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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.	5.4	31
42	Syntheses and structures of mononuclear lutetium imido complexes with very short Lu=O bonds. Chemical Communications, 2007, , 5007.	4.1	59
43	Influence of Solvent Polarity and Hydrogen Bonding on the Electronic Transition of Coumarin 120: A TDDFT Study. ChemPhysChem, 2008, 9, 1593-1602.	2.1	42
44	Mechanism of Ligand Photodissociation in Photoactivable [Ru(bpy) <sub>2</sub> LC <sub>2</sub> ] <sup>2+</sup> Complexes: A Density Functional Theory Study. Journal of the American Chemical Society, 2008, 130, 9590-9597.	13.7	149
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808	Normal coordinate analysis and vibrational spectroscopy (FT-IR and FT-Raman) studies of 5-methyl-N-[4-(trifluoromethyl) phenyl]-isoxazole-4-carboxamide using density functional method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 142-151.	3.9	6
809	Ruthenium(II) bipyridine complexes bearing quinoline-azoimine (NN <sup>2</sup> N <sup>3</sup> ) tridentate ligands: Synthesis, spectral characterization, electrochemical properties and single-crystal X-ray structure analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 125, 375-383.	3.9	8
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811	Hydrogen fluoride on the pristine, Al and Si doped BC <sub>2</sub> N nanotubes: A computational study. <i>Computational Materials Science</i> , 2014, 82, 197-201.	3.0	27
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815	Vibrational spectroscopic study and NBO analysis on tranexamic acid using DFT method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 129, 184-192.	3.9	76



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819	Spectroscopic (FT-IR, FT-Raman, and UV-visible) and quantum chemical studies on molecular geometry, Frontier molecular orbitals, NBO, NLO and thermodynamic properties of 1-acetylindole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 133, 626-638.	3.9	17
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1088	Experimental and theoretical studies on IR, Raman, and UV-Vis spectra of quinoline-7-carboxaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 134, 81-89.	3.9	26
1089	Molecular conformational stability and Spectroscopic analysis of Parared with experimental techniques and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 1194-1205.	3.9	19
1090	Vibrational analysis using FT-IR, FT-Raman spectra and HF-DFT methods and NBO, NLO, NMR, HOMO-LUMO, UV and electronic transitions studies on 2,2,4-trimethyl pentane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 138, 900-912.	3.9	10
1091	Synthesis, spectroscopic characterization and photophysics of a novel environmentally sensitive dye 3-naphthyl-1-phenyl-5-(4-carboxyphenyl)-2-pyrazoline. <i>Journal of Luminescence</i> , 2015, 159, 9-16.	3.1	26
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1093	Synthesis, structure, spectroscopic studies (FT-IR, FT-Raman and UV), normal coordinate, NBO and NLO analysis of salicylaldehyde p-chlorophenylthiosemicarbazone. <i>Journal of Molecular Structure</i> , 2015, 1081, 400-412.	3.6	62
1094	Synthesis and characterization of novel aliphatic-aromatic polyamide/Fe <sub>3</sub> O <sub>4</sub> nanocomposites containing pendent 9 <i>H</i> -xanthene groups. <i>Designed Monomers and Polymers</i> , 2015, 18, 157-169.	1.6	11
1095	N-bromosuccinimide (NBS)-promoted, three-component synthesis of 1,2-unsaturated isoxazol-5(4H)-ones, and spectroscopic investigation and computational study of 3-methyl-4-(thiophen-2-ylmethylene)isoxazol-5(4H)-one. <i>Research on Chemical Intermediates</i> , 2015, 41, 7739-7773.	2.7	47
1096	Molecular structure, vibrational spectra, AIM, HOMO-LUMO, NBO, UV, first order hyperpolarizability, analysis of 3-thiophenecarboxylic acid monomer and dimer by Hartree-Fock and density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1227-1242.	3.9	79
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1326	A highly selective fluorescent chemosensor for Mg <sup>2+</sup> ion in aqueous solution using density function theory calculations. <i>Journal of Molecular Structure</i> , 2016, 1123, 111-115.	3.6	35
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1335	Experimental (FTIR, Raman, UV-visible and PL) and theoretical (DFT and TDDFT) studies on bis(8-hydroxyquinolinium) tetrachlorocobaltate(II) compound. <i>Journal of Molecular Structure</i> , 2016, 1125, 149-161.	3.6	37
1336	Soluble Flavanthrone Derivatives: Synthesis, Characterization, and Application to Organic Light-Emitting Diodes. <i>Chemistry - A European Journal</i> , 2016, 22, 7978-7986.	3.3	15
1337	Luminescent phosphine ruthenium(II) complexes with 8-hydroxyquinoline derivative ligands. <i>Journal of Luminescence</i> , 2016, 169, 765-772.	3.1	2

