

List of Publications by Year in descending order

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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	Biodiesel production from waste cooking oil: An efficient technique to convert waste into biodiesel. <i>Sustainable Cities and Society</i> , 2018, 41, 220-226.	10.4	304
2	Designing Three-dimensional (3D) Non-Fullerene Small Molecule Acceptors with Efficient Photovoltaic Parameters. <i>ChemistrySelect</i> , 2018, 3, 12797-12804.	1.5	119
3	Designing N-phenylaniline-triazol configured donor materials with promising optoelectronic properties for high-efficiency solar cells. <i>Computational and Theoretical Chemistry</i> , 2020, 1186, 112908.	2.5	119
4	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells. <i>RSC Advances</i> , 2019, 9, 26402-26418.	3.6	115
5	Enhanced electronic and non-linear optical properties of alkali metal (Li, Na, K) doped boron nitride nano-cages. <i>Journal of Alloys and Compounds</i> , 2016, 687, 976-983.	5.5	102
6	Opto-electronic properties of non-fullerene fused-undecacyclic electron acceptors for organic solar cells. <i>Computational Materials Science</i> , 2019, 159, 150-159.	3.0	102
7	Designing indenothiophene-based acceptor materials with efficient photovoltaic parameters for fullerene-free organic solar cells. <i>Journal of Molecular Modeling</i> , 2020, 26, 137.	1.8	97
8	Enhancement in Photovoltaic Properties of <i>N,N</i> -diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. <i>ChemistrySelect</i> , 2020, 5, 5022-5034.	1.5	95
9	Designing of benzothiazole based non-fullerene acceptor (NFA) molecules for highly efficient organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020, 1181, 112833.	2.5	94
10	Phosphides or nitrides for better NLO properties? A detailed comparative study of alkali metal doped nano-cages. <i>Materials Research Bulletin</i> , 2017, 92, 113-122.	5.2	92
11	Density functional theory study of palladium cluster adsorption on a graphene support. <i>RSC Advances</i> , 2020, 10, 20595-20607.	3.6	86
12	Designing indacenodithiophene based non-fullerene acceptors with a donor-acceptor combined bridge for organic solar cells. <i>RSC Advances</i> , 2019, 9, 3605-3617.	3.6	83
13	Remarkable nonlinear optical response of alkali metal doped aluminum phosphide and boron phosphide nanoclusters. <i>Journal of Molecular Liquids</i> , 2018, 271, 51-64.	4.9	80
14	Tuning the optoelectronic properties of Subphthalocyanine (SubPc) derivatives for photovoltaic applications. <i>Optical Materials</i> , 2020, 107, 110154.	3.6	79
15	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
16	Designing alkoxy-induced based high performance near infrared sensitive small molecule acceptors for organic solar cells. <i>Journal of Molecular Liquids</i> , 2020, 305, 112829.	4.9	76
17	Benchmark study of the linear and nonlinear optical polarizabilities in proto-type NLO molecule of <i>p</i> -nitroaniline. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950030.	1.8	74
18	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

