

Javed Iqbal

List of Publications by Year in descending order

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331
papers

10,077
citations

36303

51
h-index

76900

74
g-index

333
all docs

333
docs citations

333
times ranked

6746
citing authors

#	ARTICLE	IF	CITATIONS
1	Applications of graphene-based tungsten oxide nanocomposites: a review. <i>Journal of Nanostructure in Chemistry</i> , 2023, 13, 167-196.	9.1	8
2	Investigating the nexus between critical success factors, despotic leadership, and success of renewable energy projects. <i>Environmental Science and Pollution Research</i> , 2022, 29, 10388-10398.	5.3	37
3	Exploring the potential of tetraazaacene derivatives as photovoltaic materials with enhanced photovoltaic parameters. <i>International Journal of Quantum Chemistry</i> , 2022, 122, e26817.	2.0	19
4	Tuning the optoelectronic properties of benzodithiophene based donor materials and their photovoltaic applications. <i>Materials Science in Semiconductor Processing</i> , 2022, 137, 106150.	4.0	34
5	G-C3N4/Ag@CoWO4: A novel sunlight active ternary nanocomposite for potential photocatalytic degradation of rhodamine B dye. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 161, 110437.	4.0	34
6	Designing benzothiadiazole based highly efficient non-fullerene acceptor molecules for organic solar cells. <i>Polymer</i> , 2022, 238, 124405.	3.8	26
7	DFT study of OLi3 and MgF3 doped boron nitride with enhanced nonlinear optical behavior. <i>Journal of Molecular Structure</i> , 2022, 1251, 131934.	3.6	19
8	Dative behavior of <i>N</i> -heterocyclic carbenes (NHCs) with selenium in Se-NHC compounds. <i>Reviews in Inorganic Chemistry</i> , 2022, 42, 229-238.	4.1	2
9	Dopant Free Triphenylamine-Based Hole Transport Materials with Excellent Photovoltaic Properties for High-Performance Perovskite Solar Cells. <i>Energy Technology</i> , 2022, 10, 2100838.	3.8	34
10	Identification of Marine Fungi-Based Antiviral Agents as Potential Inhibitors of SARS-CoV-2 by Molecular Docking, ADMET and Molecular Dynamic Study. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 139-153.	1.7	4
11	End-capped modification of dithienosilole based small donor molecules for high performance organic solar cells using DFT approach. <i>Journal of Molecular Liquids</i> , 2022, 345, 118138.	4.9	59
12	Social Media Tools for the Development of Pre-Service Health Sciences Researchers during COVID-19 in Pakistan. <i>International Journal of Environmental Research and Public Health</i> , 2022, 19, 581.	2.6	15
13	DFT study of 2D graphitic carbon nitride based preferential targeted delivery of levosimendan, a cardiovascular drug. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113584.	2.5	6
14	Raman spectroscopic characterization of selenium N-heterocyclic carbene compounds. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 270, 120823.	3.9	7
15	Shedding light on the optical and nonlinear optical properties of superalkali-doped borophene. <i>Journal of Molecular Modeling</i> , 2022, 28, 46.	1.8	6
16	Investigation of the adsorption properties of gemcitabine anticancer drug with metal-doped boron nitride fullerenes as a drug-delivery carrier: a DFT study. <i>RSC Advances</i> , 2022, 12, 2873-2887.	3.6	31
17	Synergistic engineering of end-capped acceptor and bridge on arylborane-arylamine macrocycles to boost the photovoltaic properties of organic solar cells. <i>Optical Materials</i> , 2022, 123, 111907.	3.6	48
18	The Impacts of Emotional Intelligence on Students' Study Habits in Blended Learning Environments: The Mediating Role of Cognitive Engagement during COVID-19. <i>Behavioral Sciences (Basel)</i> , 2022, 11, 1030.	1.0	1

