

# Ahmad Irfan

## 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.

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	Shedding light on the optical and nonlinear optical properties of superalkali-doped borophene.. <i>Journal of Molecular Modeling</i> , <b>2022</b> , 28, 46	2	0
398	Exploration of a Bimetallic NiSe <sub>2</sub> @CoSe <sub>2</sub> Nanosphere as a Proficient Electrode for Electrochemical Activity. <i>Energy &amp; Fuels</i> , <b>2022</b> , 36, 1726-1734	4.1	1
397	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> , <b>2022</b> , 1-14	1.9	1
396	Current understandings and perspectives of petroleum hydrocarbons in Alzheimer's disease and Parkinson's disease: a global concern.. <i>Environmental Science and Pollution Research</i> , <b>2022</b> , 29, 10928	5.1	0
395	Shedding Light on the Synthesis, Crystal Structure, Characterization, and Computational Study of Optoelectronic Properties and Bioactivity of Imine derivatives.. <i>ACS Omega</i> , <b>2022</b> , 7, 5217-5230	3.9	4
394	Polymer microgels for the stabilization of gold nanoparticles and their application in the catalytic reduction of nitroarenes in aqueous media.. <i>RSC Advances</i> , <b>2022</b> , 12, 5105-5117	3.7	5
393	Recent Advancement of the Current Aspects of g-C <sub>3</sub> N <sub>4</sub> for its Photocatalytic Applications in Sustainable Energy System.. <i>Chemical Record</i> , <b>2022</b> , e202100310	6.6	3
392	Antioxidant, molecular docking and computational investigation of new flavonoids. <i>Journal of Molecular Structure</i> , <b>2022</b> , 1254, 132189	3.4	2
391	Spectroscopic, quantum mechanical, electronic excitation properties (Ethanol solvent), DFT investigations and molecular docking analysis of an anti-cancer drug Bendamustine. <i>Journal of Molecular Structure</i> , <b>2022</b> , 1253, 132211	3.4	3
390	Synthesis and investigation of anti-COVID19 ability of ferrocene Schiff base derivatives by quantum chemical and molecular docking.. <i>Journal of Molecular Structure</i> , <b>2022</b> , 1253, 132242	3.4	1
389	Insighting the functionally modified C <sub>60</sub> fullerenes as an efficient nonlinear optical materials: A quantum chemical study. <i>Materials Science in Semiconductor Processing</i> , <b>2022</b> , 141, 106421	4.3	5
388	Fabrication of Ce doped TiO <sub>2</sub> for efficient organic pollutants removal from wastewater.. <i>Chemosphere</i> , <b>2022</b> , 293, 133540	8.4	3
387	Multivariate Investigation of Toxic and Essential Metals in the Serum from Various Types and Stages of Colorectal Cancer Patients. <i>Biological Trace Element Research</i> , <b>2022</b> , 200, 31-48	4.5	0
386	Anti-microbial activity, molecular profiling, electronic properties and molecular docking investigations of 5-[1-hydroxy-2-(isopropylamino)ethyl] benzene-1,3-diol. <i>Journal of Molecular Structure</i> , <b>2022</b> , 1247, 131299	3.4	5
385	Pyridine nitrogen position controlled molecular packing and stimuli-responsive solid-state fluorescence switching: supramolecular complexation facilitated turn-on fluorescence. <i>CrystEngComm</i> , <b>2022</b> , 24, 2642-2649	3.3	0
384	Anti-obesity effect and UHPLC-QTOF-MS/MS based metabolite profiling of Solanum nigrum leaf extract. <i>Asian Pacific Journal of Tropical Biomedicine</i> , <b>2022</b> , 12, 164	1.4	1
383	The photovoltaic application and optics of ZnO/TiO <sub>2</sub> and ZnO/NiO nanocomposite binary system <b>2022</b> , 207190		0

382	Molecular Structure, Spectroscopic Assessment, PDOS, Topology Evaluation and Docking Studies of 2-Chloro-5-nitrobenzophenone. <i>Analytical Chemistry Letters</i> , <b>2022</b> , 12, 198-220	1	