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1340	A Turn-on Fluorescent Chemosensor for Zn <sup>2+</sup> Based on Quinoline in Aqueous Media. <i>Journal of Fluorescence</i> , 2016, 26, 835-844.	2.5	12
1341	Synthesis and theoretical studies on new amidodithiophosphonates. <i>Journal of Molecular Structure</i> , 2016, 1111, 61-68.	3.6	4
1342	TD-DFT based fine-tuning of molecular excitation energies using evolutionary algorithms. <i>RSC Advances</i> , 2016, 6, 3661-3670.	3.6	4
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1345	Theoretical evaluation of a doubleâ€‘functional heterogeneous nano-sensor. <i>Applied Surface Science</i> , 2016, 366, 545-551.	6.1	11
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1348	Persistence of Câ€‘Hâ€‘Î€(chelate ring) interactions in the crystal structures of Pd(S <sub>2</sub> COR) <sub>2</sub> . The utility of Pd(S <sub>2</sub> COR) <sub>2</sub> as precursors for palladium sulphide materials. <i>CrystEngComm</i> , 2016, 18, 1105-1117.	2.6	26
1349	Charge-controlled switchable methane adsorption on heteroatom-doped BNNSs. <i>RSC Advances</i> , 2016, 6, 5079-5088.	3.6	18
1350	Vanillinyl thioether Schiff base as a turn-on fluorescence sensor to Zn <sup>2+</sup> ion with living cell imaging. <i>Sensors and Actuators B: Chemical</i> , 2016, 228, 287-294.	7.8	58
1351	Adsorption behavior of 5-fluorouracil on pristine, B-, Si-, and Al-doped C <sub>60</sub> fullerenes: A first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 937-941.	2.1	102
1352	Hetero aromatic donors as effective terminal groups for DPP based organic solar cells. <i>RSC Advances</i> , 2016, 6, 9023-9036.	3.6	6
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1354	FTIR, FT-Raman and UVâ€‘Vis spectral studies of d-tyrosine molecule. <i>Journal of Molecular Structure</i> , 2016, 1105, 169-177.	3.6	15
1355	Conformational, vibrational spectroscopic, nonlinear optical activity, and structureâ€‘activity studies on 2-hydroxy-3,5-dinitropyridine: Combined experimental and density functional theory approach. <i>Spectroscopy Letters</i> , 2016, 49, 155-166.	1.0	20



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1357	Donor-free™ oligo(3-hexylthiophene) dyes for efficient dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2016, 4, 2509-2516.	10.3	28
1358	Pyrene-Oxadiazoles for Organic Light-Emitting Diodes: Triplet to Singlet Energy Transfer and Role of Hole-Injection/Hole-Blocking Materials. <i>Journal of Organic Chemistry</i> , 2016, 81, 603-614.	3.2	66
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1368	Supramolecular nickel complex based on thiosemicarbazone. Synthesis, transfer hydrogenation and unexpected thermal behavior. <i>Polyhedron</i> , 2016, 110, 188-196.	2.2	11
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1371	Rhodamine hydrazone as OFF-ON type selective sequential sensor of Al <sup>3+</sup> and N <sup>3-</sup> ions. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 319-320, 78-86.	3.9	11
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1394	Distinguishing Bonds. <i>Journal of the American Chemical Society</i> , 2016, 138, 3731-3744.	13.7	48
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1401	Benzo[ <i>c</i> ][1,2,5]thiadiazole Donor-Acceptor Dyes: A Synthetic, Spectroscopic, and Computational Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1853-1866.	2.5	46
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1422	Tuning hydrogen storage of carbon nanotubes by mechanical bending: theoretical study. <i>Molecular Simulation</i> , 2016, 42, 709-714.	2.0	3
1423	The spectroscopic (FT-IR, FT-Raman, dispersive Raman and NMR) study of ethyl-6-chloronicotinate molecule by combined density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 153, 754-770.	3.9	11
1424	Synthesis, characterization and DFT studies of diethyl 4-hydroxy-6-nitro-4H-chromene-2,3-dicarboxylate. <i>Journal of Molecular Structure</i> , 2016, 1105, 118-127.	3.6	12
1425	Molecular structure, vibrational spectral assignments (FT-IR and FT-Raman), UV-Vis, NMR, NBO, HOMO-LUMO and NLO properties of 3-(3-pentyl-2,6-diphenylpiperidin-4-one picrate based on DFT calculations. <i>Journal of Molecular Structure</i> , 2016, 1105, 225-237.	3.6	31
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1431	Experimental and theoretical study of ornidazole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 153, 496-504.	3.9	12
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1434	A dual chemosensor for Zn <sup>2+</sup> and Co <sup>2+</sup> in aqueous media and living cells: Experimental and theoretical studies. <i>Sensors and Actuators B: Chemical</i> , 2016, 223, 509-519.	7.8	68
1435	Sensing properties of BN nanotube toward carcinogenic 4-chloroaniline: A computational study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2016, 76, 6-11.	2.7	131
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1438	DFT investigation on molecular structures of metal and nonmetal-doped ZnO sodalite-like cage and their electronic properties. <i>Structural Chemistry</i> , 2016, 27, 773-784.	2.0	8
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1443	Aggregation induced emission enhancement (AIEE) of fluorenyl appended Schiff base : A turn on fluorescent probe for Al <sup>3+</sup> , and its photovoltaic effect. <i>Journal of Luminescence</i> , 2017, 181, 56-62.	3.1	20
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1450	Cyclometalated platinum(II) complexes of 2,2'-bipyridine N-oxide containing a 1,1'-bis(diphenylphosphino)ferrocene ligand: structural, computational and electrochemical studies. <i>Dalton Transactions</i> , 2017, 46, 2013-2022.	3.3	11
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1454	Structural, electronic and optical properties of 2,5-dichloro-p-xylene: experimental and theoretical calculations using DFT method. <i>RSC Advances</i> , 2017, 7, 1401-1412.	3.6	39
1455	TD-DFT Study of Absorption and Emission Spectra of 2-(2'-Aminophenyl)benzothiazole Derivatives in Water. <i>Journal of Fluorescence</i> , 2017, 27, 745-754.	2.5	7
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1458	Vibrational spectroscopic, UV-Vis, molecular structure and NBO analysis of Rabeprazole. <i>Journal of Molecular Structure</i> , 2017, 1137, 277-291.	3.6	28
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1461	Spectroelectrochemistry of alternating ambipolar copolymers of 4,4'- and 2,2'-bipyridine isomers and quaterthiophene. <i>Electrochimica Acta</i> , 2017, 231, 437-452.	5.2	12
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1474	Synthesis and Optical Properties of Unsymmetrically Substituted Triarylamine Hexaazatrinaphthalenes. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 2432-2440.	2.4	16
1475	Physical and optical properties of DCJTb dye for OLED display applications: Experimental and theoretical investigation. <i>Journal of Molecular Structure</i> , 2017, 1137, 403-411.	3.6	38
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1588	A single fluorescent chemosensor for multiple targets of Cu <sup>2+</sup> , Fe <sup>2+/3+</sup> and Al <sup>3+</sup> in living cells and a near-perfect aqueous solution. <i>RSC Advances</i> , 2017, 7, 28723-28732.	3.6	38
1589	pH-Switchability and Second-Order Nonlinear Optical Properties of Monocyclopentadienylruthenium(II)/iron(II) Tetrazoles/Tetrazolates: Synthesis, Characterization, and Time-Dependent Density Functional Theory Calculations. <i>Inorganic Chemistry</i> , 2017, 56, 6849-6863.	4.0	10