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19	Exploring the inhibitory potential of novel bioactive compounds from mangrove actinomycetes against nsp10 the major activator of SARS-CoV-2 replication. <i>Chemical Papers</i> , 2022, 76, 3051-3064.	2.2	14
20	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. <i>Solar Energy</i> , 2022, 231, 793-808.	6.1	56
21	Amplifying the photovoltaic properties of azaBODIPY core based small molecules by terminal acceptors modification for high performance organic solar cells: A DFT approach. <i>Solar Energy</i> , 2022, 233, 31-45.	6.1	43
22	Theoretical investigation of X ₂ NaIO ₆ (X= Pb,Sr) double perovskites for thermoelectric and optoelectronic applications. <i>Physica B: Condensed Matter</i> , 2022, 630, 413694.	2.7	39
23	Drug delivery of carvedilol (cardiovascular drug) using phosphorene as a drug carrier: a DFT study. <i>Journal of Taibah University for Science</i> , 2022, 16, 31-46.	2.5	14
24	Identification of Halogen-Based Derivatives as Potent Inhibitors of Estrogen Receptor Alpha of Breast Cancer: An <i>in-Silico</i> Investigation. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 181-205.	1.7	6
25	A DFT approach for finding therapeutic potential of two dimensional (2D) graphitic carbon nitride (GCN) as a drug delivery carrier for curcumin to treat cardiovascular diseases. <i>Journal of Molecular Structure</i> , 2022, 1257, 132547.	3.6	16
26	Tuning the optoelectronic properties of indacenodithiophene based derivatives for efficient photovoltaic applications: A DFT approach. <i>Chemical Physics Letters</i> , 2022, 793, 139459.	2.6	44
27	Tuning of diphenylamine subphthalocyanine based small molecules with efficient photovoltaic parameters for organic solar cells. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 112, 108146.	2.4	12
28	Controlled supramolecular interaction to enhance the bioavailability of hesperetin to targeted cancer cells through graphyne: a comprehensive <i>in silico</i> study. <i>RSC Advances</i> , 2022, 12, 6336-6346.	3.6	12
29	Silver cluster doped graphyne (GY) with outstanding non-linear optical properties. <i>RSC Advances</i> , 2022, 12, 5466-5482.	3.6	29
30	A Tacit-Knowledge-Based Requirements Elicitation Model Supporting COVID-19 Context. <i>IEEE Access</i> , 2022, 10, 24481-24508.	4.2	3
31	Simultaneously enhanced efficiency of eco-friendly structural characterization of the dithienocyclopentacarbazole donor based acceptors with narrow bandgap for high-performance organic solar cells. <i>Journal Physics D: Applied Physics</i> , 2022, 55, 235501.	2.8	26
32	Impact of Self-Concept, Self-Imagination, and Self-Efficacy on English Language Learning Outcomes Among Blended Learning Students During COVID-19. <i>Frontiers in Psychology</i> , 2022, 13, 784444.	2.1	4
33	DFT Study of the Possible Reaction Path for Radical Promoted Esterification Mechanism of Free Fatty Acids of Soapnut Oil for the Production of Biodiesel. <i>Letters in Organic Chemistry</i> , 2022, 19, 1023-1033.	0.5	1
34	Impact of Destination Image Formation on Tourist Trust: Mediating Role of Tourist Satisfaction. <i>Frontiers in Psychology</i> , 2022, 13, 845538.	2.1	12
35	Designing phenyl-di-p-tolyl-amine-based asymmetric small molecular donor materials with favorable photovoltaic parameters. <i>Optik</i> , 2022, 256, 168739.	2.9	9
36	Quantum chemical study of end-capped acceptor and bridge on triphenyl diamine based molecules to enhance the optoelectronic properties of organic solar cells. <i>Polymer</i> , 2022, 245, 124675.	3.8	26

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37	Enhancement in non-linear optical properties of carbon nitride (C ₂ N) by doping superalkali (Li ₃ O): A DFT study. Computational and Theoretical Chemistry, 2022, 1211, 113654.	2.5	18
38	Designing of the indacenodithiophene core-based small molecules for optoelectronic applications: A DFT approach. Solar Energy, 2022, 237, 108-121.	6.1	37
39	Engineering of A ₂ -D-A ₁ -D-A ₂ type BT-dIDT based non-fullerene acceptors for effective organic solar cells. Computational and Theoretical Chemistry, 2022, 1211, 113666.	2.5	12
40	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
41	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
42	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
43	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
44	Synthesis, photophysical, electrochemical and computational studies of novel 2-aminoimidazolones with D- π -A framework. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 429, 113918.	3.9	5
45	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
46	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
47	Symmetrical end-capped molecular engineering of star-shaped triphenylamine-based derivatives having remarkable photovoltaic properties for efficient organic solar cells. Journal of Molecular Modeling, 2022, 28, 132.	1.8	2
48	Effect of Despotic Leadership on Employee Turnover Intention: Mediating Toxic Workplace Environment and Cognitive Distraction in Academic Institutions. Behavioral Sciences (Basel), 2022, 11, 50297.	1.5	297
49	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
50	How curriculum delivery translates into entrepreneurial skills: The mediating role of knowledge of information and communication technology. PLoS ONE, 2022, 17, e0265880.	2.5	4
51	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
52	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
53	Virtual screening of potential inhibitor against breast cancer-causing estrogen receptor alpha (ER α): molecular docking and dynamic simulations. Molecular Simulation, 2022, 48, 1163-1174.	2.0	5
54	Impact of side-chain engineering on the A- π -D- π -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