381	Fe-POM/attapulgite composite materials: Efficient catalysts for plastic pyrolysis.. <i>Waste Management and Research</i> , <b>2022</b> , 734242X221080084	4	0
380	Structural Modifications on Chalcone Framework for Developing New Class of Cholinesterase Inhibitors.. <i>International Journal of Molecular Sciences</i> , <b>2022</b> , 23,	6.3	2
379	Computational Study on the Inhibitory Effect of Natural Compounds against the SARS-CoV-2 Proteins.. <i>Bioinorganic Chemistry and Applications</i> , <b>2022</b> , 2022, 8635054	4.2	3
378	Critical role of nitric oxide in impeding COVID-19 transmission and prevention: a promising possibility.. <i>Environmental Science and Pollution Research</i> , <b>2022</b> , 1	5.1	1
377	Synthesis, Characterization, Biological Activity and Molecular Docking Studies of Novel Organotin(IV) Carboxylates.. <i>Frontiers in Pharmacology</i> , <b>2022</b> , 13, 864336	5.6	2
376	Experimental spectra, electronic energies (liquid and gaseous phases) quantum computational strategies and potential biological activity studies of (1E, 4E)-1, 5-bis (4-methoxyphenyl) penta-1,4-dien-3-one: An antiviral agent. <i>Journal of Molecular Liquids</i> , <b>2022</b> , 356, 119012	6	0
375	Synthesis of hybrid biosorbent based on 1,2-cyclohexylenedinitrilotetraacetic acid modified crosslinked chitosan and organo-functionalized calcium alginate for adsorptive removal of Cu(II).. <i>International Journal of Biological Macromolecules</i> , <b>2022</b> , 209, 132-143	7.9	3
374	Synthesis and Application of Egg Shell Biochar for As(V) Removal from Aqueous Solutions. <i>Catalysts</i> , <b>2022</b> , 12, 431	4	2
373	3D CoMoO nanoflake arrays decorated disposable pencil graphite electrode for selective and sensitive enzyme-less electrochemical glucose sensors.. <i>Mikrochimica Acta</i> , <b>2022</b> , 189, 200	5.8	2
372	Revealing the role of the benzyloxy pharmacophore in the design of a new class of monoamine oxidase-B inhibitors.. <i>Archiv Der Pharmazie</i> , <b>2022</b> , e2200084	4.3	1
371	DFT investigation of graphene quantum dot-Ixora floral natural dye (GQD-NDIX) nanocomposites as visible light harvesters in dye-sensitized solar cells. <i>Journal of Molecular Liquids</i> , <b>2022</b> , 119531	6	0
370	Modified alginate-chitosan-TiO composites for adsorptive removal of Ni(II) ions from aqueous medium. <i>International Journal of Biological Macromolecules</i> , <b>2021</b> , 194, 117-127	7.9	2
369	Coumaronochromone as antibacterial and carbonic anhydrase inhibitors from (Burm.f.) Merr.: experimental and first-principles approaches. <i>Zeitschrift Fur Naturforschung - Section C Journal of Biosciences</i> , <b>2021</b> , 76, 71-78	1.7	3
368	A DFT+U study of the effect of transition metal replacements on optoelectronic and elastic properties of TmCu <sub>3</sub> S <sub>4</sub> (Tm = V, Ta, Nb). <i>Optik</i> , <b>2021</b> , 250, 168289	2.5	0
367	Multifunctional Magnetic Nanomedicine Drug Delivery and Imaging-Based Diagnostic Systems. <i>Particle and Particle Systems Characterization</i> , <b>2021</b> , 38, 2100179	3.1	0
366	Facile Synthesis of Iron-Based MOFs MIL-100(Fe) as Heterogeneous Catalyst in Kabachnick Reaction. <i>Catalysts</i> , <b>2021</b> , 11, 1451	4	0
365	Polymer hydrogels for stabilization of inorganic nanoparticles and their application in catalysis for degradation of toxic chemicals. <i>Environmental Technology (United Kingdom)</i> , <b>2021</b> , 1-11	2.6	0

364	Nanostructure Engineering via Intramolecular Construction of Carbon Nitride as Efficient Photocatalyst for CO Reduction.. <i>Nanomaterials</i> , <b>2021</b> , 11,	5.4	7