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1594	Direct time-resolved spectroscopic investigation of intramolecular hydrogen atom transfer of deoxyblebbistatin. <i>Chemical Physics Letters</i> , 2017, 683, 431-435.	2.6	1
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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.	2.6	14
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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.	2.6	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.	3.3	17
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1637	Warped C <sub>80</sub> H <sub>30</sub> nanographene as a chemical sensor for CO gas: DFT studies. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 646-651.	2.1	51
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1639	New anthracene-based Schiff bases: Theoretical and experimental investigations of photophysical and electrochemical properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 175, 24-35.	3.9	18
1640	Glyoxalbis(2-methylmercaptoanil) complexes of nickel and ruthenium: radical versus non-radical states. <i>New Journal of Chemistry</i> , 2017, 41, 1149-1159.	2.8	3
1641	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.	3.6	8
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1645	Bulky Nature Phenanthroimidazole-Based Porphyrin Sensitizers for Dye-Sensitized Solar Cell Applications. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25691-25704.	3.1	26
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1658	Ambient-Stable Bis-Azoaromatic-Centered Diradical [(L <sup>•</sup> )M(L <sup>•</sup> )] Complexes of Rh(III): Synthesis, Structure, Redox, and Spinâ€Spin Interaction. <i>Inorganic Chemistry</i> , 2017, 56, 12764-12774.	4.0	11
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1717	DFT/TDDFT investigation on the electronic structures and spectral characteristics of C <sub>5</sub> H <sub>3</sub> XOS (X = H,) Tj ETQq1 1 0,784314 <sub>g</sub> BT /Over	1.0	1
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1864	Electronic Interactions between Ferrocenyl Units Facilitated by the Cobalt Bis(dicarbollide) Anion Linker: An Experimental and DFT Study. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 666-670.	2.0	4
1865	Thiocarbonyl-bound metallonitrosyl complexes with visible-light induced DNA cleavage and promising vasodilation activity. <i>Journal of Inorganic Biochemistry</i> , 2018, 182, 83-91.	3.5	19
1866	DFT and TD-DFT calculations of metallotetraphenylporphyrin and metallotetraphenylporphyrin fullerene complexes as potential dye sensitizers for solar cells. <i>Journal of Molecular Structure</i> , 2018, 1160, 415-427.	3.6	23
1867	Novel heat-resistant and soluble poly(amide-ether)/zinc oxide nanocomposites: synthesis, characterization and computational study. <i>Polymer Bulletin</i> , 2018, 75, 4445-4468.	3.3	5
1868	Fluorescence sensing and photocatalytic properties of a 2D stable and biocompatible Zn(II)-based polymer. <i>Journal of Molecular Structure</i> , 2018, 1158, 264-270.	3.6	20
1869	Potential application of doped hexa-peri-hexabenzocoronene as NH <sub>3</sub> gas sensor: a computational investigation. <i>Structural Chemistry</i> , 2018, 29, 929-935.	2.0	2
1870	Electronic versus steric effects of pyridinophane ligands on Pd( $\eta^3$ ) complexes. <i>Dalton Transactions</i> , 2018, 47, 1151-1158.	3.3	13
1871	Adsorption properties of chloropicrin on pristine and borazine-doped nanographenes: A theoretical study. <i>Journal of Physics and Chemistry of Solids</i> , 2018, 115, 277-282.	4.0	15
1872	Pt <sup>II</sup> Phosphors with Click-Derived 1,2,3-Triazole-Containing Tridentate Chelates. <i>Organometallics</i> , 2018, 37, 145-155.	2.3	31
1873	A DFT investigation on group 8B transition metal-doped silicon carbide nanotubes for hydrogen storage application. <i>Applied Surface Science</i> , 2018, 439, 494-505.	6.1	46
1874	Analytical hessian fitting schemes for efficient determination of force-constant parameters in molecular mechanics. <i>Journal of Computational Chemistry</i> , 2018, 39, 307-318.	3.3	8
1875	Exploring the relevance of thiophene rings as bridge unit in acceptor-bridge-donor dyes on self-aggregation and performance in DSSCs. <i>Journal of Computational Chemistry</i> , 2018, 39, 685-698.	3.3	10
1876	Adsorption properties of graphene towards the ephedrine - A frequently used molecule in sport. <i>Computational and Theoretical Chemistry</i> , 2018, 1124, 39-50.	2.5	12
1877	Optical graphene quantum dots gas sensors: Theoretical study. <i>Superlattices and Microstructures</i> , 2018, 114, 321-330.	3.1	34

