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Citation Report

#	ARTICLE	IF	CITATIONS
41	Investigation of the effects of copper ions on protein aggregation using a model system. Cellular and Molecular Life Sciences, 2004, 61, 982-991.	2.4	31
42	Syntheses and structures of mononuclear lutetium imido complexes with very short Lu–N bonds. Chemical Communications, 2007, , 5007.	2.2	59
43	Influence of Solvent Polarity and Hydrogen Bonding on the Electronic Transition of Coumarin 120: A TDDFT Study. ChemPhysChem, 2008, 9, 1593-1602.	1.0	42
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55	Search for the most stable Ca@C44 isomer: Structural stability and electronic property investigations. Journal of Chemical Physics, 2009, 130, 124705.	1.2	3
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412	Quantum chemical studies, vibrational analysis, molecular structure, first order hyper polarizability, NBO and HOMO-LUMO analysis of 3-hydroxybenzaldehyde and its cation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 789-799.	2.0	17
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655	Spectroscopic properties of Zn(salphenazine) complexes and their application in small molecule organic solar cells. <i>Dalton Transactions</i> , 2014, 43, 210-221.	1.6	21
656	Ruthenium, Rhodium, Osmium, and Iridium Complexes of Osazones (Osazones = Bis-Arylhydrazones of) Tj ETQq0 0,0 rgBT /Overlock 10	1.9	12
657	Solvent-Dependent Formation of Os(0) Complexes by Electrochemical Reduction of [Os(CO)(2,2- ϵ^2 -bipyridine)(L)Cl ₂]; L = Cl ϵ^2 , PrCN. <i>Inorganic Chemistry</i> , 2014, 53, 1382-1396.	1.9	11
658	Photocurrent Generation in Bulk vs Bilayer Devices: Quantum Treatment of Model Rubrene/7,7,8,8-Tetracyanoquinodimethane Heterojunctions for Organic Solar Cells. <i>Journal of Physical Chemistry C</i> , 2014, 118, 2287-2297.	1.5	12
659	Performance of metalloporphyrin malonic acids as dye sensitizers for use in dye-sensitized solar cells assessed by density functional theory. <i>Materials Science in Semiconductor Processing</i> , 2014, 26, 119-129.	1.9	3
660	[2+1] Cycloaddition of dichlorocarbene to finite-size graphene sheets: DFT study. <i>Monatshefte für Chemie</i> , 2014, 145, 891-896.	0.9	25
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663	Study of vibrational spectra, normal coordinate analysis and molecular structure of 6-(2,3-dichlorophenyl)-1,2,4-triazine-3,5-diamine using density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 121, 420-429.	2.0	15
664	A DFT, AIM and NBO study of adsorption and chemical sensing of iodine by S-doped fullerenes. <i>Sensors and Actuators B: Chemical</i> , 2014, 196, 624-630.	4.0	67
665	Synthesis, X-ray crystal structure, DFT calculation and catalytic activity of two new oxido-vanadium(V) complexes containing ONO tridentate Schiff bases. <i>Polyhedron</i> , 2014, 79, 138-150.	1.0	63
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667	DFT computational analysis of piracetam. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 249-255.	2.0	6
668	Spectroscopic analysis of 3-Bromodiphenylamine with experimental techniques and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 131, 432-445.	2.0	5
669	Ruthmycin, a New Tetracyclic Polyketide from <i>Streptomyces</i> sp. RM-4-15. <i>Organic Letters</i> , 2014, 16, 456-459.	2.4	23
670	On the ambiguity of 1,3,2-benzodiazaboroles as donor/acceptor functionalities in luminescent molecules. <i>Dalton Transactions</i> , 2014, 43, 3347-3363.	1.6	16
671	Theoretical Study of Novel Azo-Tetraphenylporphyrins: Potential Photovoltaic Materials. <i>Journal of Physical Chemistry A</i> , 2014, 118, 197-207.	1.1	5

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676	A novel copper(II) complex as a nitric oxide turn-on fluorosensor: intracellular applications and DFT calculation. <i>Dalton Transactions</i> , 2014, 43, 2566-2576.	1.6	44
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684	DFT computations and spectroscopic analysis of p-bromoacetanilide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 122, 542-552.	2.0	7
685	Nonplanar Donor-Acceptor Chiral Molecules with Large Second-Order Optical Nonlinearities: 1,1,4,4-Tetracyanobuta-1,3-diene Derivatives. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1094-1102.	1.1	15
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688	Monomeric and dimeric structures analysis and spectroscopic characterization of 3,5-difluorophenylboronic acid with experimental (FT-IR, FT-Raman, ¹ H and ¹³ C NMR, UV) techniques and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2014, 1058, 79-96.	1.8	48
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727	Unsymmetrical squaraine dye containing dithieno[3,2-b:2',3'-d]pyrrole as a π -spacer: A potential photosensitizer for dye-sensitized solar cells. <i>Journal of Power Sources</i> , 2014, 268, 137-145.	4.0	22
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1252	Synthesis, spectroscopic investigations, and computational study of 4-((9,10-dioxo-9,10-dihydroanthracen-1-yl)oxy)-3-methoxybenzaldehyde. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2016, 121, 246-252.	0.2	3
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1394	Distinguishing Bonds. <i>Journal of the American Chemical Society</i> , 2016, 138, 3731-3744.	6.6	48
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1476	Detection of surface-linked polychlorinated biphenyls using surface-enhanced Raman scattering spectroscopy. <i>Vibrational Spectroscopy</i> , 2017, 90, 1-6.	1.2	12
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1507	Luminescence properties of copper(I), zinc(II) and cadmium(II) coordination compounds with picoline ligands. <i>Journal of Luminescence</i> , 2017, 186, 127-134.	1.5	8
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1622	New platinum(II) one-armed Schiff base complexes for blue and orange PHOLEDs applications. <i>Organic Electronics</i> , 2017, 42, 153-162.	1.4	39
1623	Vibrational spectroscopic, molecular docking and quantum chemical studies on 6-aminonicotinamide. <i>Journal of Molecular Structure</i> , 2017, 1134, 143-156.	1.8	23
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1627	EPR interpretation, magnetism and biological study of a Cu(II) dinuclear complex assisted by a schiff base precursor. <i>Journal of Biological Inorganic Chemistry</i> , 2017, 22, 481-495.	1.1	14
1628	DFT investigation of NH ₃ , PH ₃ , and AsH ₃ adsorptions on Sc-, Ti-, V-, and Cr-doped single-walled carbon nanotubes. <i>Applied Surface Science</i> , 2017, 400, 506-514.	3.1	47
1629	Modeling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: I. <i>Ab Initio</i> Calculations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 208-220.	1.2	22
1630	The influence of halides in polyoxotitanate cages; dipole moment, splitting and expansion of d-orbitals and electronâ€“electron repulsion. <i>Dalton Transactions</i> , 2017, 46, 578-585.	1.6	17
1631	Biomarkers of cigarette smoking and DNA methylating agents: Raman, SERS and DFT study of 3-methyladenine and 7-methyladenine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 176, 1-7.	2.0	13
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1902	Theoretical studies on the potentials of some nanocages (Al ₁₂ N ₁₂ , Al ₁₂ P ₁₂ , B ₁₂ N ₁₂ , Be ₁₂ O ₁₂ , C ₁₂ Si ₁₂ ,) Tj ETQq0 0 0 rgBT /Overlock of Molecular Liquids, 2018, 260, 138-148.	2.3	58
1903	Spectroscopic investigation, hirshfeld surface analysis and molecular docking studies on anti-viral drug entecavir. Journal of Molecular Structure, 2018, 1164, 447-458.	1.8	82
1904	Structural, electrical and optical properties of Lin@C20 (n=1-6) nanoclusters. Comptes Rendus Chimie, 2018, 21, 541-546.	0.2	16
1905	Theoretical investigation on the effect of fluorine and carboxylate substitutions on the performance of benzodithiophene-diketopyrrolopyrrole-based polymer solar cells. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	3
1906	Adsorption behavior of amphetamine on the inorganic BC3 nanotube and nanosheet: DFT studies. Inorganic Chemistry Communication, 2018, 91, 95-101.	1.8	51
1907	Synthesis of a zinc(II) complex with hexadentate N 4 S 2 donor thioether ligand: X-ray structure, DNA binding study and DFT computation. Journal of Molecular Structure, 2018, 1164, 94-99.	1.8	5
1908	Tuning the field emission and electronic properties of silicon nanocones by Al and P doping: DFT studies. Journal of Molecular Graphics and Modelling, 2018, 81, 168-174.	1.3	32
1909	Theoretical, biological and in silico studies of pendant-armed heteroleptic copper(II) phenolate complexes. Journal of Molecular Structure, 2018, 1161, 306-319.	1.8	4
1910	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. Journal of Molecular Structure, 2018, 1164, 227-238.	1.8	52
1911	Complexes of DNA bases and Watson-Crick base pairs interaction with neutral silver Ag _n (n=8, 10, 12) clusters: a DFT and TDDFT study. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1050-1062.	2.0	14
1912	A theoretical study of structural, opto-electronic and nonlinear properties of arylboroxine derivatives. Indian Journal of Physics, 2018, 92, 57-68.	0.9	2
1913	The structural, electronic and spectroscopic properties of 4FPBAPE molecule: Experimental and theoretical study. Journal of Molecular Structure, 2018, 1154, 301-318.	1.8	13

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1914	Synthesis, X-ray structure, spectroscopic, DFT study and catalytic activity of cis-[RuCl ₂ (L)(EPh ₃)] complexes (E = P, As, Sb; L = NN ² N ³ tridentate azoimine-quinoline ligands). <i>Inorganica Chimica Acta</i> , 2018, 471, 186-193.		5
1915	Study of structural, optical properties and electronic structure of PTCDI-C5 organic nanostructure. <i>Chemical Physics Letters</i> , 2018, 691, 14-21.	1.2	13
1916	Proton sensitive charge-transfer excited states in bis-terdentate cyclometalated Ir(III) complexes: Spectroscopic and theoretical investigation. <i>Inorganica Chimica Acta</i> , 2018, 471, 8-16.	1.2	6
1917	Synthesis, characterization and properties of oxo-bridged diruthenium(III) complexes with thiocyanato and cyanato ligands. <i>Inorganica Chimica Acta</i> , 2018, 469, 469-477.	1.2	4
1918	Synthesis, structural characterization and theoretical studies of a new Schiff base 4-(((3-(tert-Butyl)-(1-phenyl)pyrazol-5-yl) imino)methyl)phenol. <i>Journal of Molecular Structure</i> , 2018, 1152, 163-176.	1.8	19
1919	Structural, vibrational, DFT and optical studies of a new non-centrosymmetric hybrid material (C ₄ H ₁₂ N ₂)[CoBr ₄]. <i>Journal of Molecular Structure</i> , 2018, 1152, 303-310.	1.8	23
1920	A highly sensitive and selective fluorescent chemosensor for the sequential recognition of Zn ²⁺ and S ₂ ²⁻ in living cells and aqueous media. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 3108-3116.	4.0	37
1921	A dual sensor selective for Hg ²⁺ and cysteine detection. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 2756-2763.	4.0	63
1922	Role of the Diphosphine Chelate in Emissive, Charge-Neutral Iridium(III) Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 624-635.	1.7	12
1923	The interaction of phosgene gas with different BN nanocones: DFT studies. <i>Solid State Communications</i> , 2018, 269, 23-27.	0.9	47
1924	Theoretical perspective on electronic structure and photophysical properties for three cyclometalated iridium(III) complexes bearing different substituent groups on the main ligands. <i>Canadian Journal of Chemistry</i> , 2018, 96, 18-23.	0.6	0
1925	A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene – A frequently used benzene derivative. <i>Journal of Molecular Structure</i> , 2018, 1151, 245-255.	1.8	51
1926	A DFT and QTAIM study of the adsorption of organic molecules over the copper-doped coronene and circumcoronene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 95, 59-70.	1.3	15
1927	A green and efficient synthesis of isoxazol-5(4H)-one derivatives in water and a DFT study. <i>Journal of the Iranian Chemical Society</i> , 2018, 15, 455-469.	1.2	19
1928	Selective detection of Cu ²⁺ and S ₂ ²⁻ by a colorimetric chemosensor: Experimental and theoretical calculations. <i>Inorganica Chimica Acta</i> , 2018, 471, 709-717.	1.2	12
1929	A computational study on the cisplatin drug interaction with boron nitride nanocluster. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 79, 223-229.	1.3	39
1930	DFT study on the adsorption behavior and electronic response of AlN nanotube and nanocage toward toxic halothane gas. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 98, 53-59.	1.3	26
1931	Copper-doped Al ₁₂ N ₁₂ nano-cages: potential candidates for nonlinear optical materials. <i>Applied Physics A: Materials Science and Processing</i> , 2018, 124, 1.	1.1	38