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55	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
56	DFT study of alkali and alkaline earth metal-doped benzocryptand with remarkable NLO properties. RSC Advances, 2022, 12, 16029-16045.	3.6	17
57	Physical Properties of Sr ₂ MWO ₆ (M=Ca, Mg) for Renewable Energy Applications. Physica Status Solidi (B): Basic Research, 2022, 259, .	1.5	7
58	Enhancement of NLO properties of supersalt (Al(BH ₄) ₃)-doped graphene: a DFT study. Journal of Molecular Modeling, 2022, 28, .	1.8	4
59	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
60	Engineering of A- π -D- π -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
61	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
62	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
63	Model to Cope With Requirements Engineering Issues for Software Development Outsourcing. IEEE Access, 2022, 10, 63199-63229.	4.2	3
64	Alkaline earth metals doped C ₂ N with enhanced non-linear optical properties. Optik, 2022, 265, 169514.	2.9	3
65	Enhanced non-linear optical response of alkali metal-doped nitrogenated holey graphene (C ₂ N). Journal of Molecular Structure, 2022, 1267, 133580.	3.6	3
66	Insighting isatin derivatives as potential antiviral agents against NSP3 of COVID-19. Chemical Papers, 2022, 76, 6271-6285.	2.2	6
67	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
68	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
69	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
70	A DFT study of nonlinear optical response of supersalt (Al(BH ₄) ₃) ₃ doped boron nitride. Journal of Taibah University for Science, 2022, 16, 621-631.	2.5	6
71	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
72	Towards dealing with commonly occurring requirements engineering process issues during software development outsourcing. PLoS ONE, 2022, 17, e0269607.	2.5	0

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73	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. <i>Journal of Molecular Structure</i> , 2022, 1268, 133622.	3.6	7
74	Enhanced linear and nonlinear optical response of superhalogen (Al ₇) doped graphitic carbon nitride (g-C ₃ N ₄). <i>Optik</i> , 2021, 226, 165923.	2.9	46
75	O-4-Acetylamino-benzenesulfonylated pyrimidine derivatives: synthesis, SC-XRD, DFT analysis and electronic behaviour investigation. <i>Journal of Molecular Structure</i> , 2021, 1224, 129308.	3.6	32
76	Exploring the twisted molecular configurations for tuning their optical and nonlinear optical response properties: A quantum chemical approach. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 102, 107766.	2.4	14
77	Synthesis of molybdenum oxide on AISI-316 steel using cathodic cage plasma deposition at cathodic and floating potential. <i>Surface and Coatings Technology</i> , 2021, 406, 126650.	4.8	19
78	Designing benzothiadiazole based non-fullerene acceptors with high open circuit voltage and higher LUMO level to increase the efficiency of organic solar cells. <i>Optik</i> , 2021, 228, 166138.	2.9	48
79	Use of hydrogen-bonded supramolecular eutectic solvents for eco-friendly extraction of bioactive molecules from <i>Cymbopogon citratus</i> using Boxâ€œBehnken design. <i>Journal of Food Measurement and Characterization</i> , 2021, 15, 1487-1498.	3.2	11
80	Theoretical Investigation of Perylene Diimide derivatives as Acceptors to Match with Benzodithiophene based Donors for Organic Photovoltaic Devices. <i>Zeitschrift Fur Physikalische Chemie</i> , 2021, 235, 427-449.	2.8	9
81	A Study on Mitigating the Communication and Coordination Challenges During Requirements Change Management in Global Software Development. <i>IEEE Access</i> , 2021, 9, 88217-88242.	4.2	9
82	Exploring the optoelectronic and third-order nonlinear optical susceptibility of cross-shaped molecules: insights from molecule to material level. <i>Journal of Molecular Modeling</i> , 2021, 27, 12.	1.8	33
83	DFT study of superhalogen and superalkali doped graphitic carbon nitride and its non-linear optical properties. <i>RSC Advances</i> , 2021, 11, 7779-7789.	3.6	39
84	How Toxic Workplace Environment Effects the Employee Engagement: The Mediating Role of Organizational Support and Employee Wellbeing. <i>International Journal of Environmental Research and Public Health</i> , 2021, 18, 2294.	2.6	145
85	Phase transition and thermoelectric properties of cubic KNbO ₃ under pressure: DFT approach. <i>Journal of Materials Research and Technology</i> , 2021, 11, 2106-2113.	5.8	46
86	Synthesis in combination with Biological and Computational evaluations of selenium-N-Heterocyclic Carbene compounds. <i>Computational and Theoretical Chemistry</i> , 2021, 1197, 113135.	2.5	7
87	Investigation of optical and thermoelectric properties of PbTiO ₃ under pressure. <i>Physica B: Condensed Matter</i> , 2021, 615, 412857.	2.7	16
88	Designing of small molecule non-fullerene acceptors with cyanobenzene core for photovoltaic application. <i>Computational and Theoretical Chemistry</i> , 2021, 1197, 113154.	2.5	43
89	Exploring the new potential antiviral constituents of <i>Moringa oliefera</i> for SARS-COV-2 pathogenesis: An in silico molecular docking and dynamic studies. <i>Chemical Physics Letters</i> , 2021, 767, 138379.	2.6	58
90	Theoretical investigation of supramolecular hydrogen-bonded choline chloride-based deep eutectic solvents using density functional theory. <i>Chemical Physics Letters</i> , 2021, 769, 138427.	2.6	79