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1879	Fluorescent Sensor for Sequentially Monitoring Zinc(II) and Cyanide Anion in Near-Perfect Aqueous Media. Industrial & Engineering Chemistry Research, 2018, 57, 54-62.	3.7	38
1880	Synthesis, biological evaluation, substitution behaviour and DFT study of Pd(II) complexes incorporating benzimidazole derivative. New Journal of Chemistry, 2018, 42, 2574-2589.	2.8	32
1881	Platinum(II)-glutamic acid dendrimer conjugates: Synthesis, characterization, DFT calculation, conformational analysis and catalytic properties. Inorganica Chimica Acta, 2018, 473, 245-254.	2.4	2
1882	Combined spectroscopic, molecular docking and quantum mechanics study of $\beta$ -casein and p-coumaric acid interactions following thermal treatment. Food Chemistry, 2018, 252, 163-170.	8.2	60
1883	Computational Design, Synthesis, and Structure Property Evaluation of 1,3-Thiazole-Based Color-Tunable Multi-heterocyclic Small Organic Fluorophores as Multifunctional Molecular Materials. Journal of Organic Chemistry, 2018, 83, 3453-3466.	3.2	24
1884	A new Zn(II) metal-organic framework having 3D CdSO <sub>4</sub> topology as luminescent sensor and photocatalyst for degradation of organic dyes. New Journal of Chemistry, 2018, 42, 2767-2775.	2.8	79
1885	A simple multi-responsive system based on aldehyde functionalized amino-boranes. Chemical Science, 2018, 9, 1902-1911.	7.4	99
1886	Ir-Pt-BODIPY Complexes with Platinum Attachment to Carbon Atoms C2 or C3: Spectroscopic, Structural, and (Spectro)Electrochemical Studies and Photocatalysis. Organometallics, 2018, 37, 235-253.	2.3	18
1887	Thieno[2,3-b]thiophene based polymers: Synthesis and optoelectronic properties. European Polymer Journal, 2018, 104, 72-80.	5.4	8
1888	Cobalt(II), nickel(II) and copper(II) complexes of N-[(2-pyridyl)methyliden]-6-coumarin: Characterization, DNA interaction, catecholase activity and theoretical interpretation. Inorganica Chimica Acta, 2018, 482, 659-668.	2.4	6
1889	Indolocarbazole (IC) Derivatives as Promising p-type Organic Semiconductors: A First-Principle Study of Their Anisotropic Charge Mobilities. ChemistrySelect, 2018, 3, 4624-4634.	1.5	3
1890	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.	1.7	95
1891	Theoretical and experimental studies of newly synthesized (Z)-4-(2-(3,5-dibromo-2-hydroxy-4-methoxybenzylidene)hydrazinyl)benzonitrile compound. Journal of Molecular Structure, 2018, 1166, 407-415.	3.6	6
1892	Synthesis and photovoltaic properties of new Ru(II) complexes for dye-sensitized solar cells. Journal of Materials Science: Materials in Electronics, 2018, 29, 11045-11058.	2.2	11
1893	A new molecular switch based on a symmetrical dinuclear complex of two tricarbonylrhenium(I) moieties bridged by 4,4'-azobis-(2,2'-bipyridine). Polyhedron, 2018, 149, 109-116.	2.2	5
1894	Cu(II)-Based binuclear compound for the application of photosensitive electronic devices. New Journal of Chemistry, 2018, 42, 8629-8637.	2.8	17
1895	Degradation of blue-phosphorescent organic light-emitting devices involves exciton-induced generation of polaron pair within emitting layers. Nature Communications, 2018, 9, 1211.	12.8	107



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1897	Theoretical screening and design of SM315-based porphyrin dyes for highly efficient dye-sensitized solar cells with near-IR light harvesting. Dyes and Pigments, 2018, 155, 292-299.	3.7	41
1898	Theoretical Study of the Relationship between the Geometry and the Orbital Hybridization in the CuAln <sup>+</sup> (n = 11–13) Cluster. Bulletin of the Chemical Society of Japan, 2018, 91, 940-949.	3.2	2
1899	Theoretical investigation of the photophysical properties of donor-acceptor dyes containing coumarin and naphthoquinone moieties linked by an aminomethylene bridge. Journal of Molecular Structure, 2018, 1164, 260-270.	3.6	6
1900	Ti(ÆZ5-1-SiMe3-C9H6)(Cl)2(OR): Structure and bonding. Inorganica Chimica Acta, 2018, 477, 270-276.	2.4	5
1901	Is $\pi$ -Stacking Prone To Accelerate Singlet–Singlet Energy Transfers?. Inorganic Chemistry, 2018, 57, 4291-4300.	4.0	2
1902	Theoretical studies on the potentials of some nanocages (Al12N12, Al12P12, B12N12, Be12O12, C12Si12,) Tj ETQq0 0 0 rgBT /Overlock of Molecular Liquids, 2018, 260, 138-148.	4.9	58
1903	Spectroscopic investigation, hirshfeld surface analysis and molecular docking studies on anti-viral drug entecavir. Journal of Molecular Structure, 2018, 1164, 447-458.	3.6	82
1904	Structural, electrical and optical properties of Lin@C20 (n=1–6) nanoclusters. Comptes Rendus Chimie, 2018, 21, 541-546.	0.5	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.	1.4	3
1906	Adsorption behavior of amphetamine on the inorganic BC3 nanotube and nanosheet: DFT studies. Inorganic Chemistry Communication, 2018, 91, 95-101.	3.9	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.	3.6	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.	2.4	32
1909	Theoretical, biological and in silico studies of pendant-armed heteroleptic copper(II) phenolate complexes. Journal of Molecular Structure, 2018, 1161, 306-319.	3.6	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.	3.6	52
1911	Complexes of DNA bases and Watson–Crick base pairs interaction with neutral silver Agn (n=8, 10, 12) clusters: a DFT and TDDFT study. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1050-1062.	3.5	14
1912	A theoretical study of structural, opto-electronic and nonlinear properties of arylboroxine derivatives. Indian Journal of Physics, 2018, 92, 57-68.	1.8	2
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1915	Study of structural, optical properties and electronic structure of PTCDI-C5 organic nanostructure. <i>Chemical Physics Letters</i> , 2018, 691, 14-21.	2.6	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.	2.4	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.	2.4	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.	3.6	19
1919	Structural, vibrational, DFT and optical studies of a new non-centrosymmetric hybrid material (C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> )[CoBr <sub>4</sub> ]. <i>Journal of Molecular Structure</i> , 2018, 1152, 303-310.	3.6	23
1920	A highly sensitive and selective fluorescent chemosensor for the sequential recognition of Zn <sup>2+</sup> and S <sup>2-</sup> in living cells and aqueous media. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 3108-3116.	7.8	37
1921	A dual sensor selective for Hg <sup>2+</sup> and cysteine detection. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 2756-2763.	7.8	63
1922	Role of the Diphosphine Chelate in Emissive, Charge-Neutral Iridium(III) Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 624-635.	3.3	12
1923	The interaction of phosgene gas with different BN nanocones: DFT studies. <i>Solid State Communications</i> , 2018, 269, 23-27.	1.9	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.	1.1	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.	3.6	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.	2.7	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.	2.2	19
1928	Selective detection of Cu <sup>2+</sup> and S <sup>2-</sup> by a colorimetric chemosensor: Experimental and theoretical calculations. <i>Inorganica Chimica Acta</i> , 2018, 471, 709-717.	2.4	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.	2.4	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.	2.7	26
1931	Copper-doped Al <sub>12</sub> N <sub>12</sub> nano-cages: potential candidates for nonlinear optical materials. <i>Applied Physics A: Materials Science and Processing</i> , 2018, 124, 1.	2.3	38

