

Javed Iqbal

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

306
papers

5,406
citations

38
h-index

56
g-index

333
ext. papers

7,517
ext. citations

3.5
avg, IF

6.55
L-index

#	Paper	IF	Citations
306	Shedding light on the optical and nonlinear optical properties of superalkali-doped borophene.. <i>Journal of Molecular Modeling</i> , 2022 , 28, 46	2	0
305	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	3.7	5
304	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	3.3	7
303	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, Switzerland)</i> , 2022 , 12,	2.3	2
302	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 , 1-14	1.9	1
301	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	6.8	9
300	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	6.8	12
299	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	2.8	6
298	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	3	3
297	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 , 132547	3.4	1
296	Tuning the optoelectronic properties of indacenodithiophene based derivatives for efficient photovoltaic applications: A DFT approach. <i>Chemical Physics Letters</i> , 2022 , 793, 139459	2.5	11
295	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	2.8	4
294	Designing benzothiadiazole based highly efficient non-fullerene acceptor molecules for organic solar cells. <i>Polymer</i> , 2022 , 238, 124405	3.9	5
293	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,	4.6	3
292	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	2
291	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	3.9	6
290	Tuning the optoelectronic properties of benzodithiophene based donor materials and their photovoltaic applications. <i>Materials Science in Semiconductor Processing</i> , 2022 , 137, 106150	4.3	15

289	Controlled supramolecular interaction to enhance the bioavailability of hesperetin to targeted cancer cells through graphyne: a comprehensive study.. <i>RSC Advances</i> , 2022 , 12, 6336-6346	3.7	1
288	Silver cluster doped graphyne (GY) with outstanding non-linear optical properties.. <i>RSC Advances</i> , 2022 , 12, 5466-5482	3.7	3
287	A Tacit-Knowledge-Based Requirements Elicitation Model Supporting COVID-19 Context. <i>IEEE Access</i> , 2022 , 10, 24481-24508	3.5	
286	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	3	4
285	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	3.4	0
284	Impact of Destination Image Formation on Tourist Trust: Mediating Role of Tourist Satisfaction.. <i>Frontiers in Psychology</i> , 2022 , 13, 845538	3.4	0
283	Designing phenyl-di-p-tolyl-amine-based asymmetric small molecular donor materials with favorable photovoltaic parameters. <i>Optik</i> , 2022 , 256, 168739	2.5	1
282	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	3.9	1
281	Enhancement in non-linear optical properties of carbon nitride (C ₂ N) by doping superalkali (Li ₃ O): A DFT study. <i>Computational and Theoretical Chemistry</i> , 2022 , 1211, 113654	2	1
280	Designing of the indacenodithiophene core-based small molecules for optoelectronic applications: A DFT approach. <i>Solar Energy</i> , 2022 , 237, 108-121	6.8	7
279	Engineering of A2-D-A1-D-A2 type BT-dIDT based non-fullerene acceptors for effective organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2022 , 1211, 113666	2	3
278	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	6
277	Quantum chemical approach to study TIPSTAP derivatives with anticipated minimized crystal roughness for photovoltaic application with estimated PCE of over 20%. <i>Solar Energy</i> , 2022 , 237, 96-107	6.8	0
276	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	4.1	10
275	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	2.8	11
274	Synthesis, photophysical, electrochemical and computational studies of novel 2-aminoimidazolones with D- π A framework. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022 , 429, 113918	4.7	0
273	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	3.9	5
272	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	3.7	5

