

Ahmad Irfan

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399
papers

5,523
citations

34
h-index

48
g-index

429
ext. papers

7,583
ext. citations

3.5
avg, IF

6.69
L-index

#	Paper	IF	Citations
399	Removal of Congo red dye from aqueous medium by its catalytic reduction using sodium borohydride in the presence of various inorganic nano-catalysts: A review. <i>Journal of Cleaner Production</i> , 2018 , 187, 296-307	10.3	127
398	Quantum chemical design of nonlinear optical materials by sp ² -hybridized carbon nanomaterials: issues and opportunities. <i>Journal of Materials Chemistry C</i> , 2013 , 1, 5439	7.1	116
397	Modified solvothermal synthesis of cobalt ferrite (CoFe ₂ O ₄) magnetic nanoparticles photocatalysts for degradation of methylene blue with H ₂ O ₂ /visible light. <i>Results in Physics</i> , 2018 , 8, 1046-1053	3.7	115
396	An investigation on the key features of a DA type novel chalcone derivative for opto-electronic applications. <i>RSC Advances</i> , 2015 , 5, 87320-87332	3.7	86
395	Quantum chemical study of the donor-bridge-acceptor triphenylamine based sensitizers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013 , 110, 60-6	4.4	67
394	Applications of UV/Vis Spectroscopy in Characterization and Catalytic Activity of Noble Metal Nanoparticles Fabricated in Responsive Polymer Microgels: A Review. <i>Critical Reviews in Analytical Chemistry</i> , 2018 , 48, 503-516	5.2	66
393	Tuning the push-pull configuration for efficient second-order nonlinear optical properties in some chalcone derivatives. <i>Journal of Molecular Graphics and Modelling</i> , 2016 , 68, 95-105	2.8	65
392	Chemical sensor development based on polycrystalline gold electrode embedded low-dimensional Ag ₂ O nanoparticles. <i>Electrochimica Acta</i> , 2013 , 112, 422-430	6.7	61
391	Adsorptive removal of heavy metal ions using polystyrene-poly(N-isopropylmethacrylamide-acrylic acid) core/shell gel particles: Adsorption isotherms and kinetic study. <i>Journal of Molecular Liquids</i> , 2019 , 277, 522-531	6	61
390	Catalytic reduction of toxic dyes in the presence of silver nanoparticles impregnated core-shell composite microgels. <i>Journal of Cleaner Production</i> , 2019 , 211, 855-864	10.3	59
389	First principles study for the key electronic, optical and nonlinear optical properties of novel donor-acceptor chalcones. <i>Journal of Molecular Graphics and Modelling</i> , 2017 , 72, 58-69	2.8	57
388	Quantum chemical study in the direction to design efficient donor-bridge-acceptor triphenylamine sensitizers with improved electron injection. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4893-900	2	56
387	Electro-optical, nonlinear and charge transfer properties of naphthalene based compounds: A dual approach study. <i>Optik</i> , 2017 , 132, 101-110	2.5	51
386	Role of a singlet diradical character in carbon nanomaterials: a novel hot spot for efficient nonlinear optical materials. <i>Nanoscale</i> , 2016 , 8, 17998-18020	7.7	49
385	Facile synthesis of silver nanoparticles in a crosslinked polymeric system by in situ reduction method for catalytic reduction of 4-nitroaniline. <i>Environmental Technology (United Kingdom)</i> , 2019 , 40, 2027-2036	2.6	49
384	How does hybrid bridging core modification enhance the nonlinear optical properties in donor-acceptor configuration? A case study of dinitrophenol derivatives. <i>Journal of Computational Chemistry</i> , 2015 , 36, 118-28	3.5	46
383	Chemical reduction of methylene blue in the presence of nanocatalysts: a critical review. <i>Reviews in Chemical Engineering</i> , 2020 , 36, 749-770	5	45