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1932	The structure and photocatalytic activity of the tetranuclear titanium(IV) oxo-complex with 4-aminobenzoate ligands. <i>Polyhedron</i> , 2018, 141, 110-117.	1.0	14
1933	Syntheses of Zn(II) and Cu(II) Schiff base complexes using N,O donor Schiff base ligand: Crystal structure, DNA binding, DNA cleavage, docking and DFT study. <i>Polyhedron</i> , 2018, 141, 153-163.	1.0	55
1934	Azophenine as Central Core for Efficient Light Harvesting Devices. <i>ChemPhysChem</i> , 2018, 19, 596-611.	1.0	2
1935	Spectral investigations and DFT studies of 3,7-dihydro-1,3,7-trimethyl-1 H -purine-2,6-dione (caffeine) interaction and recognition by single amino acid derived self-assembled nanostructures. <i>Journal of Molecular Structure</i> , 2018, 1156, 51-61.	1.8	3
1936	Glabralides A – C, three novel meroterpenoids from <i>Sarcandra glabra</i> . <i>Tetrahedron</i> , 2018, 74, 341-347.	1.0	12
1937	Light Harvesting and Direct Electron Injection by Interfacial Charge-Transfer Transitions between TiO ₂ and Carboxy-Anchor Dye LEG4 in Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2018, 122, 8-15.	1.5	41
1938	Adsorption behavior and mechanism of acidic blue 25 dye onto cucurbit[8]uril: A spectral and DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 193, 125-132.	2.0	24
1939	First-principles investigation on structural and electronic properties of antimonene nanoribbons and nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 97, 98-104.	1.3	51
1940	The ClCN adsorption on the pristine and Al-doped boron nitride nanosheet, nanocage, and nanocone: Density functional studies. <i>Thin Solid Films</i> , 2018, 645, 363-369.	0.8	22
1941	A visible light excitable chromone appended hydrazide chemosensor for sequential sensing of Al ³⁺ and F ⁻ in aqueous medium and in Vero cells. <i>Sensors and Actuators B: Chemical</i> , 2018, 257, 545-552.	4.0	42
1942	Syntheses, crystal structures, DNA binding, DNA cleavage, molecular docking and DFT study of Cu(II) complexes involving N ₂ O ₄ donor azo Schiff base ligands. <i>New Journal of Chemistry</i> , 2018, 42, 246-259.	1.4	33
1943	Studies on structural, optical, thermal and vibrational properties of thienyl chalcone derivative: 1-(4-Nitrophenyl)-3-(2-thienyl)prop-2-en-1-one. <i>Journal of Molecular Structure</i> , 2018, 1155, 634-645.	1.8	4
1944	The Effect of Superalkali M30 (M = Li, Na and K) on Structure, Electrical and Nonlinear Optical Properties of C20 Fullerene Nanocluster. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2018, 28, 110-120.	1.9	12
1945	Dispersion corrected density functional study of CO oxidation on pristine/functionalized/doped graphene surfaces in aqueous phase. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 79, 27-34.	1.3	5
1946	Adsorption orientation of 8-azaadenine on silver nanoparticles determined by SERS and DFT. <i>Journal of Raman Spectroscopy</i> , 2018, 49, 376-382.	1.2	7
1947	Chloropicrin sensor based on the pristine BN nanocones: DFT studies. <i>Structural Chemistry</i> , 2018, 29, 585-592.	1.0	11
1948	Investigation of NH ₃ adsorption behavior on graphdiyne nanosheet and nanotubes: A first-principles study. <i>Journal of Molecular Liquids</i> , 2018, 249, 24-32.	2.3	65
1949	Structure, spectra and electrical conductivity of copper(I) and silver(I) phosphino bridging mixed ligand complexes with coumarinyl Schiff base. <i>Inorganica Chimica Acta</i> , 2018, 469, 523-535.	1.2	14

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1950	Toxic CO detection by Li-encapsulated fullerene-like BeO. Structural Chemistry, 2018, 29, 231-241.	1.0	8
1951	Theoretical investigation on reaction pathways for ethylene epoxidation on Ti-decorated graphene. Structural Chemistry, 2018, 29, 159-170.	1.0	13
1952	Surface-decorated CdS nanoparticles for the recognition of K ⁺ in aqueous medium: DFT and antibacterial studies. Research on Chemical Intermediates, 2018, 44, 155-171.	1.3	4
1953	Quantum-Chemical Study of the Adsorption of Bi ³⁺ Ions on Au(111). Russian Journal of Electrochemistry, 2018, 54, 1201-1208.	0.3	1
1954	Quantum-Chemical Study of the Adsorption of Pb ²⁺ on Au(111). Russian Journal of Electrochemistry, 2018, 54, 902-911.	0.3	2
1955	Interaction between Thallium and the Au(111) Surface. Quantum-Chemical Analysis. Russian Journal of Electrochemistry, 2018, 54, 912-921.	0.3	0
1956	Synthesis, Reactivity Studies, and Cytotoxicity of Two trans-Iodidoplatinum(II) Complexes. Does Photoactivation Work?. Inorganics, 2018, 6, 127.	1.2	4
1957	TDDFT Investigation of the Hybrid Organic Inorganic Perovskite: CH ₃ NH ₃ PbC ₃ . , 2018, , .		0
1958	TDDFT Studies on Sheet Size-Dependency of Optoelectronic Properties of 2D Silicon. , 2018, , .		1
1959	Alkyl chain-modified cyclometalated iridium complexes as tunable anticancer and imaging agents. Dalton Transactions, 2018, 47, 15873-15881.	1.6	21
1960	Six-coordinate [Co ^{III} (L) ₂] ^{z+} (z = 1 ⁺ , 0, 1+) complexes of an azo-appended <i>o</i> -aminophenolate in amidate(2 ⁻) and iminosemiquinonate $\dot{\text{C}}$ -radical (1 ⁻) redox-levels: the existence of valence-tautomerism. Dalton Transactions, 2018, 47, 17086-17101.	1.6	12
1961	An aminoquinoline based biocompatible fluorescent and colourimetric pH sensor designed for cancer cell discrimination. New Journal of Chemistry, 2018, 42, 19818-19826.	1.4	33
1962	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. Monatshefte für Chemie, 2018, 149, 2167-2174.	0.9	7
1963	Supramolecular Chiral Helical Ribbons of Tetraphenylethylene-Appended Naphthalenediimide Controlled by Solvent and Induced by <i>l</i> - and <i>d</i> -Alanine Spacers. Chemistry - an Asian Journal, 2018, 13, 3947-3953.	1.7	18
1964	Structure, electrical and nonlinear optical properties of M@C_{20} (M = Li, Na, K). <i>Tj ETQq</i> 0,0,0 rgBT ₅ Overlock		
1965	Donor functionalized quinoline based organic sensitizers for dye sensitized solar cell (DSSC) applications: DFT and TD-DFT investigations. Journal of Molecular Modeling, 2018, 24, 343.	0.8	25
1966	DFT Calculations of Structure and Optical Properties in Wide Band-Gap Semiconductor Clusters for Dye-Sensitized Solar Cells. , 2018, , .		0
1967	CH ₂ O Adsorption on M (M = Li, Mg and Al) Atom Deposited ZnO Nano-Cage: DFT Study. Key Engineering Materials, 0, 786, 384-392.	0.4	8

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1968	Exploring the potential of iron to replace ruthenium in photosensitizers: a computational study. <i>Journal of Molecular Modeling</i> , 2018, 24, 341.	0.8	6
1969	Structural, energetic and spectroscopic studies of new luminescent complexes based on 2-(2-hydroxyphenyl)imidazo[1,2- <i>a</i>]pyridines and 1,2-phenylenediboronic acid. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 725-737.	0.5	7
1970	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
1971	Theoretical Study of the Solvent Effect on the Electronic and Vibrational Properties of [CpFe(CO) ₂ (NCS)] and [CpFe(CO) ₂ (SCN)] Linkage Isomers. <i>Journal of Structural Chemistry</i> , 2018, 59, 1058-1066.	0.3	3
1972	Two new terpenoid ester glycosides from the twigs of <i>Litsea cubeba</i> . <i>Journal of Asian Natural Products Research</i> , 2018, 20, 1129-1136.	0.7	4
1973	Theoretical Study of NO Linkage Isomers in a Rhenacarborane Nitrosyl Complex. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 2518-2523.	0.1	0
1974	Enhancing the Light Harvesting Efficiency, Open Circuit Voltage And Stability of Molybdenum Doped (Zn) ₆ Nanocluster in Dye-Sensitized Solar Cells: A DFT Study. <i>Oriental Journal of Chemistry</i> , 2018, 34, 2292-2304.	0.1	2
1975	Emission and Color Tuning of Cyanostilbenes and White Light Emission. <i>ACS Omega</i> , 2018, 3, 17376-17385.	1.6	25
1976	Kinetics of dye regeneration in liquid electrolyte unveils efficiency of 10.5% in dye-sensitized solar cells. <i>Journal of Materials Chemistry C</i> , 2018, 6, 11444-11456.	2.7	18
1977	Analysis of the Interaction Between the C ₂₀ 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
1978	A Density Functional Investigation of Geometrical and Electronic Structures, Charge Transfer, and Photoluminescent Property of a Zinc(II) Complex with 5-Amino-2-(1H-Benzoimidazol-2-yl)-Phenol. <i>Journal of Structural Chemistry</i> , 2018, 59, 1088-1094.	0.3	1
1979	Selective prebiotic conversion of pyrimidine and purine anhydronucleosides into Watson-Crick base-pairing arabino-furanosyl nucleosides in water. <i>Nature Communications</i> , 2018, 9, 4073.	5.8	36
1980	Structures and Spectral Study of Two Binuclear Cd(II) Complexes Based on 4-Nitro-1,2-Benzenedicarboxylic Acid. <i>Journal of Structural Chemistry</i> , 2018, 59, 936-942.	0.3	4
1981	4-((1,3-dioxoisindolin-2-yl)methyl)benzenesulfonamide: Full Structural and Spectroscopic Characterization and Molecular Docking with Carbonic Anhydrase II. <i>ChemistrySelect</i> , 2018, 3, 10113-10124.	0.7	16
1982	Benzodithiazole-Based Hole-Transporting Material for Efficient Perovskite Solar Cells. <i>Asian Journal of Organic Chemistry</i> , 2018, 7, 2497-2503.	1.3	8
1983	NBO, AIM, HOMO-LUMO and thermodynamic investigation of the nitrate ion adsorption on the surface of pristine, Al and Ga doped BNNTs: A DFT study. <i>Adsorption</i> , 2018, 24, 757-767.	1.4	32
1984	Supramolecular Assembly of a Zn(II)-Based 1D Coordination Polymer through Hydrogen Bonding and π - π Interactions: Crystal Structure and Device Applications. <i>ACS Omega</i> , 2018, 3, 12060-12067.	1.6	31
1985	Structural, density functional computational studies and antibacterial screening on N,N-bis-(4-hydroxy- β -methylsalicylidene)ethylenediamine nickel (II) complex. <i>Polyhedron</i> , 2018, 156, 165-173.	1.0	0