271	Symmetrical end-capped molecular engineering of star-shaped triphenylamine-based derivatives having remarkable photovoltaic properties for efficient organic solar cells.. <i>Journal of Molecular Modeling</i> , 2022 , 28, 132	2	
270	Effect of Despotic Leadership on Employee Turnover Intention: Mediating Toxic Workplace Environment and Cognitive Distraction in Academic Institutions. <i>Behavioral Sciences (Basel, Switzerland)</i> , 2022 , 12, 125	2.3	0
269	Tuning the optoelectronic properties of cross conjugated small molecules using benzodithiophene as a core unit with favorable photovoltaic parameters: a DFT study. <i>Journal Physics D: Applied Physics</i> , 2022 , 55, 295106	3	0
268	How curriculum delivery translates into entrepreneurial skills: The mediating role of knowledge of information and communication technology.. <i>PLoS ONE</i> , 2022 , 17, e0265880	3.7	1
267	A DFT approach towards therapeutic potential of phosphorene as a novel carrier for the delivery of felodipine (cardiovascular drug). <i>Computational and Theoretical Chemistry</i> , 2022 , 1212, 113724	2	1
266	Remarkable non-linear optical properties of gold cluster doped graphyne (GY): A DFT study.. <i>Journal of Molecular Graphics and Modelling</i> , 2022 , 114, 108204	2.8	0
265	Impact of side-chain engineering on the A-ED-EA type SM-BF1 donor molecule for bulk heterojunction and their photovoltaic performance: A DFT approach. <i>Solar Energy</i> , 2022 , 240, 38-56	6.8	4
264	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. <i>Computational and Theoretical Chemistry</i> , 2022 , 1213, 113747	2	2
263	DFT study of alkali and alkaline earth metal-doped benzocryptand with remarkable NLO properties. <i>RSC Advances</i> , 2022 , 12, 16029-16045	3.7	1
262	DFT study of transition metals doped calix-4-pyrrole with excellent electronic and non-linear optical properties. <i>Computational and Theoretical Chemistry</i> , 2022 , 113767	2	1
261	Engineering of A-ED-EA system based non-fullerene acceptors to enhance the photovoltaic properties of organic solar cells; A DFT Approach. <i>Chemical Physics Letters</i> , 2022 , 139750	2.5	3
260	Quantum chemical simulations of benzothiadiazole (BT) based small molecule donor materials for efficient organic solar cells. <i>Chemical Physics Letters</i> , 2022 , 801, 139726	2.5	1
259	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	4.3	4
258	A Theoretical Perspective on Strategies for Modeling High Performance Nonlinear Optical Materials. <i>Frontiers in Materials</i> , 2021 , 8,	4	4
257	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		7
256	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	3.1	
255	DFT study of OLi3 and MgF3 doped boron nitride with enhanced nonlinear optical behavior. <i>Journal of Molecular Structure</i> , 2021 , 1251, 131934	3.4	1
254	A Facile Approach for the Synthesis of SrTiO3/g-C3N4 Photo-catalyst and its Efficacy in Biodiesel Production. <i>ChemistrySelect</i> , 2021 , 6, 12082-12093	1.8	1

253	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	2.3	0
252	Secure IIoT-Enabled Industry 4.0. <i>Sustainability</i> , 2021 , 13, 12384	3.6	2
251	Production of Biodiesel from <i>Spirogyra elongata</i> , a Common Freshwater Green Algae with High Oil Content. <i>Sustainability</i> , 2021 , 13, 12737	3.6	2
250	End-capped modification of dithienosilole based small donor molecules for high performance organic solar cells using DFT approach. <i>Journal of Molecular Liquids</i> , 2021 , 345, 118138	6	17
249	Raman spectroscopic characterization of selenium N-heterocyclic carbene compounds.. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021 , 270, 120823	4.4	0
248	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	2	9
247	Tuning of a A-A-D-A-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	3.9	12
246	Synthesis in combination with Biological and Computational evaluations of selenium-N-Heterocyclic Carbene compounds. <i>Computational and Theoretical Chemistry</i> , 2021 , 1197, 113135	2	3
245	Investigation of optical and thermoelectric properties of PbTiO ₃ under pressure. <i>Physica B: Condensed Matter</i> , 2021 , 615, 412857	2.8	2
244	Designing of small molecule non-fullerene acceptors with cyanobenzene core for photovoltaic application. <i>Computational and Theoretical Chemistry</i> , 2021 , 1197, 113154	2	18
243	Exploring the new potential antiviral constituents of <i>Moringa oliefera</i> for SARS-COV-2 pathogenesis: An molecular docking and dynamic studies. <i>Chemical Physics Letters</i> , 2021 , 767, 138379	2.5	22
242	Theoretical investigation of supramolecular hydrogen-bonded choline chloride-based deep eutectic solvents using density functional theory. <i>Chemical Physics Letters</i> , 2021 , 769, 138427	2.5	22
241	Triphenylamine based donor-acceptor-donor type small molecules for organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2021 , 1198, 113176	2	7
240	DFT study of superhalogen (AlF ₄) doped boron nitride for tuning their nonlinear optical properties. <i>Optik</i> , 2021 , 231, 166464	2.5	12
239	Spectroscopic Investigation of Laser-Produced Strontium Plasma Using Fundamental and Second Harmonics of Nd:YAG Laser. <i>IEEE Transactions on Plasma Science</i> , 2021 , 49, 1564-1573	1.3	
238	Watch Out for the Tailings Pond, a Sharp Edge Hanging over Our Heads: Lessons Learned and Perceptions from the Brumadinho Tailings Dam Failure Disaster. <i>Remote Sensing</i> , 2021 , 13, 1775	5	7
237	Designing of cyanobenzene based small molecules with suitable photovoltaic parameters for organic solar cells. <i>International Journal of Quantum Chemistry</i> , 2021 , 121, e26673	2.1	2
236	DFT study of superhalogen-doped borophene with enhanced nonlinear optical properties. <i>Journal of Molecular Modeling</i> , 2021 , 27, 188	2	9

