Javed Iqbal

List of Publications by Citations

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	Biodiesel production from waste cooking oil: An efficient technique to convert waste into biodiesel. *Sustainable Cities and Society*, **2018**, 41, 220-226	10.1	200
305	Preactivated thiomers as mucoadhesive polymers for drug delivery. *Biomaterials*, **2012**, 33, 1528-35	15.6	149
304	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. *Agriculture, Ecosystems and Environment*, **2010**, 137, 294-307	5.7	131
303	Multistimuli-responsive benzothiadiazole-cored phenylene vinylene derivative with nanoassembly properties. *Langmuir*, **2011**, 27, 6323-9	4	128
302	Iron, copper and silver nanoparticles: Green synthesis using green and black tea leaves extracts and evaluation of antibacterial, antifungal and aflatoxin B1 adsorption activity. *LWT - Food Science and Technology*, **2018**, 90, 98-107	5.4	124
301	CO2 emission in a subtropical red paddy soil (Ultisol) as affected by straw and N-fertilizer applications: A case study in Southern China. *Agriculture, Ecosystems and Environment*, **2009**, 131, 292-302	5.7	111
300	Differences in soil CO2 flux between different land use types in mid-subtropical China. *Soil Biology and Biochemistry*, **2008**, 40, 2324-2333	7.5	103
299	Thiolated chitosan nanoparticles for the nasal administration of leuprolide: bioavailability and pharmacokinetic characterization. *International Journal of Pharmaceutics*, **2012**, 428, 164-70	6.5	87
298	Enhanced electronic and non-linear optical properties of alkali metal (Li, Na, K) doped boron nitride nano-cages. *Journal of Alloys and Compounds*, **2016**, 687, 976-983	5.7	72
297	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells.. *RSC Advances*, **2019**, 9, 26402-26418	3.7	68
296	N2O emissions from different land uses in mid-subtropical China. *Agriculture, Ecosystems and Environment*, **2010**, 136, 40-48	5.7	67
295	Designing Three-dimensional (3D) Non-Fullerene Small Molecule Acceptors with Efficient Photovoltaic Parameters. *ChemistrySelect*, **2018**, 3, 12797-12804	1.8	66
294	Phosphides or nitrides for better NLO properties? A detailed comparative study of alkali metal doped nano-cages. *Materials Research Bulletin*, **2017**, 92, 113-122	5.1	64
293	Microcrystalline cellulose, lactose and lignin blends: Process mapping of dry granulation via roll compaction. *Powder Technology*, **2019**, 341, 38-50	5.2	63
292	Designing indenothiophene-based acceptor materials with efficient photovoltaic parameters for fullerene-free organic solar cells. *Journal of Molecular Modeling*, **2020**, 26, 137	2	62
291	Designing N-phenylaniline-triazol configured donor materials with promising optoelectronic properties for high-efficiency solar cells. *Computational and Theoretical Chemistry*, **2020**, 1186, 112908	2	62
290	Enhancement in Photovoltaic Properties of N,N-diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. *ChemistrySelect*, **2020**, 5, 5022-5034	1.8	58

289	Synthesis and Characterization of Poly(2-hydroxyethylmethacrylate) Contact Lenses Containing Chitosan Nanoparticles as an Ocular Delivery System for Dexamethasone Sodium Phosphate. *Pharmaceutical Research*, **2016**, 33, 1638-48	4.5	58
288	Understanding the DayCent model: Calibration, sensitivity, and identifiability through inverse modeling. *Environmental Modelling and Software*, **2015**, 66, 110-130	5.2	57
287	. *IEEE Access*, **2020**, 8, 53972-53983	3.5	57
286	Remarkable nonlinear optical response of alkali metal doped aluminum phosphide and boron phosphide nanoclusters. *Journal of Molecular Liquids*, **2018**, 271, 51-64	6	57
285	Development and in vivo evaluation of an oral drug delivery system for paclitaxel. *Biomaterials*, **2011**, 32, 170-5	15.6	56
284	Density functional theory study of palladium cluster adsorption on a graphene support.. *RSC Advances*, **2020**, 10, 20595-20607	3.7	53
283	Designing of benzothiazole based non-fullerene acceptor (NFA) molecules for highly efficient organic solar cells. *Computational and Theoretical Chemistry*, **2020**, 1181, 112833	2	51
282	Thiolated chitosan: development and in vivo evaluation of an oral delivery system for leuprolide. *European Journal of Pharmaceutics and Biopharmaceutics*, **2012**, 80, 95-102	5.7	49