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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.	2.2	55
1934	Azophenine as Central Core for Efficient Light Harvesting Devices. <i>ChemPhysChem</i> , 2018, 19, 596-611.	2.1	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.	3.6	3
1936	Glabralides A – C, three novel meroterpenoids from <i>Sarcandra glabra</i> . <i>Tetrahedron</i> , 2018, 74, 341-347.	1.9	12
1937	Light Harvesting and Direct Electron Injection by Interfacial Charge-Transfer Transitions between TiO <sub>2</sub> and Carboxy-Anchored Dye LEG4 in Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2018, 122, 8-15.	3.1	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.	3.9	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.	2.7	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.	1.8	22
1941	A visible light excitable chromone appended hydrazide chemosensor for sequential sensing of Al <sup>3+</sup> and F <sup>-</sup> in aqueous medium and in Vero cells. <i>Sensors and Actuators B: Chemical</i> , 2018, 257, 545-552.	7.8	42
1942	Syntheses, crystal structures, DNA binding, DNA cleavage, molecular docking and DFT study of Cu( <sup>II</sup> ) complexes involving N <sub>2</sub> O <sub>4</sub> donor azo Schiff base ligands. <i>New Journal of Chemistry</i> , 2018, 42, 246-259.	2.8	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.	3.6	4
1944	The Effect of Superalkali M3O (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.	3.7	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.	2.4	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.	2.5	7
1947	Chloropicrin sensor based on the pristine BN nanocones: DFT studies. <i>Structural Chemistry</i> , 2018, 29, 585-592.	2.0	11
1948	Investigation of NH <sub>3</sub> adsorption behavior on graphdiyne nanosheet and nanotubes: A first-principles study. <i>Journal of Molecular Liquids</i> , 2018, 249, 24-32.	4.9	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.	2.4	14

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1951	Theoretical investigation on reaction pathways for ethylene epoxidation on Ti-decorated graphene. Structural Chemistry, 2018, 29, 159-170.	2.0	13
1952	Surface-decorated CdS nanoparticles for the recognition of K <sup>+</sup> in aqueous medium: DFT and antibacterial studies. Research on Chemical Intermediates, 2018, 44, 155-171.	2.7	4
1953	Quantum-Chemical Study of the Adsorption of Bi <sup>3+</sup> Ions on Au(111). Russian Journal of Electrochemistry, 2018, 54, 1201-1208.	0.9	1
1954	Quantum-Chemical Study of the Adsorption of Pb <sup>2+</sup> on Au(111). Russian Journal of Electrochemistry, 2018, 54, 902-911.	0.9	2
1955	Interaction between Thallium and the Au(111) Surface. Quantum-Chemical Analysis. Russian Journal of Electrochemistry, 2018, 54, 912-921.	0.9	0
1956	Synthesis, Reactivity Studies, and Cytotoxicity of Two trans-Iodidoplatinum(II) Complexes. Does Photoactivation Work?. Inorganics, 2018, 6, 127.	2.7	4
1957	TDDFT Investigation of the Hybrid Organic Inorganic Perovskite: CH <sub>3</sub> NH <sub>3</sub> PbC <sub>3</sub> . , 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.	3.3	21
1960	Six-coordinate [Co <sup>III</sup> (L) <sub>2</sub> ] <sup>z</sup> (L = 1 <sup>-</sup> , O, 1+) complexes of an azo-appended o-aminophenolate in amidate(2 <sup>-</sup> ) and iminosemiquinonate 1 <sup>-</sup> radical (1 <sup>-</sup> ) redox-levels: the existence of valence-tautomerism. Dalton Transactions, 2018, 47, 17086-17101.	3.3	12
1961	An aminoquinoline based biocompatible fluorescent and colourimetric pH sensor designed for cancer cell discrimination. New Journal of Chemistry, 2018, 42, 19818-19826.	2.8	33
1962	Influences of the substituents on the Cr=C bond in [(OC)5Cr=C(OEt)-para-C6H4X] complexes: quantum Theory of Atoms in Molecules, Energy Decomposition Analysis, and Interacting Quantum Atoms. Monatshefte für Chemie, 2018, 149, 2167-2174.	1.8	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.	3.3	18
1964	Structure, electrical and nonlinear optical properties of $\{M@C_{20}\} M@C_{20}$ (M = Li, Na, K, Tl) ETQO Org. Overlook		
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.	1.8	25
1966	DFT Calculations of Structure and Optical Properties in Wide Band-Gap Semiconductor Clusters for Dye-Sensitized Solar Cells. , 2018, , .		0
1967	CH <sub>2</sub> 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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1969	Structural, energetic and spectroscopic studies of new luminescent complexes based on 2-(2-hydroxyphenyl)imidazo[1,2-a]pyridines and 1,2-phenylenediboronic acid. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 725-737.	1.1	7
1970	Theoretical Study of the Arene Ligand Effect on the Structure and Properties of Cr(CO) <sub>3</sub> (Arene) Complexes (Arene = Benzene, Biphenyl, Triphenyl, Tetraphenyl). <i>Journal of Structural Chemistry</i> , 2018, 59, 1784-1790.	1.0	3
1971	Theoretical Study of the Solvent Effect on the Electronic and Vibrational Properties of [CpFe(CO) <sub>2</sub> (NCS)] and [CpFe(CO) <sub>2</sub> (SCN)] Linkage Isomers. <i>Journal of Structural Chemistry</i> , 2018, 59, 1058-1066.	1.0	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.	1.4	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.	0.6	0
1974	Enhancing the Light Harvesting Efficiency, Open Circuit Voltage And Stability of Molybdenum Doped (Zn) <sub>6</sub> Nanocluster in Dye-Sensitized Solar Cells: A DFT Study. <i>Oriental Journal of Chemistry</i> , 2018, 34, 2292-2304.	0.3	2
1975	Emission and Color Tuning of Cyanostilbenes and White Light Emission. <i>ACS Omega</i> , 2018, 3, 17376-17385.	3.5	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.	5.5	18
1977	Analysis of the Interaction Between the C <sub>20</sub> Cage and cis-PtCl <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub> : A DFT Investigation of the Solvent Effect, Structures, Properties, and Topologies. <i>Journal of Structural Chemistry</i> , 2018, 59, 1044-1051.	1.0	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.	1.0	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.	12.8	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.	1.0	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.	1.5	16
1982	Benzodithiazole-Based Hole-Transporting Material for Efficient Perovskite Solar Cells. <i>Asian Journal of Organic Chemistry</i> , 2018, 7, 2497-2503.	2.7	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.	3.0	32
1984	Supramolecular Assembly of a Zn(II)-Based 1D Coordination Polymer through Hydrogen Bonding and $\pi$ - $\pi$ Interactions: Crystal Structure and Device Applications. <i>ACS Omega</i> , 2018, 3, 12060-12067.	3.5	31
1985	Structural, density functional computational studies and antibacterial screening on N,N-bis-(4-hydroxy-1-methylsalicylidene)ethylenediamine nickel (II) complex. <i>Polyhedron</i> , 2018, 156, 165-173.	2.2	0