382	A review on the waste biomass derived catalysts for biodiesel production. <i>Environmental Technology and Innovation</i> , 2021 , 21, 101200	7	44
381	Inorganic nanoparticles for reduction of hexavalent chromium: Physicochemical aspects. <i>Journal of Hazardous Materials</i> , 2021 , 402, 123535	12.8	43
380	Heterocyclic azo dyes for dye sensitized solar cells: A quantum chemical study. <i>Computational and Theoretical Chemistry</i> , 2015 , 1066, 94-99	2	41
379	The DFT investigations of the electron injection in hydrazone-based sensitizers. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	41
378	Fe3O4-PDA-Lipase as Surface Functionalized Nano Biocatalyst for the Production of Biodiesel Using Waste Cooking Oil as Feedstock: Characterization and Process Optimization. <i>Energies</i> , 2020 , 13, 177	3.1	38
377	Synthesis, and characterization of metal-organic frameworks -177 for static and dynamic adsorption behavior of CO2 and CH4. <i>Microporous and Mesoporous Materials</i> , 2019 , 288, 109569	5.3	37
376	Synthesis, characterization and DFT study of methoxybenzylidene containing chromophores for DSSC materials. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 91, 239-43	4.4	37
375	A dual approach to study the electro-optical properties of a noncentrosymmetric L-asparagine monohydrate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 137, 432-41	4.4	36
374	Synthesis and Photooxygenation of Furo[3,2-c]coumarin Derivatives as Antibacterial and DNA Intercalating Agent. <i>Chinese Journal of Chemistry</i> , 2012 , 30, 316-320	4.9	36
373	Design, characterization and nonlinear optical properties of coumarin appended chalcones: Use of a dual approach. <i>Optik</i> , 2018 , 164, 5-15	2.5	35
372	Advancement in Multi-Functional Poly(styrene)-Poly(N-isopropylacrylamide) Based Core-Shell Microgels and their Applications. <i>Polymer Reviews</i> , 2018 , 58, 288-325	14	35
371	Exploring the optoelectronic and charge transfer performance of diaza[5]helicenes at molecular and bulk level. <i>Organic Electronics</i> , 2018 , 57, 211-220	3.5	35
370	Quantum chemical investigations aimed at modeling highly efficient zinc porphyrin dye sensitized solar cells. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4199-207	2	35
369	Theoretical study of triphenylamine-based organic dyes with mono-, di-, and tri-anchoring groups for dye-sensitized solar cells. <i>Organic Electronics</i> , 2018 , 63, 328-342	3.5	35
368	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	2.8	34
367	DFT and TDDFT calculations of the electronic structures and photophysical properties of newly designed pyrene-core arylamine derivatives as hole-transporting materials for perovskite solar cells. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	34
366	Fluorinated derivatives of mer-Alq3: energy decomposition analysis, optical properties, and charge transfer study. <i>Theoretical Chemistry Accounts</i> , 2009 , 122, 275-281	1.9	34
365	Push-pull effect on the charge transfer, and tuning of emitting color for disubstituted derivatives of mer-Alq3. <i>Chemical Physics</i> , 2009 , 364, 39-45	2.3	34