281	Carbon dioxide emissions from Ultisol under different land uses in mid-subtropical China. *Geoderma*, **2009**, 152, 63-73	6.7	49
280	Fungal endophyte infection increases carbon sequestration potential of southeastern USA tall fescue stands. *Soil Biology and Biochemistry*, **2012**, 44, 81-92	7.5	48
279	Marine bioactive peptides: Types, structures, and physiological functions. *Food Reviews International*, **2017**, 33, 44-61	5.5	47
278	Maize and soybean root front velocity and maximum depth in Iowa, USA. *Field Crops Research*, **2018**, 215, 122-131	5.5	47
277	Opto-electronic properties of non-fullerene fused-undecacyclic electron acceptors for organic solar cells. *Computational Materials Science*, **2019**, 159, 150-159	3.2	46
276	Theoretical study of the non linear optical properties of alkali metal (Li, Na, K) doped aluminum nitride nanocages. *RSC Advances*, **2016**, 6, 94228-94235	3.7	45
275	Tuning the optoelectronic properties of Subphthalocyanine (SubPc) derivatives for photovoltaic applications. *Optical Materials*, **2020**, 107, 110154	3.3	44
274	Evaluation of photoacoustic infrared spectroscopy for simultaneous measurement of N2 O and CO2 gas concentrations and fluxes at the soil surface. *Global Change Biology*, **2013**, 19, 327-36	11.4	44
273	Designing Triphenylamine-Configured Donor Materials with Promising Photovoltaic Properties for Highly Efficient Organic Solar Cells. *ChemistrySelect*, **2020**, 5, 7358-7369	1.8	43
272	Development of stability-enhanced ternary solid dispersions via combinations of HPMCP and Soluplus processed by hot melt extrusion. *International Journal of Pharmaceutics*, **2017**, 532, 603-611	6.5	43

271	Designing indacenodithiophene based non-fullerene acceptors with a donor-acceptor combined bridge for organic solar cells.. *RSC Advances*, **2019**, 9, 3605-3617	3.7	40
270	How Toxic Workplace Environment Effects the Employee Engagement: The Mediating Role of Organizational Support and Employee Wellbeing. *International Journal of Environmental Research and Public Health*, **2021**, 18,	4.6	40
269	In vivo evaluation of an oral drug delivery system for peptides based on S-protected thiolated chitosan. *Journal of Controlled Release*, **2012**, 160, 477-85	11.7	38
268	Design and in vitro evaluation of a novel polymeric P-glycoprotein (P-gp) inhibitor. *Journal of Controlled Release*, **2010**, 147, 62-9	11.7	38
267	Preactivated thiomers: permeation enhancing properties. *International Journal of Pharmaceutics*, **2012**, 438, 217-24	6.5	36
266	Fine Tuning the Optoelectronic Properties of Triphenylamine Based Donor Molecules for Organic Solar Cells. *Zeitschrift Fur Physikalische Chemie*, **2017**, 231, 1127-1139	3.1	35
265	The substitution effect of heterocyclic rings to tune the optical and nonlinear optical properties of hybrid chalcones: A comparative study. *Journal of Molecular Graphics and Modelling*, **2018**, 81, 25-31	2.8	34
264	Design of donor□acceptor□donor (D□A□D) type small molecule donor materials with efficient photovoltaic parameters. *International Journal of Quantum Chemistry*, **2017**, 117, e25363	2.1	33
263	Facile preparation, characterization, SC-XRD and DFT/DTDFT study of diversely functionalized unsymmetrical bis-aryl-□□unsaturated ketone derivatives. *Journal of Molecular Structure*, **2020**, 1206, 127755	3.4	33
262	Nitrous oxide emissions from yellow brown soil as affected by incorporation of crop residues with different carbon-to-nitrogen ratios: a case study in central China. *Archives of Environmental Contamination and Toxicology*, **2013**, 65, 183-92	3.2	33
261	Therapeutic potential of graphitic carbon nitride as a drug delivery system for cisplatin (anticancer drug): A DFT approach. *Biophysical Chemistry*, **2020**, 267, 106461	3.5	33
260	Effects of laser wavelengths and pulse energy ratio on the emission enhancement in dual pulse LIBS. *Laser Physics Letters*, **2015**, 12, 066102	1.5	32
259	Benchmark study of the linear and nonlinear optical polarizabilities in proto-type NLO molecule of para-nitroaniline. *Journal of Theoretical and Computational Chemistry*, **2019**, 18, 1950030	1.8	32
258	Development of fullerene free acceptors molecules for organic solar cells: A step way forward toward efficient organic solar cells. *Computational and Theoretical Chemistry*, **2019**, 1161, 26-38	2	31