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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.	2.9	16
1989	Mixed ab initio and semiempirical study of hydrogen-terminated finite germanium nanowires. <i>European Physical Journal Plus</i> , 2018, 133, 1.	2.6	3
1990	Quinolinolâ€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.	1.9	3
1991	Vibrational spectroscopic and Hirshfeld surface analysis of carvedilol crystal forms. <i>International Journal of Pharmaceutics</i> , 2018, 553, 261-271.	5.2	8
1992	The remarkable enhancement of two-photon absorption in pyrene based chalcone derivatives. <i>Optical Materials</i> , 2018, 86, 331-337.	3.6	16
1993	Zintl superalkalis as building blocks of supersalts. <i>Journal of Molecular Modeling</i> , 2018, 24, 306.	1.8	11
1994	The role of computational results databases in accelerating the discovery of catalysts. <i>Nature Catalysis</i> , 2018, 1, 809-810.	34.4	52
1995	Biotransformation of $\beta$ -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.	3.0	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.	1.3	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.	0.8	13
1998	Highly Linearized Twisted Iridium(III) Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 14450-14462.	4.0	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.	2.3	6
2000	Control of Structures and Emission Properties of (CuI) <sub>n</sub> 2-Methyldithiane Coordination Polymers. <i>Inorganic Chemistry</i> , 2018, 57, 13564-13576.	4.0	23
2001	Monocycloplatinated Solvento Complex Displays Turn-on Ratiometric Phosphorescence Responses to Histamine. <i>Inorganic Chemistry</i> , 2018, 57, 13985-13997.	4.0	7
2002	Structural, spectroscopic, and theoretical analysis of a molecular system based on		



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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.	4.0	35
2006	Effects of Ancillary Ligands on Redox and Chemical Properties of Ruthenium Coordinated Azoaromatic Pincer. <i>Inorganic Chemistry</i> , 2018, 57, 11995-12009.	4.0	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.	5.5	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.	2.8	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.	2.2	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 BT / Overlock 10 T		
2011	D- $\pi$ -A type conjugated pyrene derivatives: Third-order nonlinear absorption and excited-state dynamics. <i>Optical Materials</i> , 2018, 85, 319-328.	3.6	21
2012	Near-White Light Emission from Lead(II) Metal-Organic Frameworks. <i>Inorganic Chemistry</i> , 2018, 57, 11341-11348.	4.0	42
2013	Highly Sensitive Ratiometric Chemosensor and Biomarker for Cyanide Ions in the Aqueous Medium. <i>ACS Omega</i> , 2018, 3, 10145-10153.	3.5	46
2014	Syntheses, crystal structures, DNA binding, DNA cleavage and DFT study of Co( <sup>iii</sup> ) complexes involving azo-appended Schiff base ligands. <i>New Journal of Chemistry</i> , 2018, 42, 16571-16582.	2.8	6
2015	A multi-analyte responsive chemosensor vaniliny Schiff base: fluorogenic sensing of Zn( <sup>ii</sup> ), Cd( <sup>ii</sup> ) and I <sup>+</sup> . <i>New Journal of Chemistry</i> , 2018, 42, 16653-16665.	2.8	36
2016	Highly selective and sensitive recognition of Zn( <sup>ii</sup> ) by a novel coumarinyl scaffold following spectrofluorometric technique and its application in living cells. <i>New Journal of Chemistry</i> , 2018, 42, 16297-16306.	2.8	9
2017	Toward quantum-chemical method development for arbitrary basis functions. <i>Journal of Chemical Physics</i> , 2018, 149, 084106.	3.0	10
2018	Copper(II)-sulfonamide Schiff base complexes: Structure, biological activity and theoretical interpretation. <i>Polyhedron</i> , 2018, 151, 344-354.	2.2	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.	3.3	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.	3.7	17
2021	A quantum chemical investigation of the influence of solvent polarity on the structural, electronic, spectroscopic properties and hyperpolarizability in Molybdenum Silyldiyne complex CpMo(CO) <sub>2</sub> (Si Ph). <i>Journal of Molecular Liquids</i> , 2018, 264, 616-620.	4.9	14

