic phenazine anodes for high-performance and stable alkaline batteries. Energy and Environmental Science, 2024, 17, 114-122.	15.6	1
19956	Visualizing and characterizing excited states from time-dependent density functional theory. Physical Chemistry Chemical Physics, 2024, 26, 3755-3794.	1.3	2
20043	Towards improved comprehensive energetic properties by skeleton modification. New Journal of Chemistry, 0, , .	1.4	0
20099	Realizing one-step two-electron transfer of naphthalene diimides via a regional charge buffering strategy for aqueous organic redox flow batteries. Materials Horizons, 2024, 11, 1283-1293.	6.4	0
20122	Selective electrochemical acceptorless dehydrogenation reactions of tetrahydroisoquinoline derivatives. Organic and Biomolecular Chemistry, 0, , .	1.5	0
20172	The Thiadiazole Ring (THD) Is a Building Block for Potential Inhibitors of the SARS-CoV-2 Main Protease (Mpro): Theoretical Look into the Structure, Reactivity, and Binding Profile of Three 1,3,4-THD Derivatives toward Mpro. , 0, , .		0
20181	Upgrading of the biomass-derived platform compound 5-hydroxymethylfurfural to high-value chemicals: an environment-friendly corrosion inhibitor. Green Chemistry, 2024, 26, 1306-1316.	4.6	0
20185	Nitroiminotriazole (NIT) based potential solid propellants: Synthesis, characterization, and applications. Dalton Transactions, 0, , .	1.6	0
20247	Toxicology Studies of Anisole and Glyoxylic Acid Derivatives by Computational Methods. , 2023, , 125-158.		0
20330	Chemical Trap Orbital Analysis of Styrene-Grafted Polypropylene for HVDC Cable Insulation. Lecture Notes in Electrical Engineering, 2024, , 595-602.	0.3	0

#	ARTICLE	IF	CITATIONS
20432	A desirable coplanar energetic pentazolate salt driven by hydrogen bonds. CrystEngComm, 2024, 26, 748-752.	1.3	0
20454	Elucidating the impact of oxygen functional groups on the catalytic activity of $\text{M}^{\text{N}}_4\text{C}$ catalysts for the oxygen reduction reaction: a density functional theory and machine learning approach. Materials Horizons, 2024, 11, 1719-1731.	6.4	0
20455	Heteroatom-facilitated blue to near-infrared emission of nonconjugated polyesters. Materials Horizons, 2024, 11, 1579-1587.	6.4	1
20486	Bidentate selenium-based chalcogen bond catalyzed cationic polymerization of <i>p</i> -methoxystyrene. Chemical Communications, 2024, 60, 1321-1324.	2.2	1
20487	A donor-acceptor cage for circularly polarized TADF emission. Chemical Communications, 2024, 60, 1758-1761.	2.2	0
20515	CB_4Se_5 : a planar tetracoordinate carbon CB_4 core stabilized by peripheral Se/Se_2 bridges. Chemical Communications, 2024, 60, 1341-1344.	2.2	0
20569	Global minimum and a heap of low-lying isomers with planar tetracoordinate carbon in the Ca_3MgH_2 system. Physical Chemistry Chemical Physics, 2024, 26, 3804-3809.	1.3	1
20899	The structure-activity relationship of copper hydride nanoclusters in hydrogenation and reduction reactions. Nanoscale Advances, 2024, 6, 1374-1379.	2.2	0
21036	Can the presence of a fluorine-containing functional group in eutectic mixtures indeed bring fluorous affinity for fluorotelomer alcohol?. New Journal of Chemistry, 2024, 48, 3347-3351.	1.4	0
21724	Anti-agglomeration of gas hydrate. , 2024, , 479-522.		0