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1986	Intramolecular π - π Interactions with a Chiral Auxiliary Ligand Control Diastereoselectivity in a Cyclometalated Ir(III) Complex. <i>Inorganic Chemistry</i> , 2018, 57, 12836-12849.	1.9	8
1987	Machine Learning and Big-Data in Computational Chemistry. , 2018, , 1-24.		4
1988	Tetranuclear Oxo-Titanium Clusters with Different Carboxylate Aromatic Ligands: Optical Properties, DFT Calculations, and Photoactivity. <i>Materials</i> , 2018, 11, 1661.	1.3	16
1989	Mixed ab initio and semiempirical study of hydrogen-terminated finite germanium nanowires. <i>European Physical Journal Plus</i> , 2018, 133, 1.	1.2	3
1990	Quinolinolone-based Al/Triarylborane Dyad Assembly: Alteration of Electronic Transition States Mediated by Fluoride Anion Binding. <i>Bulletin of the Korean Chemical Society</i> , 2018, 39, 1294-1301.	1.0	3
1991	Vibrational spectroscopic and Hirshfeld surface analysis of carvedilol crystal forms. <i>International Journal of Pharmaceutics</i> , 2018, 553, 261-271.	2.6	8
1992	The remarkable enhancement of two-photon absorption in pyrene based chalcone derivatives. <i>Optical Materials</i> , 2018, 86, 331-337.	1.7	16
1993	Zintl superalkalis as building blocks of supersalts. <i>Journal of Molecular Modeling</i> , 2018, 24, 306.	0.8	11
1994	The role of computational results databases in accelerating the discovery of catalysts. <i>Nature Catalysis</i> , 2018, 1, 809-810.	16.1	52
1995	Biotransformation of \hat{I}^2 -Mangostin by an Endophytic Fungus of <i>Garcinia mangostana</i> to Furnish Xanthenes with an Unprecedented Heterocyclic Skeleton. <i>Journal of Natural Products</i> , 2018, 81, 2244-2250.	1.5	13
1996	FT-IR, Laser-Raman, UV-Vis, and NMR Spectroscopic Studies of Antidiabetic Molecule Nateglinide. <i>Journal of Spectroscopy</i> , 2018, 2018, 1-12.	0.6	5
1997	Complexes of Imino-1,2,4-triazole Derivative with Transition Metals: Synthesis and Antibacterial Study. <i>Russian Journal of General Chemistry</i> , 2018, 88, 1707-1711.	0.3	13
1998	Highly Linearized Twisted Iridium(III) Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 14450-14462.	1.9	8
1999	Experimental and theoretical spectroscopic analysis, chemical reactivity and fungicidal activity study on benalaxyl along with quantum chemical computation on metalaxyl and furalaxyl. <i>Chemical Data Collections</i> , 2018, 17-18, 370-393.	1.1	6
2000	Control of Structures and Emission Properties of $(CuI)_n$ 2-Methyldithiane Coordination Polymers. <i>Inorganic Chemistry</i> , 2018, 57, 13564-13576.	1.9	23
2001	Monocycloplatinated Solvento Complex Displays Turn-on Ratiometric Phosphorescence Responses to Histamine. <i>Inorganic Chemistry</i> , 2018, 57, 13985-13997.	1.9	7
2002	Structural, spectroscopic, and theoretical analysis of a molecular system based on		

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2004	Accurate Description of Low-Lying Excited States in a Series of Photoreactive Clusters [Os ₃ (CO) ₁₀ (f ₂ -diimine)] by DFT Calculations. <i>Inorganic Chemistry</i> , 2018, 57, 11704-11716.	1.9	3
2005	Quantum chemical design of triple hybrid organic, inorganic and organometallic materials: An efficient two-dimensional second-order nonlinear optical material. <i>Materials Chemistry and Physics</i> , 2018, 220, 286-292.	2.0	35
2006	Effects of Ancillary Ligands on Redox and Chemical Properties of Ruthenium Coordinated Azoaromatic Pincer. <i>Inorganic Chemistry</i> , 2018, 57, 11995-12009.	1.9	29
2007	Zinc/itaconate coordination polymers as first examples with long-lasting phosphorescence based on acyclic ligands. <i>Journal of Materials Chemistry C</i> , 2018, 6, 10870-10880.	2.7	10
2008	Electrical property and Schottky behavior of a flexible Schiff-base compound: X-ray structure and stabilization of 1D water chain. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 24744-24749.	1.3	9
2009	On the structural and spectroscopic properties of the thienyl chalcone derivative: 3-(5-Bromo-2-thienyl)-1-(4-nitrophenyl)-prop-2-en-1-one. <i>Vibrational Spectroscopy</i> , 2018, 99, 73-79.	1.2	3
2010	Structural, Spectroscopic, Antimicrobial Activity and DFT Studies on 4-Methyl-N-(4-methylphenylsulfonyl)-N-phenylbenzenesulfonamide. <i>Optics and Spectroscopy (English)</i> Tj ETQq0 0 0.12 BT / Overlock 10 T	1.2	3
2011	D-π-A type conjugated pyrene derivatives: Third-order nonlinear absorption and excited-state dynamics. <i>Optical Materials</i> , 2018, 85, 319-328.	1.7	21
2012	Near-White Light Emission from Lead(II) Metal-Organic Frameworks. <i>Inorganic Chemistry</i> , 2018, 57, 11341-11348.	1.9	42
2013	Highly Sensitive Ratiometric Chemosensor and Biomarker for Cyanide Ions in the Aqueous Medium. <i>ACS Omega</i> , 2018, 3, 10145-10153.	1.6	46
2014	Syntheses, crystal structures, DNA binding, DNA cleavage and DFT study of Co(III) complexes involving azo-appended Schiff base ligands. <i>New Journal of Chemistry</i> , 2018, 42, 16571-16582.	1.4	6
2015	A multi-analyte responsive chemosensor vaniliny Schiff base: fluorogenic sensing of Zn(II), Cd(II) and I ⁻ . <i>New Journal of Chemistry</i> , 2018, 42, 16653-16665.	1.4	36
2016	Highly selective and sensitive recognition of Zn(II) by a novel coumarinyl scaffold following spectrofluorometric technique and its application in living cells. <i>New Journal of Chemistry</i> , 2018, 42, 16297-16306.	1.4	9
2017	Toward quantum-chemical method development for arbitrary basis functions. <i>Journal of Chemical Physics</i> , 2018, 149, 084106.	1.2	10
2018	Copper(II)-sulfonamide Schiff base complexes: Structure, biological activity and theoretical interpretation. <i>Polyhedron</i> , 2018, 151, 344-354.	1.0	29
2019	A Computational Study on the Purinethol Drug Adsorption on the AlN Nanocone and Nanocluster. <i>Journal of Cluster Science</i> , 2018, 29, 767-775.	1.7	24
2020	Systematic design of indium-based luminophores with color-tunable emission via combined manipulation of HOMO and LUMO levels. <i>Dyes and Pigments</i> , 2018, 158, 285-294.	2.0	17
2021	A quantum chemical investigation of the influence of solvent polarity on the structural, electronic, spectroscopic properties and hyperpolarizability in Molybdenum Silyliyne complex CpMo(CO) ₂ (SiPh). <i>Journal of Molecular Liquids</i> , 2018, 264, 616-620.	2.3	14

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2022	Palladium(II) complexes with thioether containing azophenol ligands: Synthesis, characterization, X-ray structure and DNA binding study. <i>Polyhedron</i> , 2018, 150, 118-125.	1.0	11
2023	New bioactive cyclopeptide alkaloids with rare terminal unit from the root bark of <i>Ziziphus cambodiana</i> . <i>RSC Advances</i> , 2018, 8, 18204-18215.	1.7	6
2024	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
2025	Two isostructural linear coordination polymers: the size of the metal ion impacts the electrical conductivity. <i>New Journal of Chemistry</i> , 2018, 42, 10309-10316.	1.4	31
2026	Tailoring the benzotriazole (BTZ) auxiliary acceptor in a D-A- π -A type sensitizer for high performance dye-sensitized solar cells (DSSCs). <i>Dyes and Pigments</i> , 2018, 158, 195-203.	2.0	15
2027	Can bowl-like B30 nanostructure sense toxic cyanogen gas in air?: a theoretical study. <i>Molecular Physics</i> , 2018, 116, 2196-2204.	0.8	5
2028	Luminescent π -Substituted Fluoranthenes Synthesis, Structure, Electrochemistry, and Optical Properties. <i>Chemistry - A European Journal</i> , 2018, 24, 9622-9631.	1.7	10
2029	A Multi-Responsive Naphthalimide-Based Turn-on Fluorescent Chemosensor for Sensitive Detection of Trivalent Cations Ga ³⁺ , Al ³⁺ and Cr ³⁺ . <i>Journal of Fluorescence</i> , 2018, 28, 785-794.	1.3	25
2030	Adsorption of alanine with heteroatom substituted fullerene for solar cell application: A DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 202, 333-345.	2.0	7
2031	Investigation of Sarin Nerve Agent Adsorption Behavior on BN Nanostructures: DFT Study. <i>Journal of Cluster Science</i> , 2018, 29, 757-765.	1.7	31
2032	Synthesis, crystal structure, vibrational spectra, optical and DFT study of N-(3-ammonium propyl)-1, 3 diaminopropane tris iodate dehydrate [(C ₆ H ₂₀ N ₃)(IO ₃) ₃ ·2H ₂ O]. <i>Journal of Molecular Structure</i> , 2018, 1171, 76-86.	1.8	11
2033	Spectroscopic (FT-IR, FT Raman) and quantum mechanical study on N-(2,6-dimethylphenyl)-2-{4-[2-hydroxy-3-(2-methoxyphenoxy)propyl]piperazin-1-yl}acetamide. <i>Journal of Molecular Structure</i> , 2018, 1171, 268-278.	1.8	66
2034	A Flexible Rigid Rod, $\langle i \rangle$ -Pt(PMe ₃) ₂ (C ₆ H ₄ CN) ₂ (L1), to Form 2D [{Cu ₂ (μ -X) ₂] ₂ (μ -L1)] _n Polymers (X = Br, I) Exhibiting the Largest Bathochromic Emissions. <i>Inorganic Chemistry</i> , 2018, 57, 7208-7221.	1.9	8
2035	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
2036	Polymorphism in diaquatetrakis(6-chloro-2-hydroxypyridine)copper(II) perchlorate: Crystallographic, solution and theoretical studies and solid phase transformations. <i>Journal of Molecular Structure</i> , 2018, 1171, 294-304.	1.8	4
2037	Femtosecond Fluorescence Upconversion Study of a Naphthalimide Bithiophene Triphenylamine Push Pull Dye in Solution. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5533-5544.	1.1	13
2038	Mono substituted pyrenes as multifunctional materials for OLED: Analysis of the substituent effects on the charge transport properties using DFT methods. <i>Computational and Theoretical Chemistry</i> , 2018, 1138, 48-56.	1.1	6
2039	Molecular modeling, spectroscopic and structural studies on newly synthesized ligand N-benzoyl-2-isonicotinoylhydrazine-1-carboxamide. <i>Journal of Molecular Structure</i> , 2018, 1173, 332-340.	1.8	14