363	Highly enhanced dye adsorption of MoO nanoplates fabricated by hydrothermal-calcination approach in presence of chitosan and thiourea. <i>Chemosphere</i> , <b>2021</b> , 132926	8.4	0
362	Enhanced Solar Photocatalytic Reduction of Cr(VI) Using a (ZnO/CuO) Nanocomposite Grafted onto a Polyester Membrane for Wastewater Treatment. <i>Polymers</i> , <b>2021</b> , 13,	4.5	3
361	evaluation of NO donor heterocyclic vasodilators as SARS-CoV-2 M protein inhibitor. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 1-18	3.6	3
360	Developing Efficient Small Molecule Acceptors with sp <sup>2</sup> -Hybridized Nitrogen at Different Positions by Density Functional Theory Calculations, Molecular Dynamics Simulations and Machine Learning. <i>Chemistry - A European Journal</i> , <b>2021</b> ,	4.8	22
359	Structural, vibrational, electronic properties, hirshfeld surface analysis topological and molecular docking studies of N-[2-(diethylamino)ethyl]-2-methoxy-5-methylsulfonylbenzamide. <i>Heliyon</i> , <b>2021</b> , 7, e08186	3.6	5
358	Isolation of phytochemicals from Malva neglecta Wallr and their quantum chemical, molecular docking exploration as active drugs against COVID-19. <i>Journal of Saudi Chemical Society</i> , <b>2021</b> , 101358	4.3	2
357	Synthesis of pure and lanthanum-doped barium ferrite nanoparticles for efficient removal of toxic pollutants. <i>Journal of Hazardous Materials</i> , <b>2021</b> , 424, 127604	12.8	2
356	Potential of NO donor furoxan as SARS-CoV-2 main protease (M) inhibitors: analysis. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 39, 5804-5818	3.6	12
355	Excited state absorption of Cu-doped barium borate nanostructures under nanopulsed laser excitation. <i>European Physical Journal D</i> , <b>2021</b> , 75, 1	1.3	1
354	Growth of ZnSexO1x Nanorods and Their Photoelectrochemical Properties. <i>Energy &amp; Fuels</i> , <b>2021</b> , 35, 6289-6297	4.1	1
353	Quaternary CuFeSnS/PVP/rGO Composite for Supercapacitor Applications. <i>ACS Omega</i> , <b>2021</b> , 6, 9471-9484	4.9	9
352	Cobalt-based derivatives oxygen evolution reaction. <i>Applied Nanoscience (Switzerland)</i> , <b>2021</b> , 11, 1367-1378	3.7	2
351	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> , <b>2021</b> , 767, 138379	2.5	22
350	COVID-19 and Domestic Animals: Exploring the Species Barrier Crossing, Zoonotic and Reverse Zoonotic Transmission of SARS-CoV-2. <i>Current Pharmaceutical Design</i> , <b>2021</b> , 27, 1194-1201	3.3	8
349	Effect of cationic, anionic, and mixed surfactant role on manganese oxide nanoparticles for energy storage applications. <i>Applied Nanoscience (Switzerland)</i> , <b>2021</b> , 11, 1769-1775	3.3	1
348	Recyclable polymer microgel stabilized rhodium nanoparticles for reductive degradation of para-nitrophenol. <i>Zeitschrift Fur Physikalische Chemie</i> , <b>2021</b> ,	3.1	1
347	Glycerol Conversion to Solketal: Catalyst and Reactor Design, and Factors Affecting the Yield. <i>ChemBioEng Reviews</i> , <b>2021</b> , 8, 227-238	5.2	2

346	Lipase-PDA-TiO <sub>2</sub> NPs: An emphatic nano-biocatalyst for optimized biodiesel production from <i>Jatropha curcas</i> oil. <i>Renewable Energy</i> , <b>2021</b> , 169, 1026-1037	8.1	20
345	The Chronicle of COVID-19 and Possible Strategies to Curb the Pandemic. <i>Current Medicinal Chemistry</i> , <b>2021</b> , 28, 2852-2886	4.3	9
344	A Study on Optoelectronic Properties of Copper Zinc Tin Sulfur Selenide: A Promising Thin-Film Material for Next Generation Solar Technology. <i>Crystal Research and Technology</i> , <b>2021</b> , 56, 2000159	1.3	
343	Adsorption behavior of mercury over hydrated lime: Experimental investigation and adsorption process characteristic study. <i>Chemosphere</i> , <b>2021</b> , 271, 129504	8.4	13
