List of Publications by Year in descending order

201 papers	6,380 citations	53794 45 h-index	114465 63 g-index
205 all docs	205 docs citations	205 times ranked	2083 citing authors

#	Article	IF	Citations
1	Applications of graphene-based tungsten oxide nanocomposites: a review. Journal of Nanostructure in Chemistry, 2023, 13, 167-196.	9.1	8
2	Exploring the potential of tetraazaacene derivatives as photovoltaic materials with enhanced photovoltaic parameters. International Journal of Quantum Chemistry, 2022, 122, e26817.	2.0	19
3	Tuning the optoelectronic properties of benzodithiophene based donor materials and their photovoltaic applications. Materials Science in Semiconductor Processing, 2022, 137, 106150.	4.0	34
4	Improving energy harvesting efficiency of dye sensitized solar cell by using cobalt-rGO co-doped TiO2 photoanode. Journal of Alloys and Compounds, 2022, 891, 162040.	5.5	22
5	G-C3N4/Ag@CoWO4: A novel sunlight active ternary nanocomposite for potential photocatalytic degradation of rhodamine B dye. Journal of Physics and Chemistry of Solids, 2022, 161, 110437.	4.0	34
6	Coal fly ash supported CoFe2O4 nanocomposites: Synergetic Fenton-like and photocatalytic degradation of methylene blue. Environmental Research, 2022, 206, 112280.	7.5	38
7	Designing benzothiadiazole based highly efficient non-fullerene acceptor molecules for organic solar cells. Polymer, 2022, 238, 124405.	3.8	26
8	DFT study of OLi3 and MgF3 doped boron nitride with enhanced nonlinear optical behavior. Journal of Molecular Structure, 2022, 1251, 131934.	3.6	19
9	Dative behavior of N-heterocyclic carbenes (NHCs) with selenium in Se-NHC compounds. Reviews in Inorganic Chemistry, 2022, 42, 229-238.	4.1	2
10	Dopant Free Triphenylamineâ€Based Hole Transport Materials with Excellent Photovoltaic Properties for Highâ€Performance Perovskite Solar Cells. Energy Technology, 2022, 10, 2100838.	3.8	34
11	Identification of Marine Fungi-Based Antiviral Agents as Potential Inhibitors of SARS-CoV-2 by Molecular Docking, ADMET and Molecular Dynamic Study. Journal of Computational Biophysics and Chemistry, 2022, 21, 139-153.	1.7	4
12	End-capped modification of dithienosilole based small donor molecules for high performance organic solar cells using DFT approach. Journal of Molecular Liquids, 2022, 345, 118138.	4.9	59
13	DFT study of 2D graphitic carbon nitride based preferential targeted delivery of levosimendan, a cardiovascular drug. Computational and Theoretical Chemistry, 2022, 1209, 113584.	2.5	6
14	Raman spectroscopic characterization of selenium N-heterocyclic carbene compounds. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 270, 120823.	3.9	7
15	Shedding light on the optical and nonlinear optical properties of superalkali-doped borophene. Journal of Molecular Modeling, 2022, 28, 46.	1.8	6
16	Synergistic engineering of end-capped acceptor and bridge on arylborane-arylamine macrocycles to boost the photovoltaic properties of organic solar cells. Optical Materials, 2022, 123, 111907.	3.6	48
17	Exploring the inhibitory potential of novel bioactive compounds from mangrove actinomycetes against nsp10 the major activator of SARS-CoV-2 replication. Chemical Papers, 2022, 76, 3051-3064.	2.2	14
18	Environmentally compatible and highly improved hole transport materials (HTMs) based on benzotrithiophene (BTT) skeleton for perovskite as well as narrow bandgap donors for organic solar cells. Solar Energy, 2022, 231, 793-808.	6.1	56

#	Article	IF	Citations
19	Amplifying the photovoltaic properties of azaBODIPY core based small molecules by terminal acceptors modification for high performance organic solar cells: A DFT approach. Solar Energy, 2022, 233, 31-45.	6.1	43
20	Theoretical investigation of X2NaIO6 (X= Pb,Sr) double perovskites for thermoelectric and optoelectronic applications. Physica B: Condensed Matter, 2022, 630, 413694.	2.7	39
21	Drug delivery of carvedilol (cardiovascular drug) using phosphorene as a drug carrier: a DFT study. Journal of Taibah University for Science, 2022, 16, 31-46.	2.5	14