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2058	Theoretical studies on the chiral polyoxoanions [P ₂ Mo ₁₈ O ₆₂] ⁶⁻ and [PMo ₉ O ₃₁ (OH ₂) ₃] ³⁻ with histidine: chiral inversion and chiral induction. <i>Inorganic Chemistry Frontiers</i> , 2018, 5, 1992-1997.	3.0	0
2059	First-principles insights on the electronic and field emission properties of Ga and Al doped germanium nanocones. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2018, 227, 15-22.	0.8	21
2060	Fluorescent detection of Zn ²⁺ and Cu ²⁺ by a phenanthrene-based multifunctional chemosensor that acts as a basic pH indicator. <i>Inorganica Chimica Acta</i> , 2018, 482, 375-383.	1.2	14
2061	New bis 1,3,4-oxadiazole derivatives: syntheses, characterizations, computational studies, and antioxidant activities. <i>Canadian Journal of Chemistry</i> , 2018, 96, 1047-1059.	0.6	3
2062	Influence of Solvent and Electric Field on the Structure and IR, 31P NMR Spectroscopic Properties of a Titanocene-Benzyne Complex. <i>Journal of Applied Spectroscopy</i> , 2018, 85, 526-534.	0.3	14
2063	A dual target chemosensor for the fluorometric detection of In ³⁺ and colorimetric detection of Fe ³⁺ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 205, 622-629.	2.0	22
2064	Structural, vibrational and thermal studies on bis(L-glutaminato)copper(II). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 205, 603-613.	2.0	10
2065	Design and synthesis of novel ribofuranose nucleoside analogues as antiproliferative agents: A molecular docking and DFT study. <i>Journal of Molecular Liquids</i> , 2018, 269, 315-326.	2.3	20
2066	Role of Organic Ligands Orientation on the Geometrical and Optical Properties of Au ₂₅ (SCH ₃) ₁₈ . <i>Journal of Physical Chemistry A</i> , 2018, 122, 6864-6872.	1.1	9
2067	Phenothiazine-Based Oligo(<i>p</i> -phenylenevinylene)s: Substituents Affected Self-Assembly, Optical Properties, and Morphology-Induced Transport. <i>Chemistry - A European Journal</i> , 2018, 24, 13213-13222.	1.7	2
2068	A 2D Co(II) coordination polymer based on 1,3,5-tris(1H-imidazol-1-yl)benzene: photocatalytic properties and theoretical analysis. <i>Journal of Coordination Chemistry</i> , 2018, 71, 2622-2631.	0.8	1
2069	Molecular structure and absorption spectral properties of Corrole Isomers: DFT and TDDFT-IEFPCM investigations. <i>Computational and Theoretical Chemistry</i> , 2018, 1140, 73-79.	1.1	3
2070	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
2071	Complexation reactions, electronic properties, and reactivity descriptors of cysteamine-based ligands in aqueous solution: a PCM/DFT study. <i>Structural Chemistry</i> , 2018, 29, 1723-1737.	1.0	1
2072	Synthesis and characterization of a heteroleptic nickel paddlewheel complex. <i>Journal of Molecular Structure</i> , 2018, 1173, 345-348.	1.8	5
2073	The effect of electric field and Al doping on the sensitivity of hexa-peri-hexabenzocoronene nanographene to chloropicrin. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4486.	1.7	11
2074	<i>p</i> -Toluate-bridged dinuclear Cu(II) complexes in combination with tridentate chelating ligand: Crystal structure, density functional theory calculation, DNA/protein binding and catecholase activity. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4506.	1.7	17
2075	Walking the Emission Tightrope: Spectral and Computational Analysis of Some Dual-Emitting Benzothiadiazole Donor-Acceptor Dyes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7991-8006.	1.1	14

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2077	Synthesis and photophysical properties of new perylene bisimide derivatives for application as emitting materials in OLEDs. <i>Dyes and Pigments</i> , 2018, 159, 590-599.	2.0	30
2078	Alkaline-earth metal based MOFs with second scale long-lasting phosphor behavior. <i>CrystEngComm</i> , 2018, 20, 4793-4803.	1.3	29
2079	Impact of High Pressure on Metallophilic Interactions and Its Consequences for Spectroscopic Properties of a Model Tetranuclear Silver(I)-Copper(I) Complex in the Solid State. <i>Inorganic Chemistry</i> , 2018, 57, 8509-8520.	1.9	10
2080	Fluostatins Featuring a 6-5-6-6 Ring Skeleton and High Oxidized A-Rings from Marine <i>Streptomyces</i> sp. PKU-MA00045. <i>Marine Drugs</i> , 2018, 16, 87.	2.2	43
2081	HSQC-TOCSY Fingerprinting-Directed Discovery of Antiplasmodial Polyketides from the Marine Ascidian-Derived <i>Streptomyces</i> sp. (USC-16018). <i>Marine Drugs</i> , 2018, 16, 189.	2.2	17
2082	Two Chemically Stable Cd(II) Polymers as Fluorescent Sensor and Photocatalyst for Aromatic Dyes. <i>Polymers</i> , 2018, 10, 274.	2.0	5
2083	The utilization of a stable 2D bilayer MOF for simultaneous study of luminescent and photocatalytic properties: experimental studies and theoretical analysis. <i>RSC Advances</i> , 2018, 8, 23529-23538.	1.7	24
2084	Deltahedral Organozinc Superhalogens. <i>Chemistry - A European Journal</i> , 2018, 24, 13654-13658.	1.7	10
2085	The effect of ionic liquid adsorption on the electronic and optical properties of fluorographene nanosheets. <i>Journal of Molecular Liquids</i> , 2018, 268, 206-214.	2.3	15
2086	Aldehyde isomers of porphyrin: A spectroscopic and computational study. <i>Journal of Molecular Structure</i> , 2018, 1173, 665-670.	1.8	7
2087	Single sensors for multiple analytes employing fluorometric differentiation for Cr ³⁺ and Al ³⁺ in semi-aqueous medium with bio-activity and theoretical aspects. <i>Analytical Methods</i> , 2018, 10, 4063-4072.	1.3	21
2088	Electron Transfer Reactions: KO ^t Bu (but not NaO ^t Bu) Photoreduces Benzophenone under Activation by Visible Light. <i>Journal of the American Chemical Society</i> , 2018, 140, 9751-9757.	6.6	71
2089	Experimental and theoretical investigations on structural, spectroscopic, electronic and thermodynamic properties of (adamantan-1-yl)(phenylsulfanyl)methanone. <i>Journal of Molecular Structure</i> , 2018, 1173, 596-607.	1.8	2
2090	Theoretical Insights into D-D-A Sensitizers Employing N-Annulated Perylene for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6328-6342.	1.1	21
2091	A DFT study of penicillamine adsorption over pure and Al-doped C60 fullerene. <i>Adsorption</i> , 2018, 24, 471-480.	1.4	22
2092	Ethynyl-bridged porphyrin-corrole dyads and triads: Synthesis, properties and DFT calculations. <i>Tetrahedron</i> , 2018, 74, 4476-4488.	1.0	7
2093	Completely Unexpected Coordination Selectivity of Copper Iodide for Thioether Over Ethynyl. <i>Chemistry Africa</i> , 2018, 1, 67-77.	1.2	3

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2095	A multifunctional selective α -turn-on fluorescent chemosensor for detection of Group IIIA ions Al ³⁺ , Ga ³⁺ and In ³⁺ . <i>Photochemical and Photobiological Sciences</i> , 2018, 17, 1247-1255.	1.6	53
2096	New substituted imidazo[1,5-a]pyridine and imidazo[5,1-a]isoquinoline derivatives and their application in fluorescence cell imaging. <i>Dyes and Pigments</i> , 2018, 157, 298-304.	2.0	31
2097	Isoelectronic Pt(II) and Au(III)-N-heterocyclic carbene complexes: a structural and biological comparison. <i>New Journal of Chemistry</i> , 2018, 42, 10704-10711.	1.4	15
2098	What does it take to induce equilibrium in bidirectional energy transfers?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13682-13692.	1.3	1
2099	Fluorescent detection of Zn(II) and In(III) and colorimetric detection of Cu(II) and Co(II) by a versatile chemosensor. <i>Journal of Industrial and Engineering Chemistry</i> , 2018, 65, 290-299.	2.9	37
2100	A DFT study of H ₂ CO and HCN adsorptions on 3d, 4d, and 5d transition metal-doped graphene nanosheets. <i>Structural Chemistry</i> , 2018, 29, 147-157.	1.0	29
2101	First-principles study of efficient phenothiazine-based DSSCs. <i>Journal of Computational Electronics</i> , 2018, 17, 1410-1420.	1.3	35
2102	Synthesis, characterization and antimicrobial activities of Co(III) and Ni(II) complexes with 5-methyl-3-formylpyrazole-N(4)-diethylthiosemicarbazone (HMPzNHex2): X-ray crystallography and DFT calculations of [Co(MPzNHex2) ₂]ClO ₄ ·1.5H ₂ O (I) and [Ni(HMPzNHex2) ₂]Cl ₂ ·2H ₂ O (II). <i>Inorganica Chimica Acta</i> , 2018, 483, 271-283.	1.2	9
2103	Ruthenium complexes of pyridine oxime and azoimine ligands: Syntheses, crystallography, electrochemical and catalytic properties. <i>Inorganica Chimica Acta</i> , 2018, 483, 241-247.	1.2	3
2104	Synthesis, Characterization, and Nanomaterials Generated from 6,6'-((2-Hydroxyethyl)azanediyl)bis(methylene)bis(2,4-di- <i>tert</i> -butylphenol) Modified Group 4 Metal Alkoxides. <i>Inorganic Chemistry</i> , 2018, 57, 11264-11274.	1.9	8
2105	DFT/TD-DFT calculations of the electronic and optical properties of bis-N,N-dimethylaniline-based dyes for use in dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 367, 332-346.	2.0	17
2106	An experimental and theoretical investigation of the structure of synthesized ZnO powder. <i>Chemical Physics</i> , 2018, 513, 273-279.	0.9	9
2107	Explicit Aqueous Solvation Treatment of Epinephrine from Carriello 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
2108	Synthesis, characterization, theoretical simulation, and DNA-nuclease activity of a newly synthesized Mn(II) oximate complex. <i>Journal of Coordination Chemistry</i> , 2018, 71, 3250-3265.	0.8	3
2109	Improving the optical properties of [14] and [18] annulenes sandwiched between electron donor-acceptor groups. <i>Chemical Physics Letters</i> , 2018, 709, 26-32.	1.2	7
2110	Spermine-directed supramolecular self-assembly of water-soluble AIE-active tetraphenylethylene: nanobelt, nanosheet, globular and nanotubular structures. <i>New Journal of Chemistry</i> , 2018, 42, 15379-15386.	1.4	10
2111	Is it possible to use X ₁₂ Y ₁₂ (X = Al, B, and Y = N, P) nanocages for drug-delivery systems? A DFT study on the adsorption property of 4-aminopyridine drug. <i>Applied Physics A: Materials Science and Processing</i> , 2018, 124, 1.	1.1	54