342	Counteraction of Biofilm Formation and Antimicrobial Potential of Functionalized Silver Nanoparticles against and Multidrug-Resistant Gram-Negative and Gram-Positive Bacteria. <i>Antibiotics</i> , <b>2021</b> , 10,	4.9	10
341	NiMoO nanorods photocatalytic activity comparison under UV and visible light. <i>Environmental Research</i> , <b>2021</b> , 197, 111073	7.9	2
340	Leaves; UHPLC-QTOF-MS/MS Based Metabolite Profiling and Molecular Docking Insights to Explore Bioactives Role Towards Inhibition of Pancreatic Lipase. <i>Plants</i> , <b>2021</b> , 10,	4.5	2
339	Synthesis, antioxidant, and computational investigation of 2,5-dihydroxyacetophenone derived chloro-substituted hydroxychalcones, hydroxyflavanones and hydroxyflavindogenides. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 1-13	3.6	0
338	Sources, chemistry, bioremediation and social aspects of arsenic-contaminated waters: a review. <i>Environmental Chemistry Letters</i> , <b>2021</b> , 19, 3859-3886	13.3	8
337	Effects of expandable graphite on char morphology and pyrolysis of epoxy based intumescent fire-retardant coating. <i>Journal of Applied Polymer Science</i> , <b>2021</b> , 138, 51206	2.9	2
336	An Efficient Synthesis, Spectroscopic Characterization, and Optical Nonlinearity Response of Novel Salicylaldehyde Thiosemicarbazone Derivatives. <i>ACS Omega</i> , <b>2021</b> , 6, 16058-16065	3.9	8
335	Current Progress in Quinazoline Derivatives as Acetylcholinesterase and Monoamine Oxidase Inhibitors. <i>ChemistrySelect</i> , <b>2021</b> , 6, 7162-7182	1.8	3
334	A Superficial Intramolecular Alignment of Carbon Nitride through Conjugated Monomer for Optimized Photocatalytic CO <sub>2</sub> Reduction. <i>Catalysts</i> , <b>2021</b> , 11, 935	4	11
333	Influence of crystal size on structural, magnetic, mechanical, and dielectric properties of Ni-Cu-Zn nanoferrites. <i>Journal of Materials Science: Materials in Electronics</i> , <b>2021</b> , 32, 19786-19797	2.1	0
332	Deciphering the detailed structure-activity relationship of coumarins as Monoamine oxidase enzyme inhibitors-An updated review. <i>Chemical Biology and Drug Design</i> , <b>2021</b> , 98, 655-673	2.9	5
331	Exploring the potential of novel phenolic compounds as potential therapeutic candidates against SARS-CoV-2, using quantum chemistry, molecular docking and dynamic studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2021</b> , 43, 128079	2.9	9
330	Theoretical investigation of structural and magnetic properties of MnTiX (X = Si, Ge, Se, Te) half-Heusler alloys. <i>Indian Journal of Physics</i> , <b>2021</b> , 95, 841-849	1.4	3
329	Natural rubber composites containing low and high dielectric constant fillers and their application as substrates for compact flexible antennas. <i>Polymers and Polymer Composites</i> , <b>2021</b> , 29, 233-245	0.8	1

328	Comparative Adsorption of Pb <sup>2+</sup> on Nanostructured IronZirconium Oxide with Fe-to-Zr Molar Ratio of 1:1 and 1:2: Thermodynamic and Kinetic Studies. <i>Arabian Journal for Science and Engineering</i> , <b>2021</b> , 46, 287-300	2.5	1
327	Inorganic nanoparticles for reduction of hexavalent chromium: Physicochemical aspects. <i>Journal of Hazardous Materials</i> , <b>2021</b> , 402, 123535	12.8	43
326	A review on the waste biomass derived catalysts for biodiesel production. <i>Environmental Technology and Innovation</i> , <b>2021</b> , 21, 101200	7	44
325	Exploring the effect of oligothiophene and acene cores on the optoelectronic properties and enhancing p- and n-type ability of semiconductor materials. <i>Journal of Sulfur Chemistry</i> , <b>2021</b> , 42, 180-192 <sup>3</sup>	2.3	4