364	Structural parameters, electronic, linear and nonlinear optical exploration of thiopyrimidine derivatives: A comparison between DFT/TDDFT and experimental study. <i>Journal of Molecular Structure</i> , 2020 , 1201, 127183	3-4	34
363	Quantum chemical investigations of electron injection in triphenylamine-dye sensitized TiO ₂ used in dye sensitized solar cells. <i>Materials Chemistry and Physics</i> , 2013 , 142, 238-247	4-4	33
362	First principles study of the n-channel thiophene based heterocyclic chalcones. <i>Optik</i> , 2017 , 138, 349-358	3.5	32
361	Benchmark study of the linear and nonlinear optical polarizabilities in proto-type NLO molecule of para-nitroaniline. <i>Journal of Theoretical and Computational Chemistry</i> , 2019 , 18, 1950030	1.8	32
360	Modeling of efficient charge transfer materials of 4,6-di(thiophen-2-yl)pyrimidine derivatives: Quantum chemical investigations. <i>Computational Materials Science</i> , 2014 , 81, 488-492	3-2	32
359	Silver nanoparticles stabilized in polymer hydrogels for catalytic degradation of azo dyes. <i>Ecotoxicology and Environmental Safety</i> , 2020 , 202, 110924	7	32
358	Synthesis and characterization of poly(N-isopropylmethacrylamide-co-acrylic acid) microgels for in situ fabrication and stabilization of silver nanoparticles for catalytic reduction of o-nitroaniline in aqueous medium. <i>Reactive and Functional Polymers</i> , 2018 , 132, 89-97	4.6	31
357	Designing of Efficient Acceptors for Organic Solar Cells: Molecular Modelling at DFT Level. <i>Journal of Cluster Science</i> , 2018 , 29, 359-365	3	30
356	Engineering of responsive polymer based nano-reactors for facile mass transport and enhanced catalytic degradation of 4-nitrophenol. <i>Journal of Environmental Sciences</i> , 2018 , 72, 43-52	6.4	30
355	The impact of position and number of methoxy group(s) to tune the nonlinear optical properties of chalcone derivatives: a dual substitution strategy. <i>Journal of Molecular Modeling</i> , 2016 , 22, 73	2	30
354	Silver Nanoparticles Engineered Polystyrene-Poly(N-isopropylmethacrylamide-acrylic acid) Core Shell Hybrid Polymer Microgels for Catalytic Reduction of Congo Red. <i>Macromolecular Chemistry and Physics</i> , 2018 , 219, 1800211	2.6	30
353	Molecular design of new hydrazone dyes for dye-sensitized solar cells: Synthesis, characterization and DFT study. <i>Journal of Molecular Structure</i> , 2012 , 1019, 130-134	3-4	30
352	Synthesis, characterization and DFT study of 4H-benzo[h]chromene derivatives. <i>Journal of Molecular Structure</i> , 2012 , 1018, 171-175	3-4	30
351	Synthesis, characterization and density functional theory investigations of the electronic, photophysical and charge transfer properties of donor-bridge-acceptor triaminopyrazolo[1,5-a]pyrimidine dyes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017 , 171, 688-693	4-4	30
350	Exploration of adsorption behavior, electronic nature and NLO response of hydrogen adsorbed Alkali metals (Li, Na and K) encapsulated Al ₁₂ N ₁₂ nanocages. <i>Journal of Theoretical and Computational Chemistry</i> , 2020 , 19, 2050031	1.8	30
349	An unexpected reactivity during periodate oxidation of chitosan and the affinity of its 2, 3-di-aldehyde toward sulfa drugs. <i>Carbohydrate Polymers</i> , 2017 , 175, 565-574	10.3	28
348	Effect of donor and acceptor groups on radical scavenging activity of phenol by density functional theory. <i>Arabian Journal of Chemistry</i> , 2017 , 10, S1703-S1710	5.9	28
347	Push-pull effect on the electronic, optical and charge transport properties of the benzo[2,3-b]thiophene derivatives as efficient multifunctional materials. <i>Computational and Theoretical Chemistry</i> , 2014 , 1031, 76-82	2	28