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2113	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
2114	The impact of heteroatom substitution on cross-conjugation and its effect on the photovoltaic performance of DSSCs – a computational investigation of linear vs. cross-conjugated anchoring units. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22660-22673.	1.3	32
2115	A spectroscopic study of indigo dye in aqueous solution: A combined experimental and TD-DFT study. <i>Journal of Luminescence</i> , 2018, 204, 568-572.	1.5	3
2116	Dynamic multistimuli-responsive reversible chiral transformation in supramolecular helices. <i>Scientific Reports</i> , 2018, 8, 11220.	1.6	30
2117	X-ray absorption near edge structure analysis of the charge/discharge mechanisms of dithiobiuret polymer used as a high-capacity cathode material for lithium-ion batteries. <i>Electrochimica Acta</i> , 2018, 281, 99-108.	2.6	2
2118	Benzo[e]indolium derivatives in aqueous solutions: Reaction with bisulfite and successive interaction with Cu ²⁺ and Hg ²⁺ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 202, 324-332.	2.0	2
2119	Molecular dynamic simulations, ALIE surface, Fukui functions geometrical, molecular docking and vibrational spectra studies of tetra chloro p and m-xylene. <i>Journal of Molecular Structure</i> , 2018, 1171, 253-267.	1.8	53
2120	Chiral coordination polymers based on d ¹⁰ metals and 2-aminonicotinate with blue fluorescent/green phosphorescent anisotropic emissions. <i>Dalton Transactions</i> , 2018, 47, 8746-8754.	1.6	12
2121	Optical monitoring of adipose tissue destruction under encapsulated lipase action. <i>Journal of Biophotonics</i> , 2018, 11, e201800058.	1.1	10
2122	Structural, computational and Hirshfeld surface analysis of a proton transfer crystal, amino (2-(propan-2-ylidene) hydrazinyl) methaniminium picrate. <i>Journal of Molecular Structure</i> , 2018, 1171, 793-807.	1.8	4
2123	Synthesis and experimental/theoretical evaluations on redox potentials and electronic absorption spectra for copper symmetric bis(thiosemicarbazone) complexes. <i>Polyhedron</i> , 2018, 151, 221-232.	1.0	4
2124	Electrochemical, Spectroelectrochemical, MÃ¶bauer, and EPR Spectroscopic Studies on Ferrocenyl-Substituted Tritylium Dyes. <i>Chemistry - A European Journal</i> , 2018, 24, 12524-12538.	1.7	12
2125	A multi-functional chemosensor for highly selective ratiometric fluorescent detection of silver(I) ion and dual turn-on fluorescent and colorimetric detection of sulfide. <i>Royal Society Open Science</i> , 2018, 5, 180293.	1.1	19
2126	Molecular structure, Hirshfeld surface analysis, spectroscopic (FT-IR, Laser-Raman, UV-vis. and NMR), HOMO-LUMO and NBO investigations on N-(12-amino-9,10-dihydro-9,10-ethanoanthracen-11-yl)-4-methylbenzenesulfonamide. <i>Journal of Molecular Structure</i> , 2018, 1171, 696-705.	1.8	40
2127	Theoretical study of hydrogen storage reactions on nickel-decorated heterofullerene C ₅₈ B _x X _y (N _x Y _y = 0, 1, 2). <i>Molecular Physics</i> , 2018, 116, 2321-2342.		
2128	Nonlinear optical, IR and orbital properties of Ni doped MgO nanoclusters: A DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2018, 1138, 39-47.	1.1	21
2129	XRD, Spectroscopic characterization (FT-IR, UV-vis), Hirshfeld surface analysis and chemical activity of (E)-benzyl 2-((2S,3S,4R)-2,3,4-tris(benzyloxy)hex-5-enylidene) hydrazinecarboxylate. <i>Journal of Molecular Structure</i> , 2018, 1171, 375-387.	1.8	2

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2131	<i>Ab initio</i> study of C20 nanocluster effects on electrochemical properties of tetraphenylporphyrin. Journal of Porphyrins and Phthalocyanines, 2018, 22, 640-645.	0.4	2
2132	Pesticidal compound Pirimicarb: Spectral analysis, DFT computations, molecular docking study and in vitro bioactivity. Chemical Physics Letters, 2018, 706, 295-302.	1.2	8
2133	Synthesis, crystallographic structure, DFT calculations and Hirshfeld surface analysis of a fumarate bridged Co(II) coordination polymer. Journal of Molecular Structure, 2018, 1173, 42-51.	1.8	59
2134	First-principle study of ammonia molecules adsorption on boron nitride nanotubes in presence and absence of static electric field and ion field. Vacuum, 2018, 155, 456-464.	1.6	36
2135	Electronic States of Quinones for Organic Energy Devices: The Effect of Molecular Structure on Electrochemical Characteristics. ACS Applied Energy Materials, 2018, 1, 3084-3092.	2.5	9
2136	Copper (<i>scp</i>) dimers stabilized by bis(phenol) amine ligands: theoretical and experimental insights. New Journal of Chemistry, 2018, 42, 12621-12631.	1.4	12
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2141	Isothermal titration calorimetry and stopped flow circular dichroism investigations of the interaction between lomefloxacin and human serum albumin in the presence of amino acids. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2265-2282.	2.0	83
2142	ExcelAutomat 1.3: Fragment analysis based on the distortion/interaction-activation strain model. Journal of Computational Chemistry, 2019, 40, 619-624.	1.5	9
2143	Growth, Hirshfeld surfaces, spectral, quantum chemical calculations, photoconductivity and chemical etching analyses of nonlinear optical p-toluidine p-toluenesulfonate single crystal. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 206, 340-349.	2.0	38
2144	Spectroscopic investigation, molecular orbital studies, frequency and solvent dependent NLO properties of (2E)-1-(4-bromophenyl)-3-phenylprop-2-en-1-one. Materials Research Innovations, 2019, 23, 385-396.	1.0	2
2145	Optical properties of sub 20 nm long (6,5) single-walled carbon nanotubes: first principles investigation. Molecular Physics, 2019, 117, 71-78.	0.8	3
2146	Use of the fluorogenic Al ³⁺ -quinolinyl-azo-naphtholato complex for the determination of F ⁻ in aqueous medium by visible light excitation and application in ground water fluoride analysis. Analytical Methods, 2019, 11, 4440-4449.	1.3	4
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2149	Quantum chemical calculations, Hirshfeld surface analysis, and molecular docking studies of antibacterial $\text{E}^{\text{N}}\text{-}((1\text{H-Indol-3-yl)methylene})\text{-4-bromobenzohydrazide}$. <i>Spectroscopy Letters</i> , 2019, 52, 398-412.	0.5	1
2150	Theoretical UV-Vis spectra of tetracationic porphyrin: effects of environment on electronic spectral properties. <i>Journal of Molecular Modeling</i> , 2019, 25, 264.	0.8	5
2151	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells. <i>RSC Advances</i> , 2019, 9, 26402-26418.	1.7	115
2152	Quantum chemical studies and spectroscopic investigations on 2-amino-3-methyl-5-nitropyridine by density functional theory. <i>Heliyon</i> , 2019, 5, e02149.	1.4	19
2153	A comprehensive DFT study on the sensing abilities of cyclic oligothiophenes (nCTs). <i>New Journal of Chemistry</i> , 2019, 43, 14120-14133.	1.4	45
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2155	Theoretical investigation of N-trans-cinnamylidene-m-toluidine by DFT method and molecular docking studies. <i>Journal of Molecular Structure</i> , 2019, 1198, 126868.	1.8	5
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2158	Spectroscopic transitions supporting chemiluminescence in the reaction of calcium with hydrogen chloride. <i>Spectroscopy Letters</i> , 2019, 52, 330-338.	0.5	0
2159	Generation of Microsecond Charge-Separated Excited States in Rhenium(I) Diimine Complexes: Driving Force Is the Dominant Factor in Controlling Lifetime. <i>Inorganic Chemistry</i> , 2019, 58, 9785-9795.	1.9	11
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2162	Theoretical studies of nanostructures modeled by the binding of uracil derivatives to functionalized (5,5) carbon nanotubes. <i>Chemical Physics Letters</i> , 2019, 731, 136602.	1.2	17
2163	Characterization of Molybdenum Dithiocarbamates by First-Principles Calculations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7007-7015.	1.1	17
2164	Transition metals doped ZnO nanocluster for ethylene oxide detection: A DFT study. <i>Main Group Metal Chemistry</i> , 2019, 42, 113-120.	0.6	14
2165	Lithium Attachment to C60 and Nitrogen- and Boron-Doped C60: A Mechanistic Study. <i>Materials</i> , 2019, 12, 2136.	1.3	9