22	Identification of Halogen-Based Derivatives as Potent Inhibitors of Estrogen Receptor Alpha of Breast Cancer: An In-Silico Investigation. Journal of Computational Biophysics and Chemistry, 2022, 21, 181-205.	1.7	6
23	A DFT approach for finding therapeutic potential of two dimensional (2D) graphitic carbon nitride (GCN) as a drug delivery carrier for curcumin to treat cardiovascular diseases. Journal of Molecular Structure, 2022, 1257, 132547.	3.6	16
24	Tuning the optoelectronic properties of indacenodithiophene based derivatives for efficient photovoltaic applications: A DFT approach. Chemical Physics Letters, 2022, 793, 139459.	2.6	44
25	Tuning of diphenylamine subphthalocyanine based small molecules with efficient photovoltaic parameters for organic solar cells. Journal of Molecular Graphics and Modelling, 2022, 112, 108146.	2.4	12
26	Controlled supramolecular interaction to enhance the bioavailability of hesperetin to targeted cancer cells through graphyne: a comprehensive in silico study. RSC Advances, 2022, 12, 6336-6346.	3.6	12
27	Silver cluster doped graphyne (GY) with outstanding non-linear optical properties. RSC Advances, 2022, 12, 5466-5482.	3.6	29
28	Simultaneously enhanced efficiency of eco-friendly structural characterization of the dithienocyclopentacarbazole donor based acceptors with narrow bandgap for high-performance organic solar cells. Journal Physics D: Applied Physics, 2022, 55, 235501.	2.8	26
29	Designing phenyl-di-p-tolyl-amine-based asymmetric small molecular donor materials with favorable photovoltaic parameters. Optik, 2022, 256, 168739.	2.9	9
30	Quantum chemical study of end-capped acceptor and bridge on triphenyl diamine based molecules to enhance the optoelectronic properties of organic solar cells. Polymer, 2022, 245, 124675.	3.8	26
31	Enhancement in non-linear optical properties of carbon nitride (C2N) by doping superalkali (Li3O): A DFT study. Computational and Theoretical Chemistry, 2022, 1211, 113654.	2.5	18
32	Designing of the indacenodithiophene core-based small molecules for optoelectronic applications: A DFT approach. Solar Energy, 2022, 237, 108-121.	6.1	37
33	Engineering of A2-D-A1-D-A2 type BT-dIDT based non-fullerene acceptors for effective organic solar cells. Computational and Theoretical Chemistry, 2022, 1211, 113666.	2.5	12
34	Depicting the role of end-capped acceptors to amplify the photovoltaic properties of benzothiadiazole core-based molecules for high-performance organic solar cell applications. Computational and Theoretical Chemistry, 2022, 1211, 113669.	2.5	14
35	Quantum chemical approach to study TIPSTAP derivatives with anticipated minimized crystal roughness for photovoltaic application with estimated PCE of over 20%. Solar Energy, 2022, 237, 96-107.	6.1	13
36	End-capped modification of Y-Shaped dithienothiophen[3,2-b]-pyrrolobenzothiadiazole (TPBT) based non-fullerene acceptors for high performance organic solar cells by using DFT approach. Surfaces and Interfaces, 2022, 30, 101875.	3.0	31

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37	End-capped group modification on cyclopentadithiophene based non-fullerene small molecule acceptors for efficient organic solar cells; a DFT approach. Journal of Molecular Graphics and Modelling, 2022, 113, 108162.	2.4	46
38	Synthesis, photophysical, electrochemical and computational studies of novel 2-aminoimidazolones with D-Ï€-A framework. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 429, 113918.	3.9	5
39	Bithieno Thiophene-Based Small Molecules for Application as Donor Materials for Organic Solar Cells and Hole Transport Materials for Perovskite Solar Cells. ACS Omega, 2022, 7, 844-862.	3.5	43
40	Exopolysaccharides production from marine Bacillus strains and their antioxidant and bio-flocculant capacities. Archives of Microbiology, 2022, 204, 250.	2.2	3
41	Synergistic end-capped engineering on non-fused thiophene ring-based acceptors to enhance the photovoltaic properties of organic solar cells. RSC Advances, 2022, 12, 12321-12334.	3.6	19