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19	Fine Tuning the Optoelectronic Properties of Triphenylamine Based Donor Molecules for Organic Solar Cells. <i>Zeitschrift Fur Physikalische Chemie</i> , 2017, 231, 1127-1139.	2.8	67
20	Designing Triphenylamine-Configured Donor Materials with Promising Photovoltaic Properties for Highly Efficient Organic Solar Cells. <i>ChemistrySelect</i> , 2020, 5, 7358-7369.	1.5	67
21	Quantum Chemical Approach of Donor-Acceptor Based Arylborane-Arylamine Macrocycles with Outstanding Photovoltaic Properties Toward High-Performance Organic Solar Cells. <i>Energy & Fuels</i> , 2021, 35, 15018-15032.	5.1	66
22	Development of fullerene free acceptors molecules for organic solar cells: A step way forward toward efficient organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2019, 1161, 26-38.	2.5	65
23	Theoretical study of the non linear optical properties of alkali metal (Li, Na, K) doped aluminum nitride nanocages. <i>RSC Advances</i> , 2016, 6, 94228-94235.	3.6	62
24	Tuning the optoelectronic properties of triphenylamine (TPA) based small molecules by modifying central core for photovoltaic applications. <i>Journal of Molecular Modeling</i> , 2021, 27, 237.	1.8	60
25	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
26	DFT study of the therapeutic potential of phosphorene as a new drug-delivery system to treat cancer. <i>RSC Advances</i> , 2019, 9, 24325-24332.	3.6	58
27	Designing dithienothiophene (DTT)-based donor materials with efficient photovoltaic parameters for organic solar cells. <i>Journal of Molecular Modeling</i> , 2019, 25, 222.	1.8	58
28	Spirobifluorene based small molecules as an alternative to traditional fullerene acceptors for organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2019, 94, 97-106.	4.0	58
29	Tuning opto-electronic properties of alkoxy-induced based electron acceptors in infrared region for high performance organic solar cells. <i>Journal of Molecular Liquids</i> , 2020, 298, 111963.	4.9	58
30	Exploring the new potential antiviral constituents of <i>Moringa oleifera</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
31	The energy crisis in Pakistan: A possible solution via biomass-based waste. <i>Journal of Renewable and Sustainable Energy</i> , 2016, 8, .	2.0	56
32	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
33	Designing of benzodithiophene acridine based Donor materials with favorable photovoltaic parameters for efficient organic solar cell. <i>Computational and Theoretical Chemistry</i> , 2021, 1200, 113238.	2.5	55
34	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
35	Design of donor-acceptor-donor (D-A-D) type small molecule donor materials with efficient photovoltaic parameters. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25363.	2.0	54
36	A DFT study of structural, magnetic, elastic and optoelectronic properties of lanthanide based XAlO ₃ (X=Nd, Gd) compounds. <i>Journal of Materials Research and Technology</i> , 2020, 9, 16488-16496.	5.8	54

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37	Efficient tuning of small acceptor chromophores with A1-İ€A2-İ€A1 configuration for high efficacy of organic solar cells via end group manipulation. <i>Journal of Saudi Chemical Society</i> , 2021, 25, 101305.	5.2	53
38	Designing dithienonaphthalene based acceptor materials with promising photovoltaic parameters for organic solar cells. <i>RSC Advances</i> , 2019, 9, 34496-34505.	3.6	52
39	A comparative study of DFT calculated and experimental UV/Visible spectra for thirty carboline and carbazole based compounds. <i>Journal of Molecular Structure</i> , 2017, 1149, 282-298.	3.6	51
40	Facile preparation, characterization, SC-XRD and DFT/DTDFT study of diversely functionalized unsymmetrical bis-aryl-İ±, İ²-unsaturated ketone derivatives. <i>Journal of Molecular Structure</i> , 2020, 1206, 127755.	3.6	51
41	DFT study of therapeutic potential of graphitic carbon nitride (g-C3N4) as a new drug delivery system for carboplatin to treat cancer. <i>Journal of Molecular Liquids</i> , 2021, 331, 115607.	4.9	51
42	Designing of benzodithiophene (BDT) based non-fullerene small molecules with favorable optoelectronic properties for proficient organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2021, 1203, 113359.	2.5	49
43	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. <i>ACS Omega</i> , 2021, 6, 28923-28935.	3.5	49
44	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
45	Therapeutic potential of graphyne as a new drug-delivery system for daunorubicin to treat cancer: A DFT study. <i>Journal of Molecular Liquids</i> , 2021, 336, 116327.	4.9	48
46	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
47	Designing of non-fullerene 3D star-shaped acceptors for organic solar cells. <i>Journal of Molecular Modeling</i> , 2019, 25, 129.	1.8	47
48	Enhanced linear and nonlinear optical response of superhalogen (Al7) doped graphitic carbon nitride (g-C3N4). <i>Optik</i> , 2021, 226, 165923.	2.9	46
49	Phase transition and thermoelectric properties of cubic KNbO3 under pressure: DFT approach. <i>Journal of Materials Research and Technology</i> , 2021, 11, 2106-2113.	5.8	46
50	End-capped group modification on cyclopentadithiophene based non-fullerene small molecule acceptors for efficient organic solar cells; a DFT approach. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 113, 108162.	2.4	46
51	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
52	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
53	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
54	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