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91	Triphenylamine based donor-acceptor-donor type small molecules for organic solar cells. Computational and Theoretical Chemistry, 2021, 1198, 113176.	2.5	16
92	DFT study of superhalogen (AlF ₄) doped boron nitride for tuning their nonlinear optical properties. Optik, 2021, 231, 166464.	2.9	35
93	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
94	Spectroscopic Investigation of Laser-Produced Strontium Plasma Using Fundamental and Second Harmonics of Nd:YAG Laser. IEEE Transactions on Plasma Science, 2021, 49, 1564-1573.	1.3	1
95	Watch Out for the Tailings Pond, a Sharp Edge Hanging over Our Heads: Lessons Learned and Perceptions from the Brumadinho Tailings Dam Failure Disaster. Remote Sensing, 2021, 13, 1775.	4.0	24
96	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
97	DFT study of superhalogen-doped borophene with enhanced nonlinear optical properties. Journal of Molecular Modeling, 2021, 27, 188.	1.8	28
98	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
99	DFT study of therapeutic potential of graphitic carbon nitride (g-C ₃ N ₄) as a new drug delivery system for carboplatin to treat cancer. Journal of Molecular Liquids, 2021, 331, 115607.	4.9	51
100	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
101	The Effect of Emotional Intelligence and Academic Social Networking Sites on Academic Performance During the COVID-19 Pandemic. Psychology Research and Behavior Management, 2021, Volume 14, 905-920.	2.8	40
102	Pressure induced electronic, optical and thermoelectric properties of cubic SrZrO ₃ : DFT investigation. Physica B: Condensed Matter, 2021, 612, 412626.	2.7	25
103	Tuning the optoelectronic properties of oligothieryl silane derivatives and their photovoltaic properties. Journal of Molecular Graphics and Modelling, 2021, 106, 107918.	2.4	25
104	Structural, electronic, half-metallic ferromagnetic and optical properties of cubic MAIO ₃ (M=Ce, Pr) perovskites: A DFT study. Journal of Physics and Chemistry of Solids, 2021, 154, 110084.	4.0	37
105	Study of nonlinear optical properties of superhalogen and superalkali doped phosphorene. Journal of Molecular Structure, 2021, 1236, 130348.	3.6	18
106	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
107	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
108	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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109	DFT study of base catalyzed transesterification of tributyrin for biodiesel production. , 2021, , .		0
110	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
111	Pressure induced electronic, optical and thermoelectric properties of cubic BaZrO ₃ : A first principle calculations. Optik, 2021, 239, 166694.	2.9	25
112	Exploration of Nonlinear Optical Properties of Triphenylamine-Dicyanovinylene Coexisting Donor- π -Acceptor Architecture by the Modification of π -Conjugated Linker. Frontiers in Materials, 2021, 8, .	2.4	9
113	Quantum Chemical Approach of Donor- π -Acceptor Based Arylborane- π -Arylamine Macrocycles with Outstanding Photovoltaic Properties Toward High-Performance Organic Solar Cells. Energy & Fuels, 2021, 35, 15018-15032.	5.1	66
114	Efficient tuning of small acceptor chromophores with A1- π -A2- π -A1 configuration for high efficacy of organic solar cells via end group manipulation. Journal of Saudi Chemical Society, 2021, 25, 101305.	5.2	53
115	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
116	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
117	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
118	Tuning the optoelectronic properties of superalkali doped phosphorene. Journal of Molecular Graphics and Modelling, 2021, 107, 107973.	2.4	10
119	Designing and theoretical characterization of benzodithiophene dione based donor molecules for small molecule organic solar cells. Optik, 2021, 242, 167098.	2.9	24
120	Effects of Aromatic Thiol Capping Agents on the Structural and Electronic Properties of CdnTen (n =) Tj ETQq0 0 0 ggBT /Overlock 10 Tf	2.4	24
121	Computational and theoretical study of graphitic carbon nitride (g-C ₃ N ₄) as a drug delivery carrier for Ionidamine drug to treat cancer. Computational and Theoretical Chemistry, 2021, 1206, 113459.	2.5	10
122	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
123	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
124	Physical characteristics of barium based cubic perovskites. Chemical Physics Letters, 2021, 779, 138835.	2.6	11
125	Extremely large, linear, and controllable positive magnetoresistance in neodymium-doped graphene foam for magnetic sensors. Materials Today Physics, 2021, 20, 100460.	6.0	7
126	Computational study of therapeutic potential of phosphorene as a nano-carrier for drug delivery of neбиволol for the prohibition of cardiovascular diseases: a DFT study. Journal of Molecular Modeling, 2021, 27, 306.	1.8	8