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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.	3.6	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.	2.5	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.	2.8	31
2026	Tailoring the benzotriazole (BTZ) auxiliary acceptor in a D-A- $\pi$ -A type sensitizer for high performance dye-sensitized solar cells (DSSCs). <i>Dyes and Pigments</i> , 2018, 158, 195-203.	3.7	15
2027	Can bowl-like B30 nanostructure sense toxic cyanogen gas in air?: a theoretical study. <i>Molecular Physics</i> , 2018, 116, 2196-2204.	1.7	5
2028	Luminescent $\epsilon$ -Substituted Fluoranthenes Synthesis, Structure, Electrochemistry, and Optical Properties. <i>Chemistry - A European Journal</i> , 2018, 24, 9622-9631.	3.3	10
2029	A Multi-Responsive Naphthalimide-Based "Turn-on" Fluorescent Chemosensor for Sensitive Detection of Trivalent Cations Ga <sup>3+</sup> , Al <sup>3+</sup> and Cr <sup>3+</sup> . <i>Journal of Fluorescence</i> , 2018, 28, 785-794.	2.5	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.	3.9	7
2031	Investigation of Sarin Nerve Agent Adsorption Behavior on BN Nanostructures: DFT Study. <i>Journal of Cluster Science</i> , 2018, 29, 757-765.	3.3	31
2032	Synthesis, crystal structure, vibrational spectra, optical and DFT study of N-(3-ammonium propyl)-1, 3 diaminopropane tris iodate dehydrate [(C <sub>6</sub> H <sub>20</sub> N <sub>3</sub> ) (IO <sub>3</sub> ) <sub>3</sub> ·2H <sub>2</sub> O]. <i>Journal of Molecular Structure</i> , 2018, 1171, 76-86.	3.6	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.	3.6	66
2034	A flexible Rigid Rod, <i>trans</i> -Pt(PMe <sub>3</sub> ) <sub>2</sub> (C <sub>6</sub> H <sub>4</sub> CN) <sub>2</sub> (L1), to Form 2D [{Cu <sub>2</sub> ( $\mu$ -X) <sub>2</sub> }] <sub>2</sub> (L1) <sub>4</sub> Polymers (X = Br, I) Exhibiting the Largest Bathochromic Emissions. <i>Inorganic Chemistry</i> , 2018, 57, 7208-7221.	4.0	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.	2.0	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.	3.6	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.	2.5	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.	2.5	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.	3.6	14

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2058	Theoretical studies on the chiral polyoxoanions $[P_2Mo_{18}O_{62}]^{6-}$ and $[PMo_9O_{31}(OH)_2]^{3-}$ with histidine: chiral inversion and chiral induction. <i>Inorganic Chemistry Frontiers</i> , 2018, 5, 1992-1997.	6.0	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.	1.7	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.	2.4	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.	1.1	3
2062	Influence of Solvent and Electric Field on the Structure and IR, $^{31}P$ NMR Spectroscopic Properties of a Titanocene-Benzyne Complex. <i>Journal of Applied Spectroscopy</i> , 2018, 85, 526-534.	0.7	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.	3.9	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.	3.9	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.	4.9	20
2066	Role of Organic Ligands Orientation on the Geometrical and Optical Properties of $Au_{25}(SCH_3)_{18}^{0-}$ . <i>Journal of Physical Chemistry A</i> , 2018, 122, 6864-6872.	2.5	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.	3.3	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.	2.2	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.	2.5	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.	1.6	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.	2.0	1
2072	Synthesis and characterization of a heteroleptic nickel paddlewheel complex. <i>Journal of Molecular Structure</i> , 2018, 1173, 345-348.	3.6	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.	3.5	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.	3.5	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.	2.5	14

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2076	Reconstitution of Enzymatic Carbon-Sulfur Bond Formation Reveals Detoxification-Like Strategy in Fungal Toxin Biosynthesis. <i>ACS Chemical Biology</i> , 2018, 13, 2508-2512.	3.4	12
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.	3.7	30
2078	Alkaline-earth metal based MOFs with second scale long-lasting phosphor behavior. <i>CrystEngComm</i> , 2018, 20, 4793-4803.	2.6	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.	4.0	10
2080	Fluostatins: A Family of 6-5-6-6 Ring Skeleton and High Oxidized A-Rings from Marine Streptomyces sp. PKU-MA00045. <i>Marine Drugs</i> , 2018, 16, 87.	4.6	43
2081	HSQC-TOCSY Fingerprinting-Directed Discovery of Antiplasmodial Polyketides from the Marine Ascidian-Derived Streptomyces sp. (USC-16018). <i>Marine Drugs</i> , 2018, 16, 189.	4.6	17
2082	Two Chemically Stable Cd(II) Polymers as Fluorescent Sensor and Photocatalyst for Aromatic Dyes. <i>Polymers</i> , 2018, 10, 274.	4.5	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.	3.6	24
2084	Deltahedral Organozinc Superhalogens. <i>Chemistry - A European Journal</i> , 2018, 24, 13654-13658.	3.3	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.	4.9	15
2086	Aldehyde isomers of porphyrin: A spectroscopic and computational study. <i>Journal of Molecular Structure</i> , 2018, 1173, 665-670.	3.6	7
2087	Single sensors for multiple analytes employing fluorometric differentiation for Cr <sup>3+</sup> and Al <sup>3+</sup> in semi-aqueous medium with bio-activity and theoretical aspects. <i>Analytical Methods</i> , 2018, 10, 4063-4072.	2.7	21
2088	Electron Transfer Reactions: KO <sup>t</sup> Bu (but not NaO <sup>t</sup> Bu) Photoreduces Benzophenone under Activation by Visible Light. <i>Journal of the American Chemical Society</i> , 2018, 140, 9751-9757.	13.7	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.	3.6	2
2090	Theoretical Insights into D-D- $\pi$ -A Sensitizers Employing $\pi$ -N-Annulated Perylene for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6328-6342.	2.5	21
2091	A DFT study of penicillamine adsorption over pure and Al-doped C60 fullerene. <i>Adsorption</i> , 2018, 24, 471-480.	3.0	22
2092	Ethynyl-bridged porphyrin-corrole dyads and triads: Synthesis, properties and DFT calculations. <i>Tetrahedron</i> , 2018, 74, 4476-4488.	1.9	7
2093	Completely Unexpected Coordination Selectivity of Copper Iodide for Thioether Over Ethynyl. <i>Chemistry Africa</i> , 2018, 1, 67-77.	2.4	3