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55	Bithieno Thiophene-Based Small Molecules for Application as Donor Materials for Organic Solar Cells and Hole Transport Materials for Perovskite Solar Cells. <i>ACS Omega</i> , 2022, 7, 844-862.	3.5	43
56	Theoretical Calculations of the Optical and Electronic Properties of Dithienosilole and Dithiophene-Based Donor Materials for Organic Solar Cells. <i>ChemistrySelect</i> , 2018, 3, 1593-1601.	1.5	42
57	The substitution effect of heterocyclic rings to tune the optical and nonlinear optical properties of hybrid chalcones: A comparative study. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 81, 25-31.	2.4	42
58	Thermal degradation behavior and X-ray diffraction studies of chitosan based polyurethane bio-nanocomposites using different diisocyanates. <i>International Journal of Biological Macromolecules</i> , 2018, 117, 762-772.	7.5	42
59	Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study. <i>Journal of Molecular Liquids</i> , 2020, 297, 111902.	4.9	42
60	Tuning the optoelectronic properties of dibenzochrysenes (DBC) based small molecules for organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2021, 127, 105689.	4.0	41
61	End-capped engineering of bipolar diketopyrrolopyrrole based small electron acceptor molecules for high performance organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113242.	2.5	40
62	Coal fly ash-based copper ferrite nanocomposites as potential heterogeneous photocatalysts for wastewater remediation. <i>Applied Surface Science</i> , 2021, 565, 150542.	6.1	40
63	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
64	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
65	Theoretical investigation of X_2NaIO_6 (X= Pb,Sr) double perovskites for thermoelectric and optoelectronic applications. <i>Physica B: Condensed Matter</i> , 2022, 630, 413694.	2.7	39
66	Designing 2D fused ring materials for small molecules organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020, 1183, 112848.	2.5	38
67	Isatin-derived non-fullerene acceptors for efficient organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2021, 121, 105345.	4.0	38
68	Coal fly ash supported $CoFe_2O_4$ nanocomposites: Synergetic Fenton-like and photocatalytic degradation of methylene blue. <i>Environmental Research</i> , 2022, 206, 112280.	7.5	38
69	Structural, electronic, half-metallic ferromagnetic and optical properties of cubic $MAIO_3$ (M=Ce, Pr) perovskites: A DFT study. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 154, 110084.	4.0	37
70	Designing of the indacenodithiophene core-based small molecules for optoelectronic applications: A DFT approach. <i>Solar Energy</i> , 2022, 237, 108-121.	6.1	37
71	Impact of end-capped modification of MO-IDT based non-fullerene small molecule acceptors to improve the photovoltaic properties of organic solar cells. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108255.	2.4	37
72	Linear and nonlinear optical discussions of nanostructured Zn-doped CdO thin films. <i>Physica B: Condensed Matter</i> , 2017, 511, 54-60.	2.7	36