42	Symmetrical endâ€capped molecular engineering of starâ€shaped triphenylamine-based derivatives having remarkable photovoltaic properties for efficient organic solar cells. Journal of Molecular Modeling, 2022, 28, 132.	1.8	2
43	Tuning the optoelectronic properties of cross conjugated small molecules using benzodithiophene as a core unit with favorable photovoltaic parameters: a DFT study. Journal Physics D: Applied Physics, 2022, 55, 295106.	2.8	3
44	A DFT approach towards therapeutic potential of phosphorene as a novel carrier for the delivery of felodipine (cardiovascular drug). Computational and Theoretical Chemistry, 2022, 1212, 113724.	2.5	7
45	Remarkable non-linear optical properties of gold cluster doped graphyne (GY): A DFT study. Journal of Molecular Graphics and Modelling, 2022, 114, 108204.	2.4	9
46	Virtual screening of potential inhibitor against breast cancer-causing estrogen receptor alpha (ERÎ±): molecular docking and dynamic simulations. Molecular Simulation, 2022, 48, 1163-1174.	2.0	5
47	Impact of side-chain engineering on the A-Ï€-D-Ï€-A type SM-BF1 donor molecule for bulk heterojunction and their photovoltaic performance: A DFT approach. Solar Energy, 2022, 240, 38-56.	6.1	25
48	Strategies toward the end-group modifications of indacenodithiophene based non-fullerene small molecule acceptor to improve the efficiency of organic solar cells; a DFT study. Computational and Theoretical Chemistry, 2022, 1213, 113747.	2.5	9
49	DFT study of alkali and alkaline earth metal-doped benzocryptand with remarkable NLO properties. RSC Advances, 2022, 12, 16029-16045.	3.6	17
50	Physical Properties of Sr₂MWO₆ (M=Ca, Mg) for Renewable Energy Applications. Physica Status Solidi (B): Basic Research, 2022, 259, .	1.5	7
51	Enhancement of NLO properties of supersalt (Al(BH4)3)-doped graphene: a DFT study. Journal of Molecular Modeling, 2022, 28, .	1.8	4
52	DFT study of transition metals doped calix-4-pyrrole with excellent electronic and non-linear optical properties. Computational and Theoretical Chemistry, 2022, 1214, 113767.	2.5	29
53	Engineering of A-Ï€-D-Ï€-A system based non-fullerene acceptors to enhance the photovoltaic properties of organic solar cells; A DFT approach. Chemical Physics Letters, 2022, 801, 139750.	2.6	11
54	Quantum chemical simulations of benzothiadiazole (BT) based small molecule donor materials for efficient organic solar cells. Chemical Physics Letters, 2022, 801, 139726.	2.6	5

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55	Designing the optoelectronic properties of BODIPY and their photovoltaic applications for high performance of organic solar cells by using computational approach. Materials Science in Semiconductor Processing, 2022, 148, 106812.	4.0	14
56	Alkaline earth metals doped C2N with enhanced non-linear optical properties. Optik, 2022, 265, 169514.	2.9	3
57	Enhanced non-linear optical response of alkali metal-doped nitrogenated holey graphene (C2N). Journal of Molecular Structure, 2022, 1267, 133580.	3.6	3
58	Insighting isatin derivatives as potential antiviral agents against NSP3 of COVID-19. Chemical Papers, 2022, 76, 6271-6285.	2.2	6
59	Molecular Modeling of Pentacyclic Aromatic Bislactam-Based Small Donor Molecules by Altering Auxiliary End-Capped Acceptors to Elevate the Photovoltaic Attributes of Organic Solar Cells. ACS Omega, 2022, 7, 20528-20541.	3.5	5
60	Impact of end-capped modification of MO-IDT based non-fullerene small molecule acceptors to improve the photovoltaic properties of organic solar cells. Journal of Molecular Graphics and Modelling, 2022, 116, 108255.	2.4	37
61	Tuning the photovoltaic parameters of spiro[fluorenexanthene]-diol (SFX-OH)-based crosslinked donor materials for efficient organic solar cells. Computational and Theoretical Chemistry, 2022, 1214, 113778.	2.5	1
62	A DFT study of nonlinear optical response of supersalt (Al(BH₄)₃) doped boron nitride. Journal of Taibah University for Science, 2022, 16, 621-631.	2.5	6
63	Impact of end capped modification on BT-CIC molecule for high-performance photovoltaic attributes: a DFT approach. Journal of Molecular Modeling, 2022, 28, .	1.8	10