235	Tuning the optoelectronic properties of dibenzochrysene (DBC) based small molecules for organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2021 , 127, 105689	4.3	16
234	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. <i>Journal of Molecular Liquids</i> , 2021 , 331, 115607	6	19
233	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		29
232	The Effect of Emotional Intelligence and Academic Social Networking Sites on Academic Performance During the COVID-19 Pandemic. <i>Psychology Research and Behavior Management</i> , 2021 , 14, 905-920	3.8	14
231	Pressure induced electronic, optical and thermoelectric properties of cubic SrZrO ₃ : DFT investigation. <i>Physica B: Condensed Matter</i> , 2021 , 612, 412626	2.8	3
230	Tuning the optoelectronic properties of oligothieryl silane derivatives and their photovoltaic properties. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 106, 107918	2.8	8
229	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	3.9	13
228	Study of nonlinear optical properties of superhalogen and superalkali doped phosphorene. <i>Journal of Molecular Structure</i> , 2021 , 1236, 130348	3.4	5
227	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	8
226	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	20
225	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	2.5	16
224	O-4-Acetylamino-benzenesulfonylated pyrimidine derivatives: synthesis, SC-XRD, DFT analysis and electronic behaviour investigation. <i>Journal of Molecular Structure</i> , 2021 , 1224, 129308	3.4	15
223	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	2.8	5
222	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	4.4	6
221	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	2.5	18
220	Use of hydrogen-bonded supramolecular eutectic solvents for eco-friendly extraction of bioactive molecules from <i>Cymbopogon citratus</i> using BoxBehnken design. <i>Journal of Food Measurement and Characterization</i> , 2021 , 15, 1487-1498	2.8	3
219	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	3.1	4
218	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	3.5	1