- 346 Effect of one ligand substitution on charge transfer and optical properties in mer-Alq3: a theoretical study. *Theoretical Chemistry Accounts*, **2009**, 124, 339-344 1.9 28
- 345 PEDOT/NiFe2O4 nanocomposites on biochar as a free-standing anode for high-performance and durable microbial fuel cells. *New Journal of Chemistry*, **2019**, 43, 7743-7750 3.6 27
- 344 The effect of donors-acceptors on the charge transfer properties and tuning of emitting color for thiophene, pyrimidine and oligoacene based compounds. *Journal of Fluorine Chemistry*, **2014**, 157, 52-57^{2.1} 27
- 343 Synthesis, characterization, and evaluation of some novel 4(3H)-quinazolinone derivatives as anti-inflammatory and analgesic agents. *Medicinal Chemistry Research*, **2013**, 22, 440-452 2.2 27
- 342 Detailed spectra, electronic properties, qualitative non-covalent interaction analysis, solvatochromism, docking and molecular dynamics simulations in different solvent atmosphere of cenobamate. *Structural Chemistry*, **2020**, 31, 2475-2485 1.8 27
- 341 The structural, electro-optical, charge transport and nonlinear optical properties of 2-[(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)methylidene]indan-1,3-dione. *Optik*, **2016**, 127, 10148-10157^{2.5} 27
- 340 A dual approach to study the key features of nickel (II) and copper (II) coordination complexes: Synthesis, crystal structure, optical and nonlinear properties. *Inorganica Chimica Acta*, **2019**, 484, 148-159^{3.7} 27
- 339 Exploring the potential of boron-doped nanographene as efficient charge transport and nonlinear optical material: A first-principles study. *Journal of Molecular Graphics and Modelling*, **2017**, 75, 209-219^{2.8} 26
- 338 In-depth quantum chemical investigation of electro-optical and charge-transport properties of trans-3-(3,4-dimethoxyphenyl)-2-(4-nitrophenyl)prop-2-enenitrile. *Comptes Rendus Chimie*, **2015**, 18, 1289-1296^{2.7} 26
- 337 A comparative study of key properties of glycine glycinium picrate (GGP) and glycinium picrate (GP): A combined experimental and quantum chemical approach. *Journal of Saudi Chemical Society*, **2018**, 22, 352-362 4.3 26
- 336 Sensing performance optimization by tuning surface morphology of organic (D-EA) dye based humidity sensor. *Sensors and Actuators B: Chemical*, **2016**, 231, 30-37 8.5 26
- 335 Exploring the novel donor-nanotube archetype as an efficient third-order nonlinear optical material: asymmetric open-shell carbon nanotubes. *Nanoscale*, **2018**, 10, 16499-16507 7.7 26
- 334 Modeling of multifunctional donor-bridge-acceptor 4,6-di(thiophen-2-yl)pyrimidine derivatives: a first principles study. *Journal of Molecular Graphics and Modelling*, **2013**, 44, 168-76 2.8 26
- 333 Comparison of mono- and di-substituted triphenylamine and carbazole based sensitizers @TiO₂ cluster for dye-sensitized solar cells applications. *Computational and Theoretical Chemistry*, **2019**, 1159, 1-6 2 25
- 332 Combined experimental and computational insights into the key features of L-alanine L-alaninium picrate monohydrate: growth, structural, electronic and nonlinear optical properties. *RSC Advances*, **2015**, 5, 53988-54002 3.7 25
- 331 Molecular design of organic small molecules based on diindole-imide with fused aromatic heterocycles as donors for organic solar cells. *RSC Advances*, **2017**, 7, 39899-39905 3.7 25
- 330 Electronic, optical, and charge transfer properties of donor-bridge-acceptor hydrazone sensitizers. *Structural Chemistry*, **2013**, 24, 499-506 1.8 25
- 329 Packing Effect on the Transfer Integrals and Mobility in π -bis(dithieno[3,2-b:2',3'-d]thiophene) (BDT) and its Heteroatom-Substituted Analogues. *Australian Journal of Chemistry*, **2011**, 64, 1587 1.2 25