64	Synthesis, comparative theoretical and experimental characterization of some new 1,3,5 triazine based heterocyclic compounds and in vitro evaluation as promising biologically active agents. Journal of Molecular Structure, 2022, 1268, 133622.	3.6	7
65	Enhanced linear and nonlinear optical response of superhalogen (Al7) doped graphitic carbon nitride (g-C3N4). Optik, 2021, 226, 165923.	2.9	46
66	O-4-Acetylamino-benzenesulfonylated pyrimidine derivatives: synthesis, SC-XRD, DFT analysis and electronic behaviour investigation. Journal of Molecular Structure, 2021, 1224, 129308.	3.6	32
67	Exploring the twisted molecular configurations for tuning their optical and nonlinear optical response properties: A quantum chemical approach. Journal of Molecular Graphics and Modelling, 2021, 102, 107766.	2.4	14
68	Designing benzothiadiazole based non-fullerene acceptors with high open circuit voltage and higher LUMO level to increase the efficiency of organic solar cells. Optik, 2021, 228, 166138.	2.9	48
69	Theoretical Investigation of Perylene Diimide derivatives as Acceptors to Match with Benzodithiophene based Donors for Organic Photovoltaic Devices. Zeitschrift Fur Physikalische Chemie, 2021, 235, 427-449.	2.8	9
70	Exploring the optoelectronic and third-order nonlinear optical susceptibility of cross-shaped molecules: insights from molecule to material level. Journal of Molecular Modeling, 2021, 27, 12.	1.8	33
71	DFT study of superhalogen and superalkali doped graphitic carbon nitride and its non-linear optical properties. RSC Advances, 2021, 11, 7779-7789.	3.6	39
72	Phase transition and thermoelectric properties of cubic KNbO3 under pressure: DFT approach. Journal of Materials Research and Technology, 2021, 11, 2106-2113.	5.8	46

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73	Synthesis in combination with Biological and Computational evaluations of selenium-N-Heterocyclic Carbene compounds. Computational and Theoretical Chemistry, 2021, 1197, 113135.	2.5	7
74	Designing of small molecule non-fullerene acceptors with cyanobenzene core for photovoltaic application. Computational and Theoretical Chemistry, 2021, 1197, 113154.	2.5	43
75	Exploring the new potential antiviral constituents of Moringa oliefera for SARS-COV-2 pathogenesis: An in silico molecular docking and dynamic studies. Chemical Physics Letters, 2021, 767, 138379.	2.6	58
76	Theoretical investigation of supramolecular hydrogen-bonded choline chloride-based deep eutectic solvents using density functional theory. Chemical Physics Letters, 2021, 769, 138427.	2.6	79
77	Triphenylamine based donor-acceptor-donor type small molecules for organic solar cells. Computational and Theoretical Chemistry, 2021, 1198, 113176.	2.5	16
78	DFT study of superhalogen (AlF4) doped boron nitride for tuning their nonlinear optical properties. Optik, 2021, 231, 166464.	2.9	35
79	A DFT Study of Graphitic Carbon Nitride as Drug Delivery Carrier for Flutamide (Anticancer Drug). Journal of Computational Biophysics and Chemistry, 2021, 20, 347-358.	1.7	7
80	Designing of cyanobenzene based small molecules with suitable photovoltaic parameters for organic solar cells. International Journal of Quantum Chemistry, 2021, 121, e26673.	2.0	6
81	DFT study of superhalogen-doped borophene with enhanced nonlinear optical properties. Journal of Molecular Modeling, 2021, 27, 188.	1.8	28
82	Tuning the optoelectronic properties of dibenzochrysene (DBC) based small molecules for organic solar cells. Materials Science in Semiconductor Processing, 2021, 127, 105689.	4.0	41
83	DFT study of therapeutic potential of graphitic carbon nitride (g-C3N4) as a new drug delivery system for carboplatin to treat cancer. Journal of Molecular Liquids, 2021, 331, 115607.	4.9	51
84	Designing of benzodithiophene acridine based Donor materials with favorable photovoltaic parameters for efficient organic solar cell. Computational and Theoretical Chemistry, 2021, 1200, 113238.	2.5	55
85	Tuning the optoelectronic properties of oligothienyl silane derivatives and their photovoltaic properties. Journal of Molecular Graphics and Modelling, 2021, 106, 107918.	2.4	25