257	Fungal endophyte presence and genotype affect plant diversity and soil-to-atmosphere trace gas fluxes. *Plant and Soil*, **2013**, 364, 15-27	4.2	31
256	Differences in nitrous oxide fluxes from red soil under different land uses in mid-subtropical China. *Agriculture, Ecosystems and Environment*, **2012**, 146, 168-178	5.7	31
255	Laser induced breakdown spectroscopy methods and applications: A comprehensive review. *Radiation Physics and Chemistry*, **2020**, 170, 108666	2.5	31
254	Extreme weather-year sequences have nonadditive effects on environmental nitrogen losses. *Global Change Biology*, **2018**, 24, e303-e317	11.4	31

253	Thiolated chitosans: influence of various sulfhydryl ligands on permeation-enhancing and P-gp inhibitory properties. *Drug Development and Industrial Pharmacy*, **2011**, 37, 648-55	3.6	30
252	DFT study of the therapeutic potential of phosphorene as a new drug-delivery system to treat cancer.. *RSC Advances*, **2019**, 9, 24325-24332	3.7	29
251	Designing dithienothiophene (DTT)-based donor materials with efficient photovoltaic parameters for organic solar cells. *Journal of Molecular Modeling*, **2019**, 25, 222	2	29
250	Designing of benzodithiophene acridine based Donor materials with favorable photovoltaic parameters for efficient organic solar cell. *Computational and Theoretical Chemistry*, **2021**, 1200, 113238	2	29
249	Failure Mechanism and Stability Analysis of an Active Landslide in the Xiangjiaba Reservoir Area, Southwest China. *Journal of Earth Science (Wuhan, China)*, **2018**, 29, 646-661	2.2	28
248	Tuning the optoelectronic properties of triphenylamine (TPA) based small molecules by modifying central core for photovoltaic applications. *Journal of Molecular Modeling*, **2021**, 27, 237	2	28
247	Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study. *Journal of Molecular Liquids*, **2020**, 297, 111902	6	27
246	Surface modification of M2 steel by combination of cathodic cage plasma deposition and magnetron sputtered MoS2-TiN multilayer coatings. *Surface and Coatings Technology*, **2020**, 384, 125327	4.4	27
245	Spirobifluorene based small molecules as an alternative to traditional fullerene acceptors for organic solar cells. *Materials Science in Semiconductor Processing*, **2019**, 94, 97-106	4.3	26
244	Incidence of aflatoxins contamination in dry fruits and edible nuts collected from Pakistan. *Food Control*, **2017**, 78, 169-175	6.2	25
243	On the use of laser induced breakdown spectroscopy to characterize the naturally existing crystal in Pakistan and its optical emission spectrum. *Spectrochimica Acta, Part B: Atomic Spectroscopy*, **2015**, 111, 80-86	3.1	25
242	Designing alkoxy-induced based high performance near infrared sensitive small molecule acceptors for organic solar cells. *Journal of Molecular Liquids*, **2020**, 305, 112829	6	25
241	Thermal degradation behavior and X-ray diffraction studies of chitosan based polyurethane bio-nanocomposites using different diisocyanates. *International Journal of Biological Macromolecules*, **2018**, 117, 762-772	7.9	25
240	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	6	24
239	Mechanistic modelling of industrial-scale roller compactor Freund TF-MINI model *Computers and Chemical Engineering*, **2017**, 104, 141-150	4	23
238	Designing 2D fused ring materials for small molecules organic solar cells. *Computational and Theoretical Chemistry*, **2020**, 1183, 112848	2	23
237	Enhanced wear and corrosion resistance of AISI-304 steel by duplex cathodic cage plasma treatment. *Surface and Coatings Technology*, **2019**, 375, 34-45	4.4	23
236	Survey of four models of probability density functions of wind speed and directions by adaptive neuro-fuzzy methodology. *Advances in Engineering Software*, **2014**, 76, 148-153	3.6	23

235	Designing dithienonaphthalene based acceptor materials with promising photovoltaic parameters for organic solar cells.. *RSC Advances*, **2019**, 9, 34496-34505	3.7	23
234	Theoretical Calculations of the Optical and Electronic Properties of Dithienosilole- and Dithiophene-Based Donor Materials for Organic Solar Cells. *ChemistrySelect*, **2018**, 3, 1593-1601	1.8	22
