

Abdullah G Al-Sehemi

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377 papers	5,148 citations	32 h-index	45 g-index
398 ext. papers	6,550 ext. citations	3.2 avg, IF	6.37 L-index

#	Paper	IF	Citations
377	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
376	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
375	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
374	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
373	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
372	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
371	Microwave synthesis, optical properties and surface area studies of NiO nanoparticles. <i>Journal of Molecular Structure</i> , 2014 , 1058, 56-61	3.4	60
370	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
369	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
368	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
367	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
366	Synthesis of mesoporous sulfur-doped Ta ₂ O ₅ nanocomposites and their photocatalytic activities. <i>Journal of Colloid and Interface Science</i> , 2016 , 471, 145-154	9.3	50
365	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
364	Synthesis and characterization of NiO nanoparticles by thermal decomposition of nickel linoleate and their optical properties. <i>Materials Characterization</i> , 2012 , 68, 77-81	3.9	48
363	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
362	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
361	Influence of post-synthetic graphene oxide (GO) functionalization on the selective CO ₂ /CH ₄ adsorption behavior of MOF-200 at different temperatures; an experimental and adsorption isotherms study. <i>Microporous and Mesoporous Materials</i> , 2020 , 296, 110002	5.3	42

360	Heterocyclic azo dyes for dye sensitized solar cells: A quantum chemical study. <i>Computational and Theoretical Chemistry</i> , 2015 , 1066, 94-99	2	41
359	The DFT investigations of the electron injection in hydrazone-based sensitizers. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	41
358	Synthesis, and characterization of metal-organic frameworks -177 for static and dynamic adsorption behavior of CO ₂ and CH ₄ . <i>Microporous and Mesoporous Materials</i> , 2019 , 288, 109569	5.3	37
357	NiMoO ₄ nanoparticles decorated carbon nanofiber membranes for the flexible and high performance glucose sensors. <i>Sensors and Actuators B: Chemical</i> , 2020 , 312, 127886	8.5	37
356	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
355	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
354	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
353	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
352	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
351	3-(N,N-Diacylamino)quinazolin-4(3H)-ones as enantioselective acylating agents for amines. <i>Tetrahedron Letters</i> , 2000 , 41, 2239-2242	2	35
350	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
349	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
348	CO ₂ capturing, thermo-kinetic principles, synthesis and amine functionalization of covalent organic polymers for CO ₂ separation from natural gas: A review. <i>Journal of Natural Gas Science and Engineering</i> , 2020 , 77, 103203	4.6	33
347	First principles study of the n-channel thiophene based heterocyclic chalcones. <i>Optik</i> , 2017 , 138, 349-358.	5.5	32
346	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
345	Organic semiconductor photosensors. <i>Journal of Alloys and Compounds</i> , 2017 , 702, 520-530	5.7	31
344	Fabrication of non-enzymatic sensor using Co doped ZnO nanoparticles as a marker of H ₂ O ₂ . <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2014 , 62, 21-27	3	31
343	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

342	Ruthenium(II) Complex Based Photodiode for Organic Electronic Applications. <i>Journal of Electronic Materials</i> , 2018 , 47, 828-833	1.9	30
341	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
340	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
339	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
338	On-body investigation of a compact planar antenna on multilayer polymer composite for body-centric wireless communications. <i>AEU - International Journal of Electronics and Communications</i> , 2017 , 82, 20-29	2.8	30
337	Synthesis, characterization and DFT study of 4H-benzo[h]chromene derivatives. <i>Journal of Molecular Structure</i> , 2012 , 1018, 171-175	3.4	30
336	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> , 2013 , 111, 223-9	4.4	30
335	Effect of pH on solvothermal synthesis of Ni(OH) ₂ and NiO nano-architectures: Surface area studies, optical properties and adsorption studies. <i>Superlattices and Microstructures</i> , 2013 , 55, 83-97	2.8	29
334	Synthesis and characterization of mesoporous MOF UMCM-1 for CO ₂ /CH ₄ adsorption; an experimental, isotherm modeling and thermodynamic study. <i>Microporous and Mesoporous Materials</i> , 2020 , 294, 109844	5.3	29
333	Synthesis, anti-inflammatory, analgesic and anticonvulsant activities of some new 4,6-dimethoxy-5-(heterocycles)benzofuran starting from naturally occurring visnagin. <i>Arabian Journal of Chemistry</i> , 2014 , 7, 914-923	5.9	28
332	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
331	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
330	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
329	CO ₂ /CH ₄ adsorption over functionalized multi-walled carbon nanotubes; an experimental study, isotherms analysis, mechanism, and thermodynamics. <i>Microporous and Mesoporous Materials</i> , 2020 , 294, 109883	5.3	28
328	PEDOT/NiFe ₂ O ₄ nanocomposites on biochar as a free-standing anode for high-performance and durable microbial fuel cells. <i>New Journal of Chemistry</i> , 2019 , 43, 7743-7750	3.6	27
327	The effect of donors-acceptors on the charge transfer properties and tuning of emitting color for thiophene, pyrimidine and oligoacene based compounds. <i>Journal of Fluorine Chemistry</i> , 2014 , 157, 52-57 ^{2.1}		27
326	Synthesis, characterization, and evaluation of some novel 4(3H)-quinazolinone derivatives as anti-inflammatory and analgesic agents. <i>Medicinal Chemistry Research</i> , 2013 , 22, 440-452	2.2	27
325	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. <i>Optik</i> , 2016 , 127, 10148-10157	2.5	27