328	Theoretical investigations of the charge transfer properties of anthracene derivatives. <i>Theoretical Chemistry Accounts</i> , 2010 , 127, 587-594	1.9	25
327	Hybrid Microgels for Catalytic and Photocatalytic Removal of Nitroarenes and Organic Dyes From Aqueous Medium: A Review. <i>Critical Reviews in Analytical Chemistry</i> , 2020 , 50, 513-537	5.2	25
326	Flexible and small wearable antenna for wireless body area network applications. <i>Journal of Electromagnetic Waves and Applications</i> , 2017 , 31, 1063-1082	1.3	24
325	Extraction of cobalt ions from aqueous solution by microgels for in-situ fabrication of cobalt nanoparticles to degrade toxic dyes: A two fold-environmental application. <i>Chemical Physics Letters</i> , 2020 , 754, 137645	2.5	24
324	AIE active multianalyte fluorescent probe for the detection of Cu, Ni and Hg ions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018 , 201, 54-60	4.4	24
323	Anti-HIV cytotoxicity enzyme inhibition and molecular docking studies of quinoline based chalcones as potential non-nucleoside reverse transcriptase inhibitors (NNRT). <i>Bioorganic Chemistry</i> , 2016 , 65, 175-182	5.1	24
322	Computational Designing of Triphenylamine Dyes with Broad and Red-shifted Absorption Spectra for Dye-sensitized Solar Cells using Multi-Thiophene Rings in Spacer. <i>Bulletin of the Korean Chemical Society</i> , 2015 , 36, 2615-2620	1.2	24
321	Theoretical investigations of the charge transfer characteristics in dichlorotitanium phthalocyanine (TiCl ₂ Pc) and tin phthalocyanine (SnPc). <i>Chemical Physics Letters</i> , 2009 , 483, 143-146	2.5	24
320	Triphenylamine-based stimuli-responsive solid state fluorescent materials. <i>New Journal of Chemistry</i> , 2020 , 44, 8680-8696	3.6	24
319	Novel W-Shaped Oxygen Heterocycle-Fused Fluorene-Based Non-Fullerene Acceptors: First Theoretical Framework for Designing Environment-Friendly Organic Solar Cells. <i>Energy & Fuels</i> , 2021 , 35, 12436-12450	4.1	24
318	An investigation on thermal performance of wollastonite and bentonite reinforced intumescent fire-retardant coating for steel structures. <i>Construction and Building Materials</i> , 2019 , 228, 116734	6.7	23
317	Humidity dependent electrical properties of an organic material DMBHPET. <i>Measurement: Journal of the International Measurement Confederation</i> , 2015 , 61, 180-184	4.6	23
316	Extraction of Heavy Metals from Aqueous Medium by Husk Biomass: Adsorption Isotherm, Kinetic and Thermodynamic study. <i>Zeitschrift Fur Physikalische Chemie</i> , 2019 , 233, 201-223	3.1	23
315	Highly efficient renewable energy materials benzo[2,3-b]thiophene derivatives: Electronic and charge transfer properties study. <i>Optik</i> , 2014 , 125, 4825-4830	2.5	23
314	Quantum chemical approach toward the electronic, photophysical and charge transfer properties of the materials used in organic field-effect transistors. <i>Materials Chemistry and Physics</i> , 2013 , 138, 468-478	4.4	23
313	Machine learning and molecular dynamics simulation-assisted evolutionary design and discovery pipeline to screen efficient small molecule acceptors for PTB7-Th-based organic solar cells with over 15% efficiency. <i>Journal of Materials Chemistry A</i> ,	13	23
312	Impact of cerium oxide and cerium composite oxide as nano additives on the gaseous exhaust emission profile of waste cooking oil based biodiesel at full engine load conditions. <i>Renewable Energy</i> , 2019 , 143, 898-905	8.1	22
311	Poly(N-isopropylmethacrylamide-acrylic acid) microgels as adsorbent for removal of toxic dyes from aqueous medium. <i>Journal of Molecular Liquids</i> , 2018 , 268, 229-238	6	22