86	Structural, electronic, half â€“metallic ferromagnetic and optical properties of cubic MAlO3 (M=Ce, Pr) perovskites: A DFT study. Journal of Physics and Chemistry of Solids, 2021, 154, 110084.	4.0	37
87	Study of nonlinear optical properties of superhalogen and superalkali doped phosphorene. Journal of Molecular Structure, 2021, 1236, 130348.	3.6	18
88	Theoretical and computational study on electronic effect caused by electron withdrawing/electron-donating groups upon the coumarin thiourea derivatives. Computational and Theoretical Chemistry, 2021, 1201, 113271.	2.5	29
89	End-capped engineering of bipolar diketopyrrolopyrrole based small electron acceptor molecules for high performance organic solar cells. Computational and Theoretical Chemistry, 2021, 1201, 113242.	2.5	40
90	Designing and theoretical study of fluorinated small molecule donor materials for organic solar cells. Journal of Molecular Modeling, 2021, 27, 216.	1.8	31

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91	Tris-isopropyl-sily-ethynyl anthracene based small molecules for organic solar cells with efficient photovoltaic parameters. Computational and Theoretical Chemistry, 2021, 1202, 113305.	2.5	8
92	Pressure induced electronic, optical and thermoelectric properties of cubic BaZrO3: A first principle calculations. Optik, 2021, 239, 166694.	2.9	25
93	Exploration of Nonlinear Optical Properties of Triphenylamine-Dicyanovinylene Coexisting Donor-Ï€-Acceptor Architecture by the Modification of Ï€-Conjugated Linker. Frontiers in Materials, 2021, 8, .	2.4	9
94	Quantum Chemical Approach of Donorâ^'Ï€â€“Acceptor Based Arylboraneâ€“Arylamine Macrocycles with Outstanding Photovoltaic Properties Toward High-Performance Organic Solar Cells. Energy & Fuels, 2021, 35, 15018-15032.	5.1	66
95	Efficient tuning of small acceptor chromophores with A1-Ï€-A2-Ï€-A1 configuration for high efficacy of organic solar cells via end group manipulation. Journal of Saudi Chemical Society, 2021, 25, 101305.	5.2	53
96	Tuning the optoelectronic properties of triphenylamine (TPA) based small molecules by modifying central core for photovoltaic applications. Journal of Molecular Modeling, 2021, 27, 237.	1.8	60
97	Therapeutic potential of graphyne as a new drug-delivery system for daunorubicin to treat cancer: A DFT study. Journal of Molecular Liquids, 2021, 336, 116327.	4.9	48
98	Computational and theoretical study of subphthalocyanine based derivatives by varying acceptors to increase the efficiency of organic solar cells. Computational and Theoretical Chemistry, 2021, 1203, 113356.	2.5	14
99	Tuning the optoelectronic properties of superalkali doped phosphorene. Journal of Molecular Graphics and Modelling, 2021, 107, 107973.	2.4	10
100	Designing and theoretical characterization of benzodithiophene dione based donor molecules for small molecule organic solar cells. Optik, 2021, 242, 167098.	2.9	24
101	Effects of Aromatic Thiol Capping Agents on the Structural and Electronic Properties of CdnTen (n =) Tj ETQq1 1 0.784314 rgBT /Ove	2.4	1
102	Computational and theoretical study of graphitic carbon nitride (g-C3N4) as a drug delivery carrier for lonidamine drug to treat cancer. Computational and Theoretical Chemistry, 2021, 1206, 113459.	2.5	10
103	Electro-optical and charge transport properties of chalcone derivatives using a dual approach from molecule to material level simulations. Computational and Theoretical Chemistry, 2021, 1203, 113349.	2.5	10
104	Designing of benzodithiophene (BDT) based non-fullerene small molecules with favorable optoelectronic properties for proficient organic solar cells. Computational and Theoretical Chemistry, 2021, 1203, 113359.	2.5	49
105	Physical characteristics of barium based cubic perovskites. Chemical Physics Letters, 2021, 779, 138835.	2.6	11
106	Computational study of therapeutic potential of phosphorene as a nano-carrier for drug delivery of nebivolol for the prohibition of cardiovascular diseases: a DFT study. Journal of Molecular Modeling, 2021, 27, 306.	1.8	8