217	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	2	14
216	DFT study of superhalogen and superalkali doped graphitic carbon nitride and its non-linear optical properties.. <i>RSC Advances</i> , 2021 , 11, 7779-7789	3.7	18
215	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,	4.6	40
214	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	5.5	10
213	Designing and theoretical study of fluorinated small molecule donor materials for organic solar cells. <i>Journal of Molecular Modeling</i> , 2021 , 27, 216	2	14
212	Tris-isopropyl-sily-ethynyl anthracene based small molecules for organic solar cells with efficient photovoltaic parameters. <i>Computational and Theoretical Chemistry</i> , 2021 , 1202, 113305	2	3
211	Pressure induced electronic, optical and thermoelectric properties of cubic BaZrO ₃ : A first principle calculations. <i>Optik</i> , 2021 , 239, 166694	2.5	4
210	Exploration of Nonlinear Optical Properties of Triphenylamine-Dicyanovinylene Coexisting Donor-Acceptor Architecture by the Modification of EConjugated Linker. <i>Frontiers in Materials</i> , 2021 , 8,	4	3
209	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	4.1	19
208	Efficient tuning of small acceptor chromophores with A1-EA2-EA1 configuration for high efficacy of organic solar cells via end group manipulation. <i>Journal of Saudi Chemical Society</i> , 2021 , 25, 101305	4.3	11
207	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	2	28
206	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	6	15
205	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	4
204	Tuning the optoelectronic properties of superalkali doped phosphorene. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 107, 107973	2.8	4
203	Investigating the nexus between critical success factors, despotic leadership, and success of renewable energy projects. <i>Environmental Science and Pollution Research</i> , 2021 , 1	5.1	11
202	Designing and theoretical characterization of benzodithiophene dione based donor molecules for small molecule organic solar cells. <i>Optik</i> , 2021 , 242, 167098	2.5	14
201	Computational and theoretical study of graphitic carbon nitride (g-C ₃ N ₄) as a drug delivery carrier for lonidamine drug to treat cancer. <i>Computational and Theoretical Chemistry</i> , 2021 , 1206, 113459	2	1
200	Electro-optical and charge transport properties of chalcone derivatives using a dual approach from molecule to material level simulations. <i>Computational and Theoretical Chemistry</i> , 2021 , 1203, 113349	2	5

199	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	22
198	Physical characteristics of barium based cubic perovskites. <i>Chemical Physics Letters</i> , 2021 , 779, 138835	2.5	2
197	Extremely large, linear, and controllable positive magnetoresistance in neodymium-doped graphene foam for magnetic sensors. <i>Materials Today Physics</i> , 2021 , 20, 100460	8	2
196	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. <i>Journal of Molecular Modeling</i> , 2021 , 27, 306	2	3
195	Physical characteristics of NaTaO ₃ Under pressure for electronic devices. <i>Materials Science in Semiconductor Processing</i> , 2021 , 133, 105976	4.3	2
194	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	13
193	Optoelectronic properties of naphthalene bis-benzimidazole based derivatives and their photovoltaic applications. <i>Computational and Theoretical Chemistry</i> , 2021 , 1204, 113373	2	7
192	Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications. <i>Chemical Physics Letters</i> , 2021 , 782, 139018	2.5	14
191	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	2.5	5
190	Structural, optical and photovoltaic properties of unfused Non-Fullerene acceptors for efficient solution processable organic solar cell (Estimated PCE \geq 2.4%): A DFT approach. <i>Journal of Molecular Liquids</i> , 2021 , 341, 117428	6	18
189	Tuning the optoelectronic properties of naphthodithiophene (NDT) for designing of A-D-A type photovoltaic materials. <i>Optik</i> , 2021 , 247, 167892	2.5	7
188	Empirical Investigation About the Factors Affecting the Cost Estimation in Global Software Development Context. <i>IEEE Access</i> , 2021 , 9, 22274-22294	3.5	9
187	Isatin-derived non-fullerene acceptors for efficient organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2021 , 121, 105345	4.3	19
186	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	5.5	16
185	Enhancement of optical signal and characterization of palladium plasma by magnetic field-assisted laser-induced breakdown spectroscopy. <i>Optik</i> , 2020 , 224, 165746	2.5	4
184	Enhancement in Photovoltaic Properties of N,N-diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. <i>ChemistrySelect</i> , 2020 , 5, 5022-5034	1.8	58
183	Surface modification of PET fabric by plasma pre-treatment for long-lasting permethrin deposition. <i>Polymers for Advanced Technologies</i> , 2020 , 31, 2229	3.2	1
182	Designing indenothiophene-based acceptor materials with efficient photovoltaic parameters for fullerene-free organic solar cells. <i>Journal of Molecular Modeling</i> , 2020 , 26, 137	2	62