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73	DFT study of superhalogen (AlF ₄) doped boron nitride for tuning their nonlinear optical properties. <i>Optik</i> , 2021, 231, 166464.	2.9	35
74	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
75	G-C ₃ N ₄ /Ag@CoWO ₄ : 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
76	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
77	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
78	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
79	Synthesis and characterization of stable and biological active chitin-based polyurethane elastomers. <i>International Journal of Biological Macromolecules</i> , 2020, 154, 1149-1157.	7.5	31
80	Designing and theoretical study of fluorinated small molecule donor materials for organic solar cells. <i>Journal of Molecular Modeling</i> , 2021, 27, 216.	1.8	31
81	End-capped modification of Y-Shaped dithienothiophen[3,2-b]-pyrrolobenzothiadiazole (TPBT) based non-fullerene acceptors for high performance organic solar cells by using DFT approach. <i>Surfaces and Interfaces</i> , 2022, 30, 101875.	3.0	31
82	Theoretical and computational study on electronic effect caused by electron withdrawing/electron-donating groups upon the coumarin thiourea derivatives. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113271.	2.5	29
83	Silver cluster doped graphyne (GY) with outstanding non-linear optical properties. <i>RSC Advances</i> , 2022, 12, 5466-5482.	3.6	29
84	DFT study of transition metals doped calix-4-pyrrole with excellent electronic and non-linear optical properties. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113767.	2.5	29
85	Designing indaceno thiophene-based three new molecules containing non-fullerene acceptors as strong electron withdrawing groups with DFT approaches. <i>Journal of Molecular Modeling</i> , 2019, 25, 311.	1.8	28
86	Facile synthesis, crystal growth, characterization and computational study of new pyridine-based halogenated hydrazones: Unveiling the stabilization behavior in terms of noncovalent interactions. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5399.	3.5	28
87	DFT study of superhalogen-doped borophene with enhanced nonlinear optical properties. <i>Journal of Molecular Modeling</i> , 2021, 27, 188.	1.8	28
88	Advanced Ag/rGO/TiO ₂ ternary nanocomposite based photoanode approaches to highly-efficient plasmonic dye-sensitized solar cells. <i>Optics Communications</i> , 2019, 453, 124408.	2.1	27
89	Molecular designing of four high performance pyrazine-based non-fullerene acceptor materials with naphthalene diimide-based small organic solar cells. <i>Journal of Molecular Modeling</i> , 2019, 25, 50.	1.8	26
90	Theoretical calculation of selenium N-heterocyclic carbene compounds through DFT studies: Synthesis, characterization and biological potential. <i>Journal of Molecular Structure</i> , 2020, 1204, 127462.	3.6	26

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91	Designing benzothiadiazole based highly efficient non-fullerene acceptor molecules for organic solar cells. <i>Polymer</i> , 2022, 238, 124405.	3.8	26
92	A Theoretical Perspective on Strategies for Modeling High Performance Nonlinear Optical Materials. <i>Frontiers in Materials</i> , 2021, 8, .	2.4	26
93	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
94	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
95	Benchmark study of benzamide derivatives and four novel theoretically designed (L1, L2, L3, and L4) ligands and evaluation of their biological properties by DFT approaches. <i>Journal of Molecular Modeling</i> , 2019, 25, 223.	1.8	25
96	Tuning the optoelectronic properties of oligothieryl silane derivatives and their photovoltaic properties. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 106, 107918.	2.4	25
97	Pressure induced electronic, optical and thermoelectric properties of cubic BaZrO ₃ : A first principle calculations. <i>Optik</i> , 2021, 239, 166694.	2.9	25
98	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. <i>Solar Energy</i> , 2022, 240, 38-56.	6.1	25
99	Designing and theoretical characterization of benzodithiophene dione based donor molecules for small molecule organic solar cells. <i>Optik</i> , 2021, 242, 167098.	2.9	24
100	Visible light active indigo dye/graphene/WO ₃ nanocomposites with excellent photocatalytic activity. <i>Journal of Materials Research and Technology</i> , 2019, 8, 3261-3269.	5.8	23
101	Tuning the optoelectronic properties of Benzo Thiophene (BT-CIC) based non-fullerene acceptor organic solar cell. <i>Journal of Theoretical and Computational Chemistry</i> , 2020, 19, 2050003.	1.8	23
102	Super alkali (OLi ₃) doped boron nitride with enhanced nonlinear optical behavior. <i>Journal of Nonlinear Optical Physics and Materials</i> , 2020, 29, 2050004.	1.8	23
103	Green Synthesis, SC-XRD, Non-Covalent Interactive Potential and Electronic Communication via DFT Exploration of Pyridine-Based Hydrazone. <i>Crystals</i> , 2020, 10, 778.	2.2	22
104	Improving energy harvesting efficiency of dye sensitized solar cell by using cobalt-rGO co-doped TiO ₂ photoanode. <i>Journal of Alloys and Compounds</i> , 2022, 891, 162040.	5.5	22
105	Optoelectronic properties of naphthalene bis-benzimidazole based derivatives and their photovoltaic applications. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113373.	2.5	21
106	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
107	Bulk Heterojunction Organic Solar Cells with Graphene Oxide Hole Transport Layer: Effect of Varied Concentration on Photovoltaic Performance. <i>Journal of Physical Chemistry C</i> , 2017, 121, 140-146.	3.1	20
108	Benchmark study of UV/Visible spectra of coumarin derivatives by computational approach. <i>Journal of Molecular Structure</i> , 2017, 1130, 603-616.	3.6	20