233	Efficient MRI labeling of endothelial progenitor cells: design of thiolated surface stabilized superparamagnetic iron oxide nanoparticles. *European Journal of Pharmaceutics and Biopharmaceutics*, **2013**, 85, 346-55	5.7	22
232	A comparative study of DFT calculated and experimental UV/Visible spectra for thirty carboline and carbazole based compounds. *Journal of Molecular Structure*, **2017**, 1149, 282-298	3.4	22
231	Denitrification and Nitrous Oxide Emissions in Annual Croplands, Perennial Grass Buffers, and Restored Perennial Grasslands. *Soil Science Society of America Journal*, **2015**, 79, 239-250	2.5	22
230	Exploring the new potential antiviral constituents of Moringa oliefera for SARS-COV-2 pathogenesis: An molecular docking and dynamic studies. *Chemical Physics Letters*, **2021**, 767, 138379	2.5	22
229	Theoretical investigation of supramolecular hydrogen-bonded choline chloride-based deep eutectic solvents using density functional theory. *Chemical Physics Letters*, **2021**, 769, 138427	2.5	22
228	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	22
227	Development and validation of a high-performance liquid chromatography method with post-column derivatization for the detection of aflatoxins in cereals and grains. *Toxicology and Industrial Health*, **2016**, 32, 1122-34	1.8	21
226	Poly(acrylic acid)-cysteine for oral vitamin B12 delivery. *Analytical Biochemistry*, **2012**, 420, 13-9	3.1	21
225	Facile synthesis, crystal growth, characterization and computational study of new pyridine-based halogenated hydrazones: Unveiling the stabilization behavior in terms of noncovalent interactions. *Applied Organometallic Chemistry*, **2020**, 34, e5399	3.1	21
224	Advanced Ag/rGO/TiO2 ternary nanocomposite based photoanode approaches to highly-efficient plasmonic dye-sensitized solar cells. *Optics Communications*, **2019**, 453, 124408	2	20
223	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	20
222	Development and in vivo characterization of a novel peptide drug delivery system providing extended plasma half life. *Journal of Controlled Release*, **2012**, 157, 375-82	11.7	19
221	Adaptive neuro-fuzzy prediction of grasping object weight for passively compliant gripper. *Applied Soft Computing Journal*, **2014**, 22, 424-431	7.5	19
220	Aflatoxins contamination and prevention in red chillies (Capsicum annuum L.) in Pakistan. *Food Additives and Contaminants: Part B Surveillance*, **2014**, 7, 1-6	3.3	19
219	Thiomers: Inhibition of cytochrome P450 activity. *European Journal of Pharmaceutics and Biopharmaceutics*, **2011**, 78, 361-5	5.7	19
218	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	6	19

217	Quantum Chemical Approach of Donor–Acceptor Based Arylborane–Arylamine Macrocycles with Outstanding Photovoltaic Properties Toward High-Performance Organic Solar Cells. *Energy & Fuels*, **2021**, 35, 15018-15032	4.1	19
216	Isatin-derived non-fullerene acceptors for efficient organic solar cells. *Materials Science in Semiconductor Processing*, **2021**, 121, 105345	4.3	19
215	Food analysis employing high energy nanosecond laser and low pressure He ambient gas. *Microchemical Journal*, **2019**, 147, 356-364	4.8	18
214	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. *Journal of Molecular Modeling*, **2019**, 25, 223	2	18
213	Nitrous oxide emissions from rape field as affected by nitrogen fertilizer management: A case study in Central China. *Atmospheric Environment*, **2011**, 45, 1775-1779	5.3	18
212	Designing of small molecule non-fullerene acceptors with cyanobenzene core for photovoltaic application. *Computational and Theoretical Chemistry*, **2021**, 1197, 113154	2	18
211	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	2.5	18
210	DFT study of superhalogen and superalkali doped graphitic carbon nitride and its non-linear optical properties.. *RSC Advances*, **2021**, 11, 7779-7789	3.7	18
209	Structural, optical and photovoltaic properties of unfused Non-Fullerene acceptors for efficient solution processable organic solar cell (Estimated PCE greater than 12.4%): A DFT approach. *Journal of Molecular Liquids*, **2021**, 341, 117428	6	18
208	Designing of non-fullerene 3D star-shaped acceptors for organic solar cells. *Journal of Molecular Modeling*, **2019**, 25, 129	2	17
207	Development and in vivo evaluation of an oral vitamin B12 delivery system. *European Journal of Pharmaceutics and Biopharmaceutics*, **2013**, 84, 132-7	5.7	17