181	Density functional theory study of palladium cluster adsorption on a graphene support.. <i>RSC Advances</i> , 2020 , 10, 20595-20607	3.7	53
180	Designing 2D fused ring materials for small molecules organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020 , 1183, 112848	2	23
179	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	62
178	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	6	25
177	NOVEL ACTIVE SCREEN PLASMA NITRIDING OF ALUMINUM USING ALUMINUM CATHODIC CAGE. <i>Surface Review and Letters</i> , 2020 , 27, 1950205	1.1	2
176	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	16
175	Computational and experimental study of heterofunctional azo reactive dyes synthesized for cellulosic fabric. <i>Journal of Molecular Structure</i> , 2020 , 1221, 128753	3.4	4
174	Designing Triphenylamine-Configured Donor Materials with Promising Photovoltaic Properties for Highly Efficient Organic Solar Cells. <i>ChemistrySelect</i> , 2020 , 5, 7358-7369	1.8	43
173	Tuning the optoelectronic properties of Subphthalocyanine (SubPc) derivatives for photovoltaic applications. <i>Optical Materials</i> , 2020 , 107, 110154	3.3	44
172	Rational design of naphthalimide based small molecules non-fullerene acceptors for organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020 , 1187, 112916	2	9
171	. <i>IEEE Access</i> , 2020 , 8, 53972-53983	3.5	57
170	Comparison of excitation mechanisms and the corresponding emission spectra in femto second and nano second laser-induced breakdown spectroscopy in reduced ambient air and their performances in surface analysis. <i>Journal of Laser Applications</i> , 2020 , 32, 012014	2.1	2
169	Preparation and energy consumption evaluation of bifunctional energy-efficient glass with superior superhydrophobic and heat shielding properties. <i>Energy and Buildings</i> , 2020 , 215, 109913	7	4
168	Improved Mechanical Properties, Wear and Corrosion Resistance of 316L Steel by Homogeneous Chromium Nitride Layer Synthesis Using Plasma Nitriding. <i>Journal of Materials Engineering and Performance</i> , 2020 , 29, 877-889	1.6	11
167	Duplex plasma treatment of AISI D2 tool steel by combining plasma nitriding (with and without white layer) and post-oxidation. <i>Surface and Coatings Technology</i> , 2020 , 385, 125420	4.4	11
166	Design, synthesis and application of triazole ligands in suzuki miyaura cross coupling reaction of aryl chlorides. <i>Journal of Molecular Structure</i> , 2020 , 1206, 127753	3.4	11
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12	Microbial biomass, and dissolved organic carbon and nitrogen strongly affect soil respiration in different land uses: A case study at Three Gorges Reservoir Area, South China. <i>Agriculture, Ecosystems and Environment</i> , 2010 , 137, 294-307	5.7	131
11	Design and in vitro evaluation of a novel polymeric P-glycoprotein (P-gp) inhibitor. <i>Journal of Controlled Release</i> , 2010 , 147, 62-9	11.7	38
10	CO ₂ emission in a subtropical red paddy soil (Ultisol) as affected by straw and N-fertilizer applications: A case study in Southern China. <i>Agriculture, Ecosystems and Environment</i> , 2009 , 131, 292-302	5.7	111
9	Carbon dioxide emissions from Ultisol under different land uses in mid-subtropical China. <i>Geoderma</i> , 2009 , 152, 63-73	6.7	49
8	Differences in soil CO ₂ flux between different land use types in mid-subtropical China. <i>Soil Biology and Biochemistry</i> , 2008 , 40, 2324-2333	7.5	103
7	Applications of graphene-based tungsten oxide nanocomposites: a review. <i>Journal of Nanostructure in Chemistry</i> , 1	7.6	2
6	Identification of Halogen-Based Derivatives as Potent Inhibitors of Estrogen Receptor Alpha of Breast Cancer: An In-Silico Investigation. <i>Journal of Computational Biophysics and Chemistry</i> , 1-25		1
5	Dopant Free Triphenylamine-Based Hole Transport Materials with Excellent Photovoltaic Properties for High-Performance Perovskite Solar Cells. <i>Energy Technology</i> , 2100838	3.5	3
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3	A DFT Study of Graphitic Carbon nitride as Drug Delivery Carrier for Flutamide (Anticancer Drug). <i>Journal of Computational Biophysics and Chemistry</i> ,		3
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1	Virtual screening of potential inhibitor against breast cancer-causing estrogen receptor alpha (ER α) by molecular docking and dynamic simulations. <i>Molecular Simulation</i> ,1-12	2	1
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