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109	Electronic, optical and magnetic properties of PrXO_3 ($\text{X} = \text{V}, \text{Cr}$): first-principle calculations. <i>Philosophical Magazine</i> , 2020, 100, 3125-3140.	1.6	20
110	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
111	A dual approach to study the synthesis, crystal structure and nonlinear optical properties of binuclear Pd(II) complex of 3-methyl-5-(trifluoromethyl) pyrazole and its potential quantum chemical analogues. <i>Inorganica Chimica Acta</i> , 2019, 494, 160-167.	2.4	19
112	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
113	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
114	Synergistic end-capped engineering on non-fused thiophene ring-based acceptors to enhance the photovoltaic properties of organic solar cells. <i>RSC Advances</i> , 2022, 12, 12321-12334.	3.6	19
115	Linear and non-linear optics of nano-scale 2×7 dichloro-fluorescein/FTO optical system: Bandgap and dielectric analysis. <i>Optical Materials</i> , 2016, 62, 527-533.	3.6	18
116	Tuning of optoelectronic properties of triphenylamines-based donor materials for organic solar cells. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950036.	1.8	18
117	Rational design of naphthalimide based small molecules non-fullerene acceptors for organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020, 1187, 112916.	2.5	18
118	Study of nonlinear optical properties of superhalogen and superalkali doped phosphorene. <i>Journal of Molecular Structure</i> , 2021, 1236, 130348.	3.6	18
119	Enhancement in non-linear optical properties of carbon nitride (C_2N) by doping superalkali (Li_3O): A DFT study. <i>Computational and Theoretical Chemistry</i> , 2022, 1211, 113654.	2.5	18
120	Investigation on the surface modification of TiO_2 nanohexagon arrays based photoanode with SnO_2 nanoparticles for highly-efficient dye-sensitized solar cells. <i>Materials Research Bulletin</i> , 2019, 109, 21-28.	5.2	17
121	Evaluation of mustard oil for the synthesis of biodiesel: Pretreatment and optimization study. <i>Environmental Progress and Sustainable Energy</i> , 2018, 37, 1829-1835.	2.3	17
122	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
123	DFT study of alkali and alkaline earth metal-doped benzocryptand with remarkable NLO properties. <i>RSC Advances</i> , 2022, 12, 16029-16045.	3.6	17
124	Triphenylamine based donor-acceptor-donor type small molecules for organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2021, 1198, 113176.	2.5	16
125	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
126	An arylene-vinylene based donor-acceptor-donor small molecule for the donor compound in high-voltage organic solar cells. <i>Solar Energy Materials and Solar Cells</i> , 2016, 155, 348-355.	6.2	14

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127	Tuning the Optoelectronic Properties of Naphthoâ€Dithiopheneâ€Based Aâ€Dâ€A Type Small Donor Molecules for Bulk Heteroâ€Junction Organic Solar Cells. <i>ChemistrySelect</i> , 2018, 3, 2352-2358.	1.5	14
128	Molecular designing of naphthalene diimide based fullerene-free small organic solar cell - Acceptors with high photovoltaic performance by density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117685.	3.9	14
129	Comparison of Photoâ€Esterification Capability of Bismuth Vanadate with Reduced Graphene Oxide Bismuth Vanadate (RGO/BiVO ₄) Composite for Biodiesel Production from High Free Fatty Acid Containing Nonâ€Edible Oil. <i>ChemistrySelect</i> , 2020, 5, 9245-9253.	1.5	14
130	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
131	Computational and theoretical study of subphthalocyanine based derivatives by varying acceptors to increase the efficiency of organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2021, 1203, 113356.	2.5	14
132	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
133	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
134	Depicting the role of end-capped acceptors to amplify the photovoltaic properties of benzothiadiazole core-based molecules for high-performance organic solar cell applications. <i>Computational and Theoretical Chemistry</i> , 2022, 1211, 113669.	2.5	14
135	Designing the optoelectronic properties of BODIPY and their photovoltaic applications for high performance of organic solar cells by using computational approach. <i>Materials Science in Semiconductor Processing</i> , 2022, 148, 106812.	4.0	14
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