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2095	A multifunctional selective "turn-on" fluorescent chemosensor for detection of Group IIIA ions Al <sup>3+</sup> , Ga <sup>3+</sup> and In <sup>3+</sup> . <i>Photochemical and Photobiological Sciences</i> , 2018, 17, 1247-1255.	2.9	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.	3.7	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.	2.8	15
2098	What does it take to induce equilibrium in bidirectional energy transfers?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13682-13692.	2.8	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.	5.8	37
2100	A DFT study of H <sub>2</sub> CO and HCN adsorptions on 3d, 4d, and 5d transition metal-doped graphene nanosheets. <i>Structural Chemistry</i> , 2018, 29, 147-157.	2.0	29
2101	First-principles study of efficient phenothiazine-based "A organic sensitizers with various spacers for DSSCs. <i>Journal of Computational Electronics</i> , 2018, 17, 1410-1420.	2.5	35
2102	Synthesis, characterization and antimicrobial activities of Co(III) and Ni(II) complexes with 5-methyl-3-formylpyrazole-N(4)-dihexylthiosemicarbazone (HMPzNH <sub>2</sub> ): X-ray crystallography and DFT calculations of [Co(MPzNH <sub>2</sub> ) <sub>2</sub> ]ClO <sub>4</sub> ·1.5H <sub>2</sub> O (I) and [Ni(HMPzNH <sub>2</sub> ) <sub>2</sub> ]Cl <sub>2</sub> ·2H <sub>2</sub> O (II). <i>Inorganica Chimica Acta</i> , 2018, 483, 271-283.	2.4	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.	2.4	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.	4.0	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.	3.9	17
2106	An experimental and theoretical investigation of the structure of synthesized ZnO powder. <i>Chemical Physics</i> , 2018, 513, 273-279.	1.9	9
2107	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.	2.6	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.	2.2	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.	2.6	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.	2.8	10
2111	Is it possible to use X <sub>12</sub> Y <sub>12</sub> (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.	2.3	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.	4.9	21
2114	The impact of heteroatom substitution on cross-conjugation and its effect on the photovoltaic performance of DSSCs – a computational investigation of linear <i>vs.</i> cross-conjugated anchoring units. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22660-22673.	2.8	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.	3.1	3
2116	Dynamic multistimuli-responsive reversible chiral transformation in supramolecular helices. <i>Scientific Reports</i> , 2018, 8, 11220.	3.3	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.	5.2	2
2118	Benzo[e]indolium derivatives in aqueous solutions: Reaction with bisulfite and successive interaction with Cu <sup>2+</sup> and Hg <sup>2+</sup> . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 202, 324-332.	3.9	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.	3.6	53
2120	Chiral coordination polymers based on d <sup>10</sup> metals and 2-aminonicotinate with blue fluorescent/green phosphorescent anisotropic emissions. <i>Dalton Transactions</i> , 2018, 47, 8746-8754.	3.3	12
2121	Optical monitoring of adipose tissue destruction under encapsulated lipase action. <i>Journal of Biophotonics</i> , 2018, 11, e201800058.	2.3	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.	3.6	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.	2.2	4
2124	Electrochemical, Spectroelectrochemical, Mössbauer, and EPR Spectroscopic Studies on Ferrocenyl-Substituted Tritylium Dyes. <i>Chemistry - A European Journal</i> , 2018, 24, 12524-12538.	3.3	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.	2.4	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.	3.6	40
2127	Theoretical study of hydrogen storage reactions on nickel-decorated heterofullerene C <sub>58</sub> B <sub>1</sub> X <sub>57</sub> N <sub>1</sub> Y <sub>57</sub> (X<Y=H, C, Si, Ge, Sn, Pb, Bi, Sb, As, Se, Te, Po, At, Rn). <i>Molecular Physics</i> , 2018, 116, 2321-2342.	3.6	6
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.	2.5	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(benzoyloxy)hex-5-enylidene) hydrazinecarboxylate. <i>Journal of Molecular Structure</i> , 2018, 1171, 375-387.	3.6	2

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2507	Hydrogen abstraction of methanimine by X12N12 (X = B, Al) nanoclusters: a DFT study. <i>Structural Chemistry</i> , 2020, 31, 447-454.	2.0	0
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3244	Metal incorporated aminothiazole-derived compounds: synthesis, density function theory analysis, <i>in vitro</i> antibacterial and antioxidant evaluation. <i>Royal Society Open Science</i> , 2021, 8, 210910.	2.4	32
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