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2167	Designing dithienothiophene (DTT)-based donor materials with efficient photovoltaic parameters for organic solar cells. <i>Journal of Molecular Modeling</i> , 2019, 25, 222.	0.8	58
2168	The Binary Iodine- κ -Chlorine Octahalide Series $[\text{I}_n\text{Cl}_{8-n}]^{2+}$ ($n=3, 3.6, 4$). <i>Chemistry - A European Journal</i> , 2019, 25, 11650-11658.	1.7	12
2169	Selective chemosensor capable of sensing both CN^- and Zn^{2+} : Its application to zebrafish. <i>Sensors and Actuators B: Chemical</i> , 2019, 297, 126814.	4.0	19
2170	Experimental and quantum chemical investigations of 4-bromoanilinium hydrogen phthalate crystal for optoelectronic applications. <i>Materials Research Express</i> , 2019, 6, 095105.	0.8	8
2171	Theoretical and experimental investigation on the electrochemical properties, structural and spectroscopic parameters of 6,7-dihydroxy-9-thia-1,4a-diaza fluoren-2-one (DTDFO). <i>Journal of Sulfur Chemistry</i> , 2019, 40, 598-613.	1.0	0
2172	The influence of water molecules on the stability of mineral green pigments in Chinese ancient painting. <i>Chemical Physics Letters</i> , 2019, 731, 136592.	1.2	5
2173	Photophysical and biological investigation of phenol substituted rhenium tetrazolato complexes. <i>Dalton Transactions</i> , 2019, 48, 15613-15624.	1.6	8
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2430	DFT/TD-DFT calculation, photophysical properties, DNA/protein binding and catecholase activity of chelating ligand based trigonal bipyramidal copper(II) complexes. <i>Journal of Molecular Structure</i> , 2019, 1179, 558-567.	1.8	14
2431	Preventive agents for neurodegenerative diseases from resin of <i>Dracaena cochinchinensis</i> attenuate LPS-induced microglia over-activation. <i>Journal of Natural Medicines</i> , 2019, 73, 318-330.	1.1	18
2432	Growth, structural, optical, thermal, laser damage threshold and theoretical investigations of organic nonlinear optical 2-aminopyridinium 4-nitrophenolate 4-nitrophenol (2AP4N) single crystal. <i>Journal of Materials Science: Materials in Electronics</i> , 2019, 30, 1553-1570.	1.1	14
2433	A fluorescent and colorimetric Schiff base chemosensor for the detection of Zn ²⁺ and Cu ²⁺ : Application in live cell imaging and colorimetric test kit. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 211, 34-43.	2.0	33
2434	Tailoring the Optical Properties of Organic D-π-A Photosensitizers: Effect of Sulfur Introduction in the Acceptor Group. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 812-825.	1.2	3
2435	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
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2438	Synthesis, X-ray crystal structure, DFT calculations, spectroscopic characterization and redox behaviour of a rhodium(III) complex of an anthracene-pyridylhydrazone ligand. <i>Transition Metal Chemistry</i> , 2019, 44, 341-347.	0.7	4
2439	Synthesis and spectroscopic study of two new pyrazole derivatives with detailed computational evaluation of their reactivity and pharmaceutical potential. <i>Journal of Molecular Structure</i> , 2019, 1181, 599-612.	1.8	59
2440	Monomeric zinc(II) amide complexes supported by bidentate, benzannulated phenanthridine amido ligands. <i>Polyhedron</i> , 2019, 161, 261-267.	1.0	13
2441	Mixed thioalkyl-azoimine (SNN [±])-diimine-ruthenium complexes: synthesis, characterization, DFT calculations, crystal structure and application as pre-catalysts for hydrogenation of acetophenone. <i>Transition Metal Chemistry</i> , 2019, 44, 355-367.	0.7	7
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2443	Spectroscopic (FT-IR, FT-Raman, UV-Vis), quantum chemical calculation and molecular docking evaluation of liquiritigenin: an influenza A (H1N1) neuraminidase inhibitor. <i>Research on Chemical Intermediates</i> , 2019, 45, 2135-2166.	1.3	21
2444	Synthesis, molecular modeling and antioxidant activity of new phenolic bis-azobenzene derivatives. <i>Journal of Molecular Structure</i> , 2019, 1182, 22-30.	1.8	19
2445	A study of the optical, electrical and structural properties of poly(pyrrole-3,4-dicarboxylic acid). <i>Polymer</i> , 2019, 164, 142-153.	1.8	10
2446	Dehydrogenation of formic acid catalysed by M-embedded nitrogen-doped graphene (M = Fe, Ru, Os): a DFT study. <i>New Journal of Chemistry</i> , 2019, 43, 1440-1448.	1.4	15
2447	Research of the substituent effect on non-linear optical properties of bis(difluoroboron)-1,2-bis((1H-pyrrol-2-yl)methylene)hydrazine (BOPHY) derivatives: Molecular simulation analyses. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 212, 380-387.	2.0	7
2448	Effect of Planarity of Aromatic Rings Appended to o-Carborane on Photophysical Properties: A Series of o-Carboranyl Compounds Based on 2-Phenylpyridine- and 2-(Benzo[b]thiophen-2-yl)pyridine. <i>Molecules</i> , 2019, 24, 201.	1.7	9
2449	Synthesis of new star-like triply ferrocenylated compounds. <i>Inorganica Chimica Acta</i> , 2019, 486, 95-100.	1.2	1
2450	Experimental and density functional theory (MEP, FMO, NLO, Fukui functions) and antibacterial activity studies on 2-amino-4-(4-nitrophenyl)-5,6-dihydrobenzo[h]quinoline-3-carbonitrile. <i>Journal of Molecular Structure</i> , 2019, 1178, 450-457.	1.8	73
2451	Deep red PhOLED from dimeric salophen Platinum(II) complexes. <i>Dyes and Pigments</i> , 2019, 162, 590-598.	2.0	65
2452	Effect of H-bond and molecular geometry towards innocent and non-innocent behavior of 3,5-di-tert-butyl-2-aminophenol units attached to a piperazine backbone: Co(III) and Cu(II) complexes. <i>Inorganica Chimica Acta</i> , 2019, 486, 213-220.	1.2	4
2453	Synthetic and structural investigations of Cd(II) complexes of tetradentate pyrimidine based Schiff base ligand: Insight through non-covalent interactions, TDDFT calculation and Hirshfeld surface analysis. <i>Journal of Molecular Structure</i> , 2019, 1178, 682-691.	1.8	10
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2456	Gold(I) Complexes of Fulvenyl-Functionalized Arylisocyanides. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 42-50.	1.0	3
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2459	A bi-nuclear Cu(II)-complex for selective epoxidation of alkenes: Crystal structure, thermal, photoluminescence and cyclic voltammetry. <i>Inorganica Chimica Acta</i> , 2019, 486, 352-360.	1.2	7
2460	Structure, vibrational, electrical and optical study of [C ₂ H ₁₀ N ₂] (IO ₃) ₂ ·4HIO ₃ . <i>Journal of Molecular Structure</i> , 2019, 1179, 18-32.	1.8	7
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2464	Theoretical study of high-efficiency organic dyes with the introduction of different auxiliary heterocyclic acceptors based on IQ1 toward dye-sensitized solar cells. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 86, 170-178.	1.3	19
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2466	Matrix Coordination Induced Emission in a Three-Dimensional Silver Cluster-Assembled Material. <i>Chemistry - A European Journal</i> , 2019, 25, 2750-2756.	1.7	38
2467	Electronic properties of B ₁₂ N ₁₂ fullerene-like nanoclusters functionalized with Schiff bases: a DFT study. <i>Structural Chemistry</i> , 2019, 30, 979-987.	1.0	2
2468	Four new luminescent-organic frameworks exhibiting highly sensing of nitroaromatics: An experimental and computational insight. <i>Inorganica Chimica Acta</i> , 2019, 487, 257-263.	1.2	15
2469	A Comparative Computational Investigation of Phosgene Adsorption on (XY) ₁₂ (X = Al, B and Y = N, P) Nanoclusters: DFT Investigations. <i>Journal of Cluster Science</i> , 2019, 30, 203-218.	1.7	34
2470	Theoretical insight into the photophysical properties of six phosphorescent heteroleptic iridium(III) complexes with different monodentate ligands. <i>Polyhedron</i> , 2019, 157, 131-135.	1.0	1
2471	Effect of C ₂₀ nanocage on electrical, optical and structural properties of tetraphenylporphyrin with Zn and Mg central metal. <i>Polyhedron</i> , 2019, 157, 310-315.	1.0	7
2472	Synthesis, spectroscopic properties and DFT studies of copper(II) complex of (E)-1-((2,4-dichlorophenylimino)methyl)naphthalen-2-ol. <i>Inorganica Chimica Acta</i> , 2019, 484, 297-304.	1.2	1

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2474	Structures and photocatalytic performance of two d10 metal-based coordination polymers containing mixed building units. <i>Transition Metal Chemistry</i> , 2019, 44, 107-114.	0.7	3
2475	Effective degradation of Reactive Red 195 via heterogeneous electro-Fenton treatment: theoretical study and optimization. <i>International Journal of Environmental Science and Technology</i> , 2019, 16, 6329-6346.	1.8	19
2476	Adsorption of mercaptopurine drug on the BN nanotube, nanosheet and nanocluster: a density functional theory study. <i>Molecular Physics</i> , 2019, 117, 531-538.	0.8	24
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2478	A new synthesis of limonene copolymer: experimental and theoretical analysis. <i>Polymer Bulletin</i> , 2019, 76, 3297-3327.	1.7	4
2479	Targeting human telomeric DNA quadruplex with novel berberrubine derivatives: insights from spectroscopic and docking studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 1375-1389.	2.0	15
2480	Boron substitution effect on adsorption of H ₂ molecules on organometallic complexes. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 345-353.	3.8	38
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2482	Structural and Optical Properties of New Naphthalene and Perylene Imide Imidazoles. <i>Polycyclic Aromatic Compounds</i> , 2019, 39, 363-373.	1.4	7
2483	Aryl ferrocenylmethylesters: Synthesis, solid-state structure and electrochemical investigations. <i>Arabian Journal of Chemistry</i> , 2020, 13, 3546-3557.	2.3	7
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2485	Efficient H ₂ gas sensor based on 2D SnO ₂ disks: Experimental and theoretical studies. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 26388-26401.	3.8	57
2486	X-ray crystal structure, spectroscopic and DFT computational studies of H-bonded charge transfer complexes of tris (hydroxymethyl)aminomethane (THAM) with chloranilic acid (CLA). <i>Journal of Molecular Structure</i> , 2020, 1200, 127066.	1.8	28
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2488	Crystal structure, Hirshfeld surface, spectroscopic analyses, electronic properties, NLO profile and thermochemical study of an antispasmodic agent trimebutine. <i>Journal of Molecular Structure</i> , 2020, 1199, 127043.	1.8	7
2489	Ga-doped phagraphene as a superior media for sensing of carbon monoxide: A detailed theoretical investigation. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 116, 113710.	1.3	29
2490	Synthesis, spectral properties, chemical descriptors and light harvesting studies of a new bioactive azo imidazole compound. <i>Journal of Molecular Structure</i> , 2020, 1199, 127035.	1.8	75

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2492	Determination of H ₂ S, COS, CS ₂ and SO ₂ by an aluminium nitride nanocluster: DFT studies. <i>Molecular Physics</i> , 2020, 118, e1658909.	0.8	17
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2494	Turn-on fluorescence study of a highly selective acridine-based chemosensor for Zn ²⁺ in aqueous solutions. <i>Inorganica Chimica Acta</i> , 2020, 499, 119191.	1.2	27
2495	A combined DFT and FT-IR study on the surface interactions in alumina supported ionic liquid [H ⁺ Pyrr]+[HSO ₄] ⁻ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 226, 117545.	2.0	7
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2497	Optical and electronic properties of nickel(II) coordinated to chiral amino-alcohols. An experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2020, 1202, 127200.	1.8	1
2498	Solvent effects on UV-Vis and FT-IR spectra of indapamide combined with DFT calculations. <i>Chemical Papers</i> , 2020, 74, 1103-1111.	1.0	2
2499	A rare flattened tetrahedral Mn(II) salen type complex: Synthesis, crystal structure, biomimetic catalysis and DFT study. <i>Inorganica Chimica Acta</i> , 2020, 499, 119176.	1.2	17
2500	Structural parameters, electronic, linear and nonlinear optical exploration of thiopyrimidine derivatives: A comparison between DFT/TDDFT and experimental study. <i>Journal of Molecular Structure</i> , 2020, 1201, 127183.	1.8	53
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2503	Synthesis, spectroscopic characterization, DFT computations, nonlinear optical profile and molecular docking study of a novel chalcone derivative. <i>Journal of Molecular Structure</i> , 2020, 1202, 127270.	1.8	18
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2505	Chromogenic hydrazide Schiff base reagent: Spectrophotometric determination of CN ⁻ ion. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 225, 117471.	2.0	23
2506	New small organic molecules based on thieno[2,3-b]indole for efficient bulk heterojunction organic solar cells: a computational study. <i>Molecular Physics</i> , 2020, 118, e1662956.	0.8	36
2507	Hydrogen abstraction of methanimine by X ₁₂ N ₁₂ (X = B, Al) nanoclusters: a DFT study. <i>Structural Chemistry</i> , 2020, 31, 447-454.	1.0	0
2508	A combined experimental (XRD, FT-IR, UV-VIS and NMR) and theoretical (NBO, NLO, local & global) Tj ETQq1 1 0.784314 rgBT /Ome acetate. <i>Journal of Molecular Structure</i> , 2020, 1199, 126970.	1.8	10