206	Does nitrogen fertilizer application rate to corn affect nitrous oxide emissions from the rotated soybean crop?. *Journal of Environmental Quality*, **2015**, 44, 711-9	3.4	17
205	Development and in vivo evaluation of a new oral nanoparticulate dosage form for leuprolide based on polyacrylic acid. *Drug Delivery*, **2011**, 18, 432-40	7	17
204	End-capped modification of dithienosilole based small donor molecules for high performance organic solar cells using DFT approach. *Journal of Molecular Liquids*, **2021**, 345, 118138	6	17
203	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	5.5	16
202	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	16
201	Spatial diagnostics of the laser-produced tin plasma in air. *Laser Physics*, **2016**, 26, 076001	1.2	16
200	Fabrication of hexagonal boron nitride quantum dots via a facile bottom-up technique. *Ceramics International*, **2019**, 45, 22765-22768	5.1	16

199	Impacts of inorganic ions and temperature on lead adsorption onto variable charge soils. *Catena*, **2013**, 109, 103-109	5.8	16
198	Tuning the optoelectronic properties of dibenzochrysene (DBC) based small molecules for organic solar cells. *Materials Science in Semiconductor Processing*, **2021**, 127, 105689	4.3	16
197	Enhanced linear and nonlinear optical response of superhalogen (Al7) doped graphitic carbon nitride (g-C3N4). *Optik*, **2021**, 226, 165923	2.5	16
196	Designing indaceno thiophene-based three new molecules containing non-fullerene acceptors as strong electron withdrawing groups with DFT approaches. *Journal of Molecular Modeling*, **2019**, 25, 311	2	15
195	Molecular designing of four high performance pyrazine-based non-fullerene acceptor materials with naphthalene diimide-based small organic solar cells. *Journal of Molecular Modeling*, **2019**, 25, 50	2	15
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193	O-4-Acetylamino-benzenesulfonylated pyrimidine derivatives: synthesis, SC-XRD, DFT analysis and electronic behaviour investigation. *Journal of Molecular Structure*, **2021**, 1224, 129308	3.4	15
192	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	6	15
191	Tuning the optoelectronic properties of benzodithiophene based donor materials and their photovoltaic applications. *Materials Science in Semiconductor Processing*, **2022**, 137, 106150	4.3	15
190	Aflatoxins contamination in Pakistani brown rice: a comparison of TLC, HPLC, LC-MS/MS and ELISA techniques. *Toxicology Mechanisms and Methods*, **2014**, 24, 544-51	3.6	14
189	The Effect of Emotional Intelligence and Academic Social Networking Sites on Academic Performance During the COVID-19 Pandemic. *Psychology Research and Behavior Management*, **2021**, 14, 905-920	3.8	14
188	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	2	14
187	Designing and theoretical study of fluorinated small molecule donor materials for organic solar cells. *Journal of Molecular Modeling*, **2021**, 27, 216	2	14
186	Designing and theoretical characterization of benzodithiophene dione based donor molecules for small molecule organic solar cells. *Optik*, **2021**, 242, 167098	2.5	14
185	Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications. *Chemical Physics Letters*, **2021**, 782, 139018	2.5	14
184	Visible light active indigo dye/graphene/WO3 nanocomposites with excellent photocatalytic activity. *Journal of Materials Research and Technology*, **2019**, 8, 3261-3269	5.5	13
183	Taxonomy of Factors Causing Integration Failure during Global Software Development. *IEEE Access*, **2018**, 6, 22228-22239	3.5	13
182	Structural, electronic, half-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	3.9	13

181	Molecular engineering strategy of naphthalimide based small donor molecules for high-performance organic solar cells. *Computational and Theoretical Chemistry*, **2021**, 1204, 113416	2	13
180	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	6.8	12
179	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. *ACS Omega*, **2021**, 6, 28923-28935	3.9	12
178	DFT study of superhalogen (AlF4) doped boron nitride for tuning their nonlinear optical properties. *Optik*, **2021**, 231, 166464	2.5	12