107	Physical characteristics of NaTaO3Under pressure for electronic devices. Materials Science in Semiconductor Processing, 2021, 133, 105976.	4.0	11
108	Molecular engineering strategy of naphthalimide based small donor molecules for high-performance organic solar cells. Computational and Theoretical Chemistry, 2021, 1204, 113416.	2.5	43

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109	Optoelectronic properties of naphthalene bis-benzimidazole based derivatives and their photovoltaic applications. Computational and Theoretical Chemistry, 2021, 1204, 113373.	2.5	21
110	Coal fly ash-based copper ferrite nanocomposites as potential heterogeneous photocatalysts for wastewater remediation. Applied Surface Science, 2021, 565, 150542.	6.1	40
111	Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications. Chemical Physics Letters, 2021, 782, 139018.	2.6	39
112	Designing and comparative analysis of 3D subphthalocyanines based non-fullerene acceptor molecules as an efficient material for organic solar cells. Optik, 2021, 246, 167845.	2.9	13
113	Structural, optical and photovoltaic properties of unfused Non-Fullerene acceptors for efficient solution processable organic solar cell (Estimated PCEÂgreater thanÂ12.4%): A DFT approach. Journal of Molecular Liquids, 2021, 341, 117428.	4.9	55
114	Tuning the optoelectronic properties of naphthodithiophene (NDT) for designing of A-D-A type photovoltaic materials. Optik, 2021, 247, 167892.	2.9	21
115	Isatin-derived non-fullerene acceptors for efficient organic solar cells. Materials Science in Semiconductor Processing, 2021, 121, 105345.	4.0	38
116	Designing of 5,10-Dihydroindolo [3,2-b] Indole (DINI) Based Donor Materials for Small Molecule Organic Solar Cells. Journal of Computational Biophysics and Chemistry, 2021, 20, 71-84.	1.7	17
117	Tuning the optoelectronic properties of ZOPTAN core-based derivatives by varying acceptors to increase efficiency of organic solar cell. Journal of Molecular Modeling, 2021, 27, 316.	1.8	20
118	Tuning of a Aâ€“Aâ€“Dâ€“Aâ€“A-Type Small Molecule with Benzodithiophene as a Central Core with Efficient Photovoltaic Properties for Organic Solar Cells. ACS Omega, 2021, 6, 28923-28935.	3.5	49
119	The theoretical investigation of the opto-electronic properties of designed molecules having 2-(2-Methylene-3-oxo-indane-1-ylidene)malononitrile as end-capped acceptors. Zeitschrift Fur Physikalische Chemie, 2021, 235, 785-804.	2.8	0
120	A Facile Approach for the Synthesis of SrTiO₃/gâ€C₃N₄ Photoâ€catalyst and its Efficacy in Biodiesel Production. ChemistrySelect, 2021, 6, 12082-12093.	1.5	6
121	A Theoretical Perspective on Strategies for Modeling High Performance Nonlinear Optical Materials. Frontiers in Materials, 2021, 8, .	2.4	26
122	Tuning opto-electronic properties of alkoxy-induced based electron acceptors in infrared region for high performance organic solar cells. Journal of Molecular Liquids, 2020, 298, 111963.	4.9	58
123	Molecular designing of naphthalene diimide based fullerene-free small organic solar cell - Acceptors with high photovoltaic performance by density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117685.	3.9	14
124	Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study. Journal of Molecular Liquids, 2020, 297, 111902.	4.9	42
125	Synthesis and characterization of stable and biological active chitin-based polyurethane elastomers. International Journal of Biological Macromolecules, 2020, 154, 1149-1157.	7.5	31
126	Facile synthesis, crystal growth, characterization and computational study of new pyridineâ€based halogenated hydrazones: Unveiling the stabilization behavior in terms of noncovalent interactions. Applied Organometallic Chemistry, 2020, 34, e5399.	3.5	28

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127	Theoretical calculation of selenium N-heterocyclic carbene compounds through DFT studies: Synthesis, characterization and biological potential. Journal of Molecular Structure, 2020, 1204, 127462.	3.6	26
128	Therapeutic potential of graphitic carbon nitride as a drug delivery system for cisplatin (anticancer) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	2.8	72