324	A dual approach to study the key features of nickel (II) and copper (II) coordination complexes: Synthesis, crystal structure, optical and nonlinear properties. <i>Inorganica Chimica Acta</i> , 2019 , 484, 148-159	3.7	27
323	Exploring the potential of boron-doped nanographene as efficient charge transport and nonlinear optical material: A first-principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2017 , 75, 209-219	2.8	26
322	In-depth quantum chemical investigation of electro-optical and charge-transport properties of trans-3-(3,4-dimethoxyphenyl)-2-(4-nitrophenyl)prop-2-enenitrile. <i>Comptes Rendus Chimie</i> , 2015 , 18, 1289-1296	3.7	26
321	A comparative study of key properties of glycine glycinium picrate (GGP) and glycinium picrate (GP): A combined experimental and quantum chemical approach. <i>Journal of Saudi Chemical Society</i> , 2018 , 22, 352-362	4.3	26
320	Sensing performance optimization by tuning surface morphology of organic (D-EA) dye based humidity sensor. <i>Sensors and Actuators B: Chemical</i> , 2016 , 231, 30-37	8.5	26
319	Exploring the novel donor-nanotube archetype as an efficient third-order nonlinear optical material: asymmetric open-shell carbon nanotubes. <i>Nanoscale</i> , 2018 , 10, 16499-16507	7.7	26
318	Modeling of multifunctional donor-bridge-acceptor 4,6-di(thiophen-2-yl)pyrimidine derivatives: a first principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2013 , 44, 168-76	2.8	26
317	Combined experimental and computational insights into the key features of L-alanine L-alaninium picrate monohydrate: growth, structural, electronic and nonlinear optical properties. <i>RSC Advances</i> , 2015 , 5, 53988-54002	3.7	25
316	Electronic, optical, and charge transfer properties of donorBridgeAcceptor hydrazone sensitizers. <i>Structural Chemistry</i> , 2013 , 24, 499-506	1.8	25
315	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. <i>Australian Journal of Chemistry</i> , 2011 , 64, 1587	1.2	25
314	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
313	Ti doped amorphous carbon (Al/Ti-a:C/p-Si/Al) photodiodes for optoelectronic applications. <i>Journal of Molecular Structure</i> , 2018 , 1155, 813-818	3.4	24
312	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
311	Computational Designing of Triphenylamine Dyes with Broad and Red-shifted Absorption Spectra for Dye-sensitized Solar Cells using Multi-Thiophene Rings in π Spacer. <i>Bulletin of the Korean Chemical Society</i> , 2015 , 36, 2615-2620	1.2	24
310	Triphenylamine-based stimuli-responsive solid state fluorescent materials. <i>New Journal of Chemistry</i> , 2020 , 44, 8680-8696	3.6	24
309	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
308	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
307	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

306	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
305	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
304	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
303	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
302	Recent Trends in Chemistry of Thiazolopyridines. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2006 , 181, 631-674	1	22
301	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
300	Silicon based photodetector with Ru(II) complexes organic interlayer. <i>Materials Science in Semiconductor Processing</i> , 2019 , 91, 422-430	4.3	22
299	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
298	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
297	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
296	Parallel kinetic resolution of racemic amines using 3-N,N-diacylaminoquinazolin-4(3H)-ones. <i>Chemical Communications</i> , 2001 , 2684-2685	5.8	21
295	Lead and cadmium removal from wastewater using eco-friendly biochar adsorbent derived from rice husk, wheat straw, and corncob. <i>Cleaner Engineering and Technology</i> , 2020 , 1, 100006	2.7	21
294	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
293	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
292	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
291	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
290	Transformations of naproxen into pyrazolecarboxamides: search for potent anti-inflammatory, analgesic and ulcerogenic agents. <i>Medicinal Chemistry Research</i> , 2014 , 23, 827-838	2.2	20
289	Chitosan/sulfonated graphene oxide/silica nanocomposite membranes for direct methanol fuel cells. <i>Solid State Ionics</i> , 2019 , 338, 153-160	3.3	19