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2511	Theoretical calculation of simple and doped CNTs with the potential adsorption of various ions for water desalination technologies. Structural Chemistry, 2020, 31, 399-409.	1.0	4
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2516	Substituent effect on the cell voltage of nanographene based Li-ion batteries: A DFT study. Solid State Communications, 2020, 306, 113770.	0.9	31
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2520	Synthesis and photophysical studies on a new fluorescent phenothiazineàbased derivative. Luminescence, 2020, 35, 608-617.	1.5	8
2521	Spectroscopic, quantum chemical, QTAIM analysis, molecular dynamics simulation, docking studies and solvent effect of pyridin-2-yl oxyacetic acid herbicide and its derivatives. Journal of Molecular Structure, 2020, 1206, 127677.	1.8	12
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2526	Rhodium assisted peri-Cà“H activation in benzothiazolyl-hydrazone derivatized pyrene. Polyhedron, 2020, 179, 114352.	1.0	2

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2528	Dinuclear μ_2 -Phenoxy and μ_2 -Hydroxo Bridged Copper Complexes Exhibiting Oxidation of Phenols and Isoelectronic Compounds: Cytotoxicity and Evidences for Cellular Apoptosis. <i>ChemistrySelect</i> , 2020, 5, 463-475.	0.7	1
2529	Rational design of novel N-doped polyaromatic hydrocarbons as donors for the perylene based dye-sensitized solar cells. <i>Journal of Chemical Sciences</i> , 2020, 132, 1.	0.7	12
2530	Investigation of electrical conductance properties, non-covalent interactions and TDDFT calculation of a newly synthesized copper(II) metal complex. <i>Journal of Molecular Structure</i> , 2020, 1206, 127663.	1.8	5
2531	Perturbing the AIEE activity of pyridine functionalized μ_2 -cyanostilbenes with donor substitutions: an experimental and DFT study. <i>New Journal of Chemistry</i> , 2020, 44, 218-230.	1.4	25
2532	Exploring solvent dependent catecholase activity in transition metal complexes: an experimental and theoretical approach. <i>New Journal of Chemistry</i> , 2020, 44, 1371-1388.	1.4	25
2533	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
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2535	New pyran-based molecules as both n- and p-type sensitizers in semi-transparent Dye Sensitized Solar Cells. <i>Dyes and Pigments</i> , 2020, 175, 108140.	2.0	16
2536	Synthesis, characterization and DFT studies of complexes bearing $[\text{Re}(\text{CO})_3]^+$ core and reactivity towards cyanide ion. <i>Journal of Organometallic Chemistry</i> , 2020, 908, 121098.	0.8	5
2537	Structural, spectroscopic and thermal characterizations combined with DFT calculations and Hirshfeld analysis of a novel hydrogen-bonded complex: p-phenylenediammonium dinitrate. <i>Journal of Molecular Structure</i> , 2020, 1205, 127624.	1.8	7
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2539	Molecular structure of 1,4-bis(substituted-carbonyl)benzene: A combined experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2020, 1205, 127633.	1.8	26
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2542	Development of Rhodamine 6G-Based Fluorescent Chemosensors for Al^{3+} -Ion Detection: Effect of Ring Strain and Substituent in Enhancing Its Sensing Performance. <i>ACS Omega</i> , 2020, 5, 145-157.	1.6	30
2543	Growth, structural, Hirshfeld surface, optical, laser damage threshold, dielectric and chemical etching analysis of 4-dimethylaminopyridinium 4-nitrophenolate 4-nitrophenol (DMAPNP) single crystal. <i>Journal of Materials Science: Materials in Electronics</i> , 2020, 31, 373-386.	1.1	7
2544	A naproxen derived schiff-base for highly selective sensing of fluoride. <i>Journal of Molecular Structure</i> , 2020, 1203, 127364.	1.8	5

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2545	Oxidovanadium (V and IV) complexes incorporating coumarin based O ^N O ligand: Synthesis, structure and catalytic activities. <i>Polyhedron</i> , 2020, 176, 114241.	1.0	3
2546	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
2547	Novel Î ² -ketoenamines versus azomethines for organic electronics: characterization of optical and electrochemical properties supported by theoretical studies. <i>Journal of Materials Science</i> , 2020, 55, 3812-3832.	1.7	9
2548	Square disks-based crossed architectures of SnO ₂ for ethanol gas sensing applications—An experimental and theoretical investigation. <i>Sensors and Actuators B: Chemical</i> , 2020, 304, 127352.	4.0	34
2549	Spectral, DFT/B3LYP and molecular docking analyses on ethyl 2-(5-methyl-1,2,4-triazolo[1,5-a]pyrimidin-7-yl)pent-4-enoate. <i>Journal of Molecular Structure</i> , 2020, 1206, 127680.	1.8	9
2550	New push-pull dyes based on 2-(3-oxo-2,3-dihydro-1H-cyclopenta[b]naphthalen-1-ylidene)malononitrile: An amine-directed synthesis. <i>Dyes and Pigments</i> , 2020, 175, 108182.	2.0	16
2551	Syntheses and photocatalytic properties of two new d10- and d9-based 2D coordination polymers. <i>Inorganica Chimica Acta</i> , 2020, 502, 119334.	1.2	5
2552	Experimental and theoretical approach: Chemical activity, charge transfer of DNA/ECT, thermodynamic, spectroscopic, structural and electronic properties of N-(4-(3-methyl-3-phenylcyclobutyl)thiazol-2-yl)acetamide molecule. <i>Journal of Molecular Structure</i> , 2020, 1204, 127513.	1.8	9
2553	Computational investigation of solvent polarity effect on the structure and properties of a (OC)4Cr-biscarbene complex in the singlet ground state and lowest singlet excited state. <i>Journal of Molecular Liquids</i> , 2020, 300, 112327.	2.3	6
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3291	Theoretical (Hirshfeld surface, molecular docking, structural, electronic properties, NBO and NLO) Tj ETQq1 1 0.784314 rgBT /Overloc of <i>Journal of Molecular Structure</i> , 2021, 1245, 130981.	1.8	5
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3320	Impact of chemical modifications on the luminescence properties of organic neutral radical emitters. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10794-10801.	2.7	13
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3507	Nature of electronic excitations in small non-stoichiometric quantum dots. <i>Journal of Materials Chemistry A</i> , 2022, 10, 5212-5220.	5.2	10
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3807	Crystal Prediction and Design of Tunable Light Emission in BTB-Based Metal-Organic Frameworks. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	3
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3835	Silicon Carbide Based Nanotubes as a Sensing Material for Gaseous H ₂ SiCl ₂ . <i>Silicon</i> , 2023, 15, 177-186.	1.8	3
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3839	Theoretical investigation of lithium-based clusters Lin (where n = 3, 5, 7) with remarkable electronic and frequency-dependent NLO properties. <i>European Physical Journal Plus</i> , 2022, 137, .	1.2	2
3840	Metal-Doped Al ₁₂ X ₁₂ (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

#	ARTICLE	IF	CITATIONS
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3914	3D supramolecular assembly of Cu(II) CP containing 1D zig-zag chain and 2D paddle-wheel net: Structural elucidation and investigation of band gap. <i>Inorganica Chimica Acta</i> , 2022, 543, 121206.	1.2	0
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3967	Dispersion corrected-DFT investigation on the adsorption and selective detection of organic solvent vapors by Cu ₂ (HCOO) ₄ paddle wheel of metal organic framework. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100749.	1.3	2
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3978	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
3979	Computational investigations on acceptor substituent influence of metal-free efficient chromophores for optoelectronic properties. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	3
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4097	The Study of Interaction of Melphalan with SWCNT- BNNT Through Force Fields Molecular Mechanics and Quantum Calculations in Different Solvents and Temperatures. <i>Letters in Organic Chemistry</i> , 2023, 20, 657-671.	0.2	0
4098	Pure and Cu, Fe, and Zn-doped CNTs as novel drug carriers for dacarbazine. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	0
4099	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
4100	Studying Ga and Ge-doped AIP nanotube as a drug carrier for ciclopirox anticancer drug using DFT. <i>Computational and Theoretical Chemistry</i> , 2023, 1221, 114025.	1.1	0
4101	Investigation of aluminum nitride nanocarrier for drug delivery process of Favipiravir: A DFT study. <i>Journal of Molecular Liquids</i> , 2023, 372, 121209.	2.3	7
4102	Adsorption, sensing and catalytic properties of the pristine C24N24 nanocage to small gas molecules: A DFT-D3 investigation. <i>Vacuum</i> , 2023, 209, 111798.	1.6	4
4103	A new cyano ($\hat{\sim}$ 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
4104	Binuclear Cu(II), Ni(II) and Zn(II) complexes of hydrazone Schiff bases: Synthesis, spectroscopy, DFT calculations, and SOD mimetic activity. <i>Journal of Molecular Structure</i> , 2023, 1278, 134926.	1.8	10
4105	Structure/function relationships of a new stannate (IV) complex based on 5,7-dichloro-8-hydroxyquinolinium, accomplished with DFT calculations. <i>Journal of Molecular Structure</i> , 2023, 1277, 134811.	1.8	3
4106	Multiple Ti and Li doped carbon nanoring for hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2022, , .	3.8	2
4109	Synthesis, Quantum Computational Analysis and Molecular Docking of 3-(2-Hydroxyphenyl)-1-Phenyl Propanone: A Combined Experimental and Theoretical Analysis. <i>Polycyclic Aromatic Compounds</i> , 2023, 43, 8903-8932.	1.4	1
4110	Metalation of Tellurophene: Reactivity of 21,23-Ditelluraporphodimethene toward Palladium(II), Platinum(II), and Rhodium(I). <i>Inorganic Chemistry</i> , 0, , .	1.9	1
4111	Luminescent Anionic Cyclometalated Organoplatinum (II) Complexes with Terminal and Bridging Cyanide Ligand: Structural and Photophysical Properties. <i>Inorganic Chemistry</i> , 2023, 62, 1513-1529.	1.9	4
4112	New palladium(\langle sc \rangle ii \langle /sc \rangle) and platinum(\langle sc \rangle ii \langle /sc \rangle) complexes with an ONS donor azo-thioether pincer ligand: synthesis, characterization, protein binding study and <i>in vitro</i> cytotoxicity. <i>New Journal of Chemistry</i> , 2023, 47, 4931-4943.	1.4	5
4113	The study of roselle flower (<i>Hibiscus sabdariffa</i> L.) antioxidants reactivity based on Frontier Molecular Orbital (FMO) theory. <i>AIP Conference Proceedings</i> , 2023, , .	0.3	1
4114	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
4115	A comparative study on optical properties of AlCl-Pc, AlH-Pc, Al-Pc, and phthalocyanine organic compounds. <i>Journal of Porphyrins and Phthalocyanines</i> , 0, , .	0.4	0