310	Structural, electronic and charge transfer studies of dianthra[2,3-b:2',3'-f]thieno[3,2-b]thiophene and its analogues: Quantum chemical investigations. <i>Journal of Molecular Structure</i> , 2013 , 1049, 198-204	3.4	22
309	Push-pull effect on the geometries, electronic and optical properties of thiophene based dye-sensitized solar cell materials. <i>Journal of Saudi Chemical Society</i> , 2014 , 18, 914-919	4.3	22
308	Developing Efficient Small Molecule Acceptors with sp ² -Hybridized Nitrogen at Different Positions by Density Functional Theory Calculations, Molecular Dynamics Simulations and Machine Learning. <i>Chemistry - A European Journal</i> , 2021 ,	4.8	22
307	Exploring the new potential antiviral constituents of Moringa oliefera for SARS-COV-2 pathogenesis: An molecular docking and dynamic studies. <i>Chemical Physics Letters</i> , 2021 , 767, 138379	2.5	22
306	Syntheses, characterizations, crystal structures and efficient NLO applications of new organic compounds bearing 2-methoxy-4-nitrobenzeneamine moiety and copper (II) complex of (E)-N'-(3,5-dichloro-2-hydroxybenzylidene) benzohydrazide. <i>Journal of Molecular Structure</i> , 2019 , 1190, 54-67	3.4	21
305	Facile green synthesis, optical and photocatalytic properties of zinc oxide nanosheets via microwave assisted hydrothermal technique. <i>Journal of Electroceramics</i> , 2013 , 31, 324-330	1.5	21
304	First-principles study of nitrogen-doped nanographene as an efficient charge transport and nonlinear optical material. <i>RSC Advances</i> , 2017 , 7, 36632-36643	3.7	21
303	Linear, second and third order nonlinear optical properties of novel noncentrosymmetric donor-acceptor configure chalcone derivatives: A dual approach study. <i>Optik</i> , 2019 , 199, 163354	2.5	20
302	The effect of anchoring groups on the electro-optical and charge injection in triphenylamine derivatives@TiO ₂ . <i>Journal of Theoretical and Computational Chemistry</i> , 2015 , 14, 1550027	1.8	20
301	Designed synthesis of silver nanoparticles in responsive polymeric system for their thermally tailored catalytic activity towards hydrogenation reaction. <i>Korean Journal of Chemical Engineering</i> , 2018 , 35, 1099-1107	2.8	20
300	Electronic and optoelectronic properties of Al/coumarin doped Pr ₂ Se ₃ /In ₂ Se ₃ /p-Si devices. <i>Journal of Materials Science: Materials in Electronics</i> , 2018 , 29, 12561-12572	2.1	20
299	Push-pull effect on the charge transport properties in anthra[2,3-b]thiophene derivatives used as dye-sensitized and hetero-junction solar cell materials. <i>Synthetic Metals</i> , 2014 , 190, 27-33	3.6	20
298	Theoretical study of coumarin derivatives as chemosensors for fluoride anion. <i>Computational and Theoretical Chemistry</i> , 2012 , 986, 93-98	2	20
297	Effect of fluorination on exciton binding energy and electronic coupling in small molecule acceptors for organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020 , 1179, 112797	2	20
296	Lipase-PDA-TiO ₂ NPs: An emphatic nano-biocatalyst for optimized biodiesel production from <i>Jatropha curcas</i> oil. <i>Renewable Energy</i> , 2021 , 169, 1026-1037	8.1	20
295	Effect of heteroatoms substitution on electronic, photophysical and charge transfer properties of naphtha [2,1-b:6,5-b'] difuran analogues by density functional theory. <i>Computational and Theoretical Chemistry</i> , 2014 , 1045, 123-134	2	19
294	Effects of Electron Withdrawing Groups on Transfer Integrals, Mobility, Electronic and Photo-Physical Properties of Naphtho[2,1-b:6,5-b']Difuran Derivatives: A Theoretical Study. <i>Science of Advanced Materials</i> , 2014 , 6, 1727-1739	2.3	19
293	Waste paper derived three-dimensional carbon aerogel integrated with ceria/nitrogen-doped reduced graphene oxide as freestanding anode for high performance and durable microbial fuel cells. <i>Bioprocess and Biosystems Engineering</i> , 2020 , 43, 97-109	3.7	19