177	Evaluation of mustard oil for the synthesis of biodiesel: Pretreatment and optimization study. *Environmental Progress and Sustainable Energy*, **2018**, 37, 1829-1835	2.5	12
176	Improved Mechanical Properties, Wear and Corrosion Resistance of 316L Steel by Homogeneous Chromium Nitride Layer Synthesis Using Plasma Nitriding. *Journal of Materials Engineering and Performance*, **2020**, 29, 877-889	1.6	11
175	Duplex plasma treatment of AISI D2 tool steel by combining plasma nitriding (with and without white layer) and post-oxidation. *Surface and Coatings Technology*, **2020**, 385, 125420	4.4	11
174	Design, synthesis and application of triazole ligands in suzuki miyaura cross coupling reaction of aryl chlorides. *Journal of Molecular Structure*, **2020**, 1206, 127753	3.4	11
173	Software SMEs□unofficial readiness for CMMI□ -based software process improvement. *Software Quality Journal*, **2016**, 24, 997-1023	1.2	11
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171	Benchmark study of UV/Visible spectra of coumarin derivatives by computational approach. *Journal of Molecular Structure*, **2017**, 1130, 603-616	3.4	11
170	Tuning the optoelectronic properties of indacenodithiophene based derivatives for efficient photovoltaic applications: A DFT approach. *Chemical Physics Letters*, **2022**, 793, 139459	2.5	11
169	Theoretical calculation of selenium N-heterocyclic carbene compounds through DFT studies: Synthesis, characterization and biological potential. *Journal of Molecular Structure*, **2020**, 1204, 127462	3.4	11
168	Green Synthesis, SC-XRD, Non-Covalent Interactive Potential and Electronic Communication via DFT Exploration of Pyridine-Based Hydrazone. *Crystals*, **2020**, 10, 778	2.3	11
167	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	4.4	11
166	Efficient tuning of small acceptor chromophores with A1-□A2-□A1 configuration for high efficacy of organic solar cells via end group manipulation. *Journal of Saudi Chemical Society*, **2021**, 25, 101305	4.3	11
165	Investigating the nexus between critical success factors, despotic leadership, and success of renewable energy projects. *Environmental Science and Pollution Research*, **2021**, 1	5.1	11
164	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	2.8	11

163	Tuning the Optoelectronic Properties of Naphtho-Dithiophene-Based A-D-A Type Small Donor Molecules for Bulk Hetero-Junction Organic Solar Cells. *ChemistrySelect*, **2018**, 3, 2352-2358	1.8	10
162	Designing Benzodithiophene-Based Donor Materials with Favorable Photovoltaic Parameters for Bulk Heterojunction Organic Solar Cells. *ChemistrySelect*, **2017**, 2, 5628-5639	1.8	10
161	Calibration-free laser-induced breakdown spectroscopic analysis of copper-rich mineral collected from the Gilgit-Baltistan region of Pakistan. *Applied Optics*, **2020**, 59, 68-76	1.7	10
160	Fungal flora and aflatoxin contamination in Pakistani wheat kernels (Triticum aestivum L.) and their attribution in seed germination. *Journal of Food and Drug Analysis*, **2016**, 24, 635-643	7	10
159	Investigation on the surface modification of TiO2 nanohexagon arrays based photoanode with SnO2 nanoparticles for highly-efficient dye-sensitized solar cells. *Materials Research Bulletin*, **2019**, 109, 21-28	5.1	10
158	Phase transition and thermoelectric properties of cubic KNbO3 under pressure: DFT approach. *Journal of Materials Research and Technology*, **2021**, 11, 2106-2113	5.5	10
157	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	4.1	10
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155	Effect of pulsed duty cycle control on tribological and corrosion properties of AISI-316 in cathodic cage plasma nitriding. *Materials Research Express*, **2017**, 4, 116507	1.7	9
154	Designing difluoro substituted benzene ring based fullerene free acceptors for small Naphthalene Di-Imide based molecules with DFT approaches. *Optical and Quantum Electronics*, **2019**, 51, 1	2.4	9
153	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. *Inorganica Chimica Acta*, **2019**, 494, 160-167	2.7	9
152	Rational design of naphthalimide based small molecules non-fullerene acceptors for organic solar cells. *Computational and Theoretical Chemistry*, **2020**, 1187, 112916	2	9
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1 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 2