129	Comparison of Photoâ€Esterification Capability of Bismuth Vanadate with Reduced Graphene Oxide Bismuth Vanadate (RGO/BiVO₄) Composite for Biodiesel Production from High Free Fatty Acid Containing Nonâ€Edible Oil. ChemistrySelect, 2020, 5, 9245-9253.	1.5	14
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131	Green Synthesis, SC-XRD, Non-Covalent Interactive Potential and Electronic Communication via DFT Exploration of Pyridine-Based Hydrazone. Crystals, 2020, 10, 778.	2.2	22
132	Manganese Incorporated Eosin Y Dye/Graphene Nanocomposite: an Efficient Visible Light Active Photocatalyst. Russian Journal of Physical Chemistry B, 2020, 14, 552-558.	1.3	6
133	A DFT study of structural, magnetic, elastic and optoelectronic properties of lanthanide based XAlO3 (X=Nd, Gd) compounds. Journal of Materials Research and Technology, 2020, 9, 16488-16496.	5.8	54
134	Enhancement in Photovoltaic Properties of N,Nâ€diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. ChemistrySelect, 2020, 5, 5022-5034.	1.5	95
135	Designing indenothiophene-based acceptor materials with efficient photovoltaic parameters for fullerene-free organic solar cells. Journal of Molecular Modeling, 2020, 26, 137.	1.8	97
136	Density functional theory study of palladium cluster adsorption on a graphene support. RSC Advances, 2020, 10, 20595-20607.	3.6	86
137	Designing 2D fused ring materials for small molecules organic solar cells. Computational and Theoretical Chemistry, 2020, 1183, 112848.	2.5	38
138	Designing N-phenylaniline-triazol configured donor materials with promising optoelectronic properties for high-efficiency solar cells. Computational and Theoretical Chemistry, 2020, 1186, 112908.	2.5	119
139	Designing alkoxy-induced based high performance near infrared sensitive small molecule acceptors for organic solar cells. Journal of Molecular Liquids, 2020, 305, 112829.	4.9	76
140	Tuning the optoelectronic properties of Benzo Thiophene (BT-CIC) based non-fullerene acceptor organic solar cell. Journal of Theoretical and Computational Chemistry, 2020, 19, 2050003.	1.8	23
141	Computational and experimental study of heterofunctional azo reactive dyes synthesized for cellulosic fabric. Journal of Molecular Structure, 2020, 1221, 128753.	3.6	13
142	Designing Triphenylamineâ€Configured Donor Materials with Promising Photovoltaic Properties for Highly Efficient Organic Solar Cells. ChemistrySelect, 2020, 5, 7358-7369.	1.5	67
143	Tuning the optoelectronic properties of Subphthalocyanine (SubPc) derivatives for photovoltaic applications. Optical Materials, 2020, 107, 110154.	3.6	79
144	Rational design of naphthalimide based small molecules non-fullerene acceptors for organic solar cells. Computational and Theoretical Chemistry, 2020, 1187, 112916.	2.5	18

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145	Design, synthesis and application of triazole ligands in suzuki miyaura cross coupling reaction of aryl chlorides. Journal of Molecular Structure, 2020, 1206, 127753.	3.6	12
146	Facile preparation, characterization, SC-XRD and DFT/DTDFT study of diversely functionalized unsymmetrical bis-aryl-Î±, Î²-unsaturated ketone derivatives. Journal of Molecular Structure, 2020, 1206, 127755.	3.6	51
147	Designing of benzothiazole based non-fullerene acceptor (NFA) molecules for highly efficient organic solar cells. Computational and Theoretical Chemistry, 2020, 1181, 112833.	2.5	94
148	Super alkali (OLi₃) doped boron nitride with enhanced nonlinear optical behavior. Journal of Nonlinear Optical Physics and Materials, 2020, 29, 2050004.	1.8	23
149	The theoretical investigation of the opto-electronic properties of designed molecules having 2-(2-Methylene-3-oxo-indane-1-ylidene)malononitrile as end-capped acceptors. Zeitschrift Fur Physikalische Chemie, 2020, .	2.8	0
150	Isolation of Several Indigenous Microalgae from Kallar Kahar Lake, Chakwal Pakistan. Iranian Journal of Biotechnology, 2020, 18, e2214.	0.3	0
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