292	AIE active turn-off fluorescent probe for the detection of Cu ions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017 , 183, 84-89	4.4	18
291	Quantum chemical approach toward rational designing of highly efficient oxadiazole based oligomers used in organic field effect transistors. <i>Journal of Computational Electronics</i> , 2012 , 11, 374-384	1.8	18
290	Electronic, optical and charge transfer properties of β -bis(dithieno[3,2-b:2',3'-d]thiophene) (BDT) and its heteroatom-substituted analogues. <i>Computational and Theoretical Chemistry</i> , 2011 , 968, 8-11	2	18
289	Optoelectronic properties of naphtho[2, 1-b:6, 5-b']difuran derivatives for photovoltaic application: a computational study. <i>Journal of Molecular Modeling</i> , 2016 , 22, 248	2	18
288	Tuning of optoelectronic and charge transport properties in star shaped anthracenothiophene-pyrimidine derivatives as multifunctional materials. <i>Optik</i> , 2017 , 149, 321-331	2.5	17
287	DFT investigations of the ground and excited state geometries of the benzothiazine and benzisothiazol based anticancer drugs. <i>Journal of Saudi Chemical Society</i> , 2015 , 19, 318-321	4.3	17
286	Synthesis, antihyperglycemic activity and computational studies of antioxidant chalcones and flavanones derived from 2,5 dihydroxyacetophenone. <i>Journal of Molecular Structure</i> , 2017 , 1148, 512-520	3.4	17
285	A study on the electronic and charge transfer properties in tin phthalocyanine (SnPc) derivatives by density functional theory. <i>Computational and Theoretical Chemistry</i> , 2011 , 977, 9-12	2	17
284	Computational analysis to understand the performance difference between two small-molecule acceptors differing in their terminal electron-deficient group. <i>Journal of Computational Electronics</i> , 2020 , 19, 931-939	1.8	17
283	Cadmium Oxide: Titanium Dioxide Composite Based Photosensitive Diode. <i>Journal of Electronic Materials</i> , 2018 , 47, 7159-7169	1.9	17
282	Computational study and in vitro evaluation of the anti-proliferative activity of novel naproxen derivatives. <i>Journal of King Saud University - Science</i> , 2017 , 29, 311-319	3.6	16
281	Diradical character and nonlinear optical properties of buckyferrocenes: focusing on the use of suitably modified fullerene fragments. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 5805-16	3.6	16
280	Peculiar behavior of starch 2,3-dialdehyde towards sulfanilamide and sulfathiazole. <i>Carbohydrate Polymers</i> , 2016 , 152, 624-631	10.3	16
279	Investigating the effect of acene-fusion and trifluoroacetyl substitution on the electronic and charge transport properties by density functional theory. <i>Journal of Saudi Chemical Society</i> , 2016 , 20, 336-342	4.3	16
278	DFT study of the electronic and charge transfer properties of perfluoroarene-thiophene oligomers. <i>Journal of Saudi Chemical Society</i> , 2014 , 18, 574-580	4.3	16
277	Explaining the HOMO and LUMO distribution on individual ligands in mer-Alq3 and its $\text{C}_{60}\text{H}_{12}\text{N}$ substituted derivatives. <i>Computational and Theoretical Chemistry</i> , 2008 , 850, 79-83		16
276	Catalytic degradation of malachite green using a crosslinked colloidal polymeric system loaded with silver nanoparticles. <i>International Journal of Environmental Analytical Chemistry</i> , 2020 , 1-17	1.8	16
275	Evaluation of humidity sensing properties of TMBHPET thin film embedded with spinel cobalt ferrite nanoparticles. <i>Journal of Nanoparticle Research</i> , 2016 , 18, 1	2.3	16

274	High-temperature CO ₂ removal from CH ₄ using silica membrane: experimental and neural network modeling 2019 , 9, 1010-1026		15
273	Exploring the effect of oligocene elongation on photovoltaic, optoelectronic and charge transfer properties in TPA dyes tethered to the semiconductor surface. <i>Results in Physics</i> , 2019 , 13, 102304	3.7	15
272	The structural, electro-optical, charge transport and nonlinear optical properties of oxazole (4Z)-4-Benzylidene-2-(4-methylphenyl)-1,3-oxazol-5(4H)-one derivative. <i>Journal of King Saud University - Science</i> , 2018 , 30, 75-82	3.6	15
271	The electro-optical and charge transport study of imidazolidin derivative: Quantum chemical investigations. <i>Journal of Saudi Chemical Society</i> , 2016 , 20, 680-685	4.3	15
270	Charge carrier and optoelectronic properties of phenylimidazo[1,5-a]pyridine-containing small molecules at molecular and solid-state bulk scales. <i>Computational Materials Science</i> , 2019 , 170, 109179	3.2	15
269	Donor-enhanced bridge effect on the electronic properties of triphenylamine based dyes: density functional theory investigations. <i>Journal of Molecular Modeling</i> , 2012 , 18, 3609-15	2	15
268	Exploring the impact of central core modifications among several push-pull configurations to enhance nonlinear optical response. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 100, 107665	2.8	15
267	Surfactant and binder free hierarchical NCNPs@CuO nanostructures on ITO for the cost effective enzyme-free glucose sensor applications. <i>Applied Physics A: Materials Science and Processing</i> , 2019 , 125, 1	2.6	14
266	Spectroscopic investigation, photophysical parameters and DFT calculations of 4,4'-(1E,1'E)-2,2'-(pyrazine-2,5-diyl)bis(ethene-2,1-diyl)bis(N,N-dimethylaniline) (PENDA) in different solvents. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 149, 722-30	4.4	14
265	Quantum chemical investigation of spectroscopic studies and hydrogen bonding interactions between water and methoxybenzylidene-based humidity sensor. <i>Journal of Theoretical and Computational Chemistry</i> , 2015 , 14, 1550029	1.8	14
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