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4118	DFT, ADMET, molecular docking and molecular dynamics studies of pyridoxal. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100926.	1.3	8
4119	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
4120	Design and Mechanism of Rare-Earth Singlet Oxygen Sensing: An Experimental and Quantum Chemical Approach. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1130-1140.	1.1	0
4121	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. <i>ACS Omega</i> , 2023, 8, 4767-4781.	1.6	8
4122	A comparative DFT study on Al- and Si- doped single-wall carbon nanotubes (SWCNTs) for Ribavirin drug sensing and detection. <i>Materials Science in Semiconductor Processing</i> , 2023, 158, 107360.	1.9	3
4123	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
4124	Synthesis, structural elucidation and optical activity of symmetric Schiff base-functionalized ferrocenes: Synergetic experimental and DFT insights. <i>Journal of Molecular Structure</i> , 2023, 1280, 135052.	1.8	2
4125	Tris chelated meridional isomers of Co(III) complexes: Synthesis, crystal structure, protein binding, cytotoxicity studies and DFT/TDDFT calculation. <i>Inorganica Chimica Acta</i> , 2023, 550, 121423.	1.2	4
4126	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
4127	Azanylylidene-based tetradentate Schiff base as a new ON-OFF fluorescent probe for the detection of Cu(II) ion: Synthesis, characterization and real sample analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 292, 122435.	2.0	9
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4129	New nitrosyl ruthenium complexes with combined activities for multiple cardiovascular disorders. <i>Dalton Transactions</i> , 2023, 52, 5176-5191.	1.6	2
4130	Synthesis and Optical Properties of a Series of Push-Pull Dyes Based on Pyrene as the Electron Donor. <i>Molecules</i> , 2023, 28, 1489.	1.7	1
4131	Transition metals doped ZnS nanocluster for carbon monoxide detection: A DFT study. <i>Materials Today Communications</i> , 2023, 34, 105491.	0.9	2
4133	He adsorption and sensing properties of graphene nanoflakes doped with Mo and Nb. <i>Physica Scripta</i> , 0, , .	1.2	1
4134	A density functional study on the sensing behavior of copper doped BC ₃ nanosheet toward COS gas. <i>Inorganic Chemistry Communication</i> , 2023, 152, 110689.	1.8	3
4135	Green synthesized ZnO/NiO heterostructures based quick responsive LPG sensor for the detection of below LEL with DFT calculations. <i>Results in Surfaces and Interfaces</i> , 2023, 11, 100103.	1.0	3

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4138	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. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2023, 291, 116392.	1.7	24
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4140	Biological determination, molecular docking and Hirshfeld surface analysis of rhodium(I)-N-heterocyclic carbene complex: Synthesis, crystal structure, DFT calculations, optical and non linear optical properties. Inorganica Chimica Acta, 2023, 551, 121459.	1.2	3
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4144	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
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4148	Design and synthesis of piano-stool ruthenium(II) complexes and their studies on the inhibition of amyloid β (1-42) peptide aggregation. International Journal of Biological Macromolecules, 2023, 239, 124197.	3.6	2
4149	DFT theoretical and experimental studies unraveling the structural and electronic properties of niobium doped calcium apatite ceramics. Materials Today Communications, 2023, 35, 105873.	0.9	0
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4152	Boron-rich triphenylene COF based electrides having excellent nonlinear optical activity. Materials Science in Semiconductor Processing, 2023, 160, 107468.	1.9	4
4153	Synthesis and spectral studies of some polysubstituted cyclohexanone oximes; DFT approach for the optimization. Journal of Molecular Structure, 2023, 1283, 135299.	1.8	1

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4156	Quantum chemical investigation of choline chloride-based deep eutectic solvents. <i>Chemical Physics</i> , 2023, 571, 111936.	0.9	10
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4159	A computational study on the potential application of metal-doped AlN nanotubes for chloroform detection. <i>Computational and Theoretical Chemistry</i> , 2023, 1222, 114047.	1.1	0
4160	Antitumor and antimicrobial effect of syringic acid urea cocrystal: Structural and spectroscopic characterization, DFT calculation and biological evaluation. <i>Journal of Molecular Structure</i> , 2023, 1282, 135113.	1.8	13
4161	Synthesis, spectroscopic, and molecular interaction study of lead(II) complex of DL-alanine using experimental techniques and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2023, 1283, 135208.	1.8	4
4162	Novel merocyanine-derived receptor: Synthesis, crystal structure and picric acid recognition, spectroscopic and theoretical study. <i>Journal of Molecular Structure</i> , 2023, 1284, 135382.	1.8	1
4163	Adsorption mechanism investigation of methylthionium chloride dye onto some metal phosphates using Monte Carlo dynamic simulations and DFT calculations. <i>Inorganic Chemistry Communication</i> , 2023, 149, 110436.	1.8	8
4164	Quantum mechanical survey on the electronic sensitivity of aluminium phosphide monolayer toward halogen gases. <i>Molecular Simulation</i> , 2023, 49, 427-432.	0.9	1
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4166	Tetraphenylethylene Based Fluorescent Chemosensor for the Selective Detection of Explosive Nitroaromatic Compounds. <i>ChemistrySelect</i> , 2023, 8, .	0.7	4
4167	A computational investigation on the cyclohexylamine recognition using the pure and Cu-doped BN nanotube. <i>Molecular Simulation</i> , 2023, 49, 386-392.	0.9	0
4168	The potential of pure and atom-decorated AlP nano-sheet as a drug delivery system for procarbazine: A DFT approach. <i>Computational and Theoretical Chemistry</i> , 2023, 1222, 114048.	1.1	1
4169	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
4170	Explosive and pollutant nitroaromatic sensing through a Cd(II) based ladder shaped 1D coordination polymer. <i>Heliyon</i> , 2023, 9, e13504.	1.4	4
4171	Synthesis, spectroscopic profiling, biological evaluation, DFT, molecular docking and mathematical studies of 3,5-diethyl-2r,6c-diphenylpiperidin-4-one picrate. <i>Molecular Physics</i> , 2023, 121, .	0.8	1

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4173	Molecular β -amino butyric acid and its crystals: Structural, electronic and optical properties. <i>Journal of Solid State Chemistry</i> , 2023, 321, 123900.	1.4	0
4174	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
4175	Cyclophosphamide drug sensing characteristics by using pure and Ti-doped graphyne-like BN-yne. <i>Inorganic Chemistry Communication</i> , 2023, 150, 110535.	1.8	0
4176	Vibrational spectra of neutral and doped oligothiophenes and polythiophene. <i>RSC Advances</i> , 2023, 13, 5419-5427.	1.7	3
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4178	A simple uric acid assay by using 3-hydroxytyramine as a chromogenic colorimetric sensor in human serum samples: Density functional theory supported mechanistic approach. <i>Journal of the Chinese Chemical Society</i> , 2023, 70, 894-908.	0.8	0
4179	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
4180	Structural and electronic properties of H ₂ , CO, CH ₄ , NO, and NH ₃ adsorbed onto Al ₁₂ Si ₁₂ nanocages using density functional theory. <i>Frontiers in Chemistry</i> , 0, 11, .	1.8	0
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4182	Ru Monoimines with Extended Excited-State Lifetimes and Geometrical Modulation of Photoinduced Mixed-Valence Interactions. <i>Inorganic Chemistry</i> , 2023, 62, 3808-3816.	1.9	0
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4184	A Density Functional Study on Adrucil Drug Sensing Based on the Rh-Decorated Gallium Nitride Nanotube. <i>Journal of Electronic Materials</i> , 2023, 52, 3156-3164.	1.0	2
4185	Neutral, Heteroleptic [Cu(I)(PPh ₃) ₂ (4-H-imidazolato)] Complexes: Ligand Exchange Reactivity, Redox Properties, Excited-State Dynamics. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	0
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4187	A DFT study on the selective adsorption and separation of CO ₂ /CH ₄ on the Mg-decorated 2-D covalent organic framework (COF-5). <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100949.	1.3	0
4188	Delivery of Cisplatin Anti-cancer Drug by Si-Decorated Al ₂₄ N ₂₄ Nanocage: DFT Evaluation of Electronic and Structural Features. <i>Journal of Electronic Materials</i> , 2023, 52, 3281-3290.	1.0	1
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4192	Donor Influence on the Optoelectronic Properties of N-Substituted Tetraphenylimidazole Derivatives. <i>ChemistrySelect</i> , 2023, 8, .	0.7	0
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4195	Theoretical descriptions of novel silicon analogs of cyclo[18]carbon. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	1
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4198	Nonlinear optical response and characteristic Raman spectra of phagraphene quantum dots. <i>Physica Scripta</i> , 2023, 98, 045109.	1.2	2
4199	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
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4201	First-principles study of nitrogen-doped porous graphene for Na ⁺ , K ⁺ , Mg ²⁺ , and Ca ²⁺ cations adsorption. <i>Structural Chemistry</i> , 0, , .	1.0	0
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4205	1,4-Divinylphenylene-bridged diruthenium complexes with 2-hydroxypyridine- and 2- or 8-hydroxyquinoline-olate ligands. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2023, 78, 75-93.	0.3	0
4207	Determination of the molecular structure and spectroscopic properties of capsaicin. <i>Radiation Physics and Chemistry</i> , 2023, 208, 110879.	1.4	4
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4211	New Bisabolane-Type Sesquiterpenoids from <i>Curcuma longa</i> and Their Anti-Atherosclerotic Activity. <i>Molecules</i> , 2023, 28, 2704.	1.7	1
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4215	Quantum Chemical Study the Removal of Acetone by Using the Pristine and Si-doped C ₂ N Monolayer. <i>Silicon</i> , 2023, 15, 5105-5113.	1.8	2
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4218	Efficient Synthesis of Imine-Carboxylic Acid Functionalized Compounds: Single Crystal, Hirshfeld Surface and Quantum Chemical Exploration. <i>Molecules</i> , 2023, 28, 2967.	1.7	17
4219	Chiral diketopyrrolopyrrole dyes showing light emission in solid and aggregate states. <i>Journal of Materials Chemistry C</i> , 2023, 11, 5701-5713.	2.7	1
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4222	Application of Low-Frequency Raman Spectroscopy to Probe Dynamics of Lipid Mesophase Transformations upon Hydration. <i>Journal of Physical Chemistry B</i> , 2023, 127, 3223-3230.	1.2	2
4223	Electronic Interaction between Aromatic Chromophores in Dibenzo-Crown Ether Complexes with Alkali Metal Ions Investigated via Cold Gas-Phase Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3210-3220.	1.1	0
4224	Photocatalytic ability of visible-light-responsive hybrid ZrO ₂ particles. <i>Sustainable Energy and Fuels</i> , 2023, 7, 2279-2287.	2.5	3
4225	Efficient Synthesis, Spectroscopic Characterization, and Nonlinear Optical Properties of Novel Salicylaldehyde-Based Thiosemicarbazones: Experimental and Theoretical Studies. <i>ACS Omega</i> , 2023, 8, 13982-13992.	1.6	14
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4228	Aluminum Carbide Sheet-Like Materials as Promising Drug Delivery Systems for Anticancer Drug. <i>Journal of Cluster Science</i> , 0, , .	1.7	0
4229	Deep Red Emitting Heteroleptic Ir(III) Complexes that Incorporate Unsymmetrical 4-quinoline Carboxylic Acid Derived Ligands. <i>European Journal of Inorganic Chemistry</i> , 2023, 26, .	1.0	4
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