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127	Physical characteristics of NaTaO ₃ Under pressure for electronic devices. <i>Materials Science in Semiconductor Processing</i> , 2021, 133, 105976.	4.0	11
128	Molecular engineering strategy of naphthalimide based small donor molecules for high-performance organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113416.	2.5	43
129	Optoelectronic properties of naphthalene bis-benzimidazole based derivatives and their photovoltaic applications. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113373.	2.5	21
130	Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications. <i>Chemical Physics Letters</i> , 2021, 782, 139018.	2.6	39
131	Designing and comparative analysis of 3D subphthalocyanines based non-fullerene acceptor molecules as an efficient material for organic solar cells. <i>Optik</i> , 2021, 246, 167845.	2.9	13
132	Structural, optical and photovoltaic properties of unfused Non-Fullerene acceptors for efficient solution processable organic solar cell (Estimated PCE > 12.4%): A DFT approach. <i>Journal of Molecular Liquids</i> , 2021, 341, 117428.	4.9	55
133	Tuning the optoelectronic properties of naphthodithiophene (NDT) for designing of A-D-A type photovoltaic materials. <i>Optik</i> , 2021, 247, 167892.	2.9	21
134	Empirical Investigation About the Factors Affecting the Cost Estimation in Global Software Development Context. <i>IEEE Access</i> , 2021, 9, 22274-22294.	4.2	17
135	Isatin-derived non-fullerene acceptors for efficient organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2021, 121, 105345.	4.0	38
136	Designing of 5,10-Dihydroindolo [3,2-b] Indole (DINI) Based Donor Materials for Small Molecule Organic Solar Cells. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 71-84.	1.7	17
137	Tuning the optoelectronic properties of ZOPTAN core-based derivatives by varying acceptors to increase efficiency of organic solar cell. <i>Journal of Molecular Modeling</i> , 2021, 27, 316.	1.8	20
138	Tuning of a A-A-D-A-Type Small Molecule with Benzodithiophene as a Central Core with Efficient Photovoltaic Properties for Organic Solar Cells. <i>ACS Omega</i> , 2021, 6, 28923-28935.	3.5	49
139	The theoretical investigation of the opto-electronic properties of designed molecules having 2-(2-Methylene-3-oxo-indane-1-ylidene)malononitrile as end-capped acceptors. <i>Zeitschrift Fur Physikalische Chemie</i> , 2021, 235, 785-804.	2.8	0
140	A Facile Approach for the Synthesis of SrTiO ₃ /g-C ₃ N ₄ Photocatalyst and its Efficacy in Biodiesel Production. <i>ChemistrySelect</i> , 2021, 6, 12082-12093.	1.5	6
141	Investigation of Fe-Doped Graphitic Carbon Nitride-Silver Tungstate as a Ternary Visible Light Active Photocatalyst. <i>Journal of Chemistry</i> , 2021, 2021, 1-18.	1.9	11
142	Secure IIoT-Enabled Industry 4.0. <i>Sustainability</i> , 2021, 13, 12384.	3.2	11
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