288	Design and performance analysis of dual-band wearable compact low-profile antenna for body-centric wireless communications. <i>International Journal of Microwave and Wireless Technologies</i> , 2018 , 10, 1175-1185	0.8	19
287	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
286	Cyanoacetanilides Intermediates in Heterocyclic Synthesis. Part 5: Preparation of Hitherto Unknown 5-Aminopyrazole and Pyrazolo[1,5-a]pyrimidine Derivatives Containing Sulfamoyl Moiety. <i>Journal of the Chinese Chemical Society</i> , 2009 , 56, 1064-1071	1.5	19
285	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
284	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
283	Exploration the effect of metal and electron withdrawing groups on charge transport and optoelectronic nature of schiff base Ni(II), Cu(II) and Zn(II) complexes at molecular and solid-state bulk scales. <i>Materials Science in Semiconductor Processing</i> , 2020 , 107, 104855	4.3	19
282	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
281	Sol-gel synthesis of poly(o-toluidine)@Sn(II)silicate/CNT composites for ion selective membrane electrodes. <i>Journal of Molecular Liquids</i> , 2015 , 208, 71-77	6	18
280	Synthesis and characterization of iso-reticular metal-organic Framework-3 (IRMOF-3) for CO ₂ /CH ₄ adsorption: Impact of post-synthetic aminomethyl propanol (AMP) functionalization. <i>Journal of Natural Gas Science and Engineering</i> , 2019 , 72, 103014	4.6	18
279	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
278	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
277	A functional material based photodiode for solar tracking systems. <i>Physica B: Condensed Matter</i> , 2017 , 520, 76-81	2.8	17
276	A photodiode based on PbS nanocrystallites for FYTRONIX solar panel automatic tracking controller. <i>Physica B: Condensed Matter</i> , 2017 , 527, 44-51	2.8	17
275	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
274	DFT investigations of the ground and excited state geometries of the benzothiazine and benisothiazol based anticancer drugs. <i>Journal of Saudi Chemical Society</i> , 2015 , 19, 318-321	4.3	17
273	Optoelectrical properties of Al/p-Si/Fe:N doped ZnO/Al diodes. <i>Thin Solid Films</i> , 2018 , 653, 236-248	2.2	17
272	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	2.4	17
271	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

270	Synthesis and spectroscopic studies of some new metal carbonyl derivatives of 1-(2-pyridylazo)-2-naphthol. <i>Journal of Coordination Chemistry</i> , 2009 , 62, 1293-1301	1.6	17
269	Cyanoacetanilides Intermediates in Heterocyclic Synthesis. Part 2: Preparation of Some Hitherto Unknown Ketene Dithioacetal, Benzoazole and Pyridone Derivatives. <i>Journal of the Chinese Chemical Society</i> , 2005 , 52, 553-558	1.5	17
268	Elastic and optoelectronic properties of CaTa ₂ O ₆ compounds: Cubic and orthorhombic phases. <i>Journal of Alloys and Compounds</i> , 2019 , 785, 232-239	5.7	17
267	Cadmium Oxide: Titanium Dioxide Composite Based Photosensitive Diode. <i>Journal of Electronic Materials</i> , 2018 , 47, 7159-7169	1.9	17
266	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
265	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
264	Peculiar behavior of starch 2,3-dialdehyde towards sulfanilamide and sulfathiazole. <i>Carbohydrate Polymers</i> , 2016 , 152, 624-631	10.3	16
263	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
262	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
261	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
260	Effect of Coulomb interactions on optoelectronic and magnetic properties of novel A ₂ V ₂ O ₇ (A= Fe and Co) compounds. <i>Journal of Alloys and Compounds</i> , 2018 , 766, 536-545	5.7	16
259	Frequency and electric field controllable photodevice: FYTRONIX device. <i>Physica B: Condensed Matter</i> , 2017 , 519, 53-58	2.8	15
258	High-temperature CO ₂ removal from CH ₄ using silica membrane: experimental and neural network modeling 2019 , 9, 1010-1026		15
257	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
256	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
255	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
254	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
253	Synthesis, crystal structure, spectroscopic, electronic and nonlinear optical properties of potent thiazole based derivatives: Joint experimental and computational insight. <i>Journal of Molecular Structure</i> , 2020 , 1202, 127354	3.4	15

252	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
251	Experimental measurements of carbon dioxide, methane and nitrogen high-pressure adsorption properties onto Malaysian coals under various conditions. <i>Energy</i> , 2020 , 210, 118575	7.9	15
250	Effect of calcination and carbon incorporation on NiO nanowires for photodiode performance. <i>Microelectronic Engineering</i> , 2018 , 202, 51-59	2.5	15
249	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
248	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
247	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
246	Density functional theory investigations of radical scavenging activity of 3?-Methyl-quercetin. <i>Journal of Saudi Chemical Society</i> , 2016 , 20, S21-S28	4.3	14
245	A Combined Experimental and Computational Investigation on Spectroscopic and Photophysical Properties of a Coumarinyl Chalcone. <i>Journal of Fluorescence</i> , 2016 , 26, 1357-65	2.4	14
244	Synthesis of amorphous ZnO/BiO ₂ nanocomposite with enhanced chemical sensing properties. <i>Thin Solid Films</i> , 2016 , 605, 277-282	2.2	14
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