324	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> , <b>2021</b> , 102, 107766	2.8	5
323	An exploration of the optoelectronic nature of 4,4-difluoro-8-(C <sub>4</sub> H <sub>3</sub> X)-4-bora-3a,4a-diaza-s-indacene (X = O, S, Se) (BODIPY) systems. <i>Journal of Computational Electronics</i> , <b>2021</b> , 20, 368-376	1.8	1
322	Superior supercapacitive performance of Cu <sub>2</sub> MnSnS <sub>4</sub> asymmetric devices. <i>Nanoscale Advances</i> , <b>2021</b> , 3, 486-498	5.1	10
321	Stabilization of silver nanoparticles in crosslinked polymer colloids through chelation for catalytic degradation of p-nitroaniline in aqueous medium. <i>Chemical Physics Letters</i> , <b>2021</b> , 763, 138263	2.5	11
320	Effect of expandable graphite and ammonium polyphosphate on the thermal degradation and weathering of intumescent fire-retardant coating. <i>Journal of Applied Polymer Science</i> , <b>2021</b> , 138, 50310	2.9	4
319	Design, facile synthesis, spectroscopic characterization, and medicinal probing of metal-based new sulfonamide drugs: A theoretical and spectral study. <i>Applied Organometallic Chemistry</i> , <b>2021</b> , 35,	3.1	11
318	Synthesis of Urease Inhibitory 2, 4-bis (4-cyanobenzyl)glycoluril using Sandmeyer Reaction and Density Functional Theory Investigation. <i>Current Organic Synthesis</i> , <b>2021</b> , 18, 592-597	1.9	
317	Molecular structure controlled self-assembly of pyridine appended fluorophores: multi-stimuli fluorescence responses and fabricating rewritable/self-erasable fluorescent platforms. <i>Materials Advances</i> , <b>2021</b> , 2, 996-1005	3.3	12
316	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> , <b>2021</b> , 27, 12	2	14
315	Recent advances in excited state intramolecular proton transfer mechanism-based solid state fluorescent materials and stimuli-responsive fluorescence switching. <i>CrystEngComm</i> , <b>2021</b> , 23, 3771-3789 <sup>3</sup>	2.3	13
314	Digera muricata (L.) Mart. mediated synthesis of antimicrobial and enzymatic inhibitory zinc oxide bionanoparticles. <i>Green Processing and Synthesis</i> , <b>2021</b> , 10, 476-484	3.9	1
313	Design of a flexible waterproof antenna for Internet of Things applications. <i>Journal of Electromagnetic Waves and Applications</i> , <b>2021</b> , 35, 874-887	1.3	1
312	A butterfly shaped organic heterojunction photocatalyst for effective photocatalytic CO <sub>2</sub> reduction. <i>CrystEngComm</i> , <b>2021</b> , 23, 4963-4974	3.3	3
311	Exploring the electron-hole transport nature and optoelectronic properties of 4-nitro-4'-amino-azobenzene-based dyes. <i>Structural Chemistry</i> , <b>2021</b> , 32, 1113-1121	1.8	



310	Nanobiocatalysts for Biodiesel Synthesis through Transesterification: A Review. <i>Catalysts</i> , <b>2021</b> , 11, 171	4	4
309	Push-pull effect on the charge transport characteristics in V-shaped organic semiconductor materials. <i>Bulletin of Materials Science</i> , <b>2021</b> , 44, 1	1.7	1
308	SARS-CoV-2 Genome from the Khyber Pakhtunkhwa Province of Pakistan. <i>ACS Omega</i> , <b>2021</b> , 6, 6588-6599	3.9	2
307	Novel W-Shaped Oxygen Heterocycle-Fused Fluorene-Based Non-Fullerene Acceptors: First Theoretical Framework for Designing Environment-Friendly Organic Solar Cells. <i>Energy &amp; Fuels</i> , <b>2021</b> , 35, 12436-12450	4.1	24
306	Effect of the Active Layer Thickness of Pentacene Thin Film Transistor; Illumination Effect. <i>Journal of Electronic Materials</i> , <b>2021</b> , 50, 5701-5712	1.9	
305	Design and investigation of novel Maraviroc analogues as dual inhibition of CCR-5/SARS-CoV-2 M. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 1-16	3.6	3
304	Investigation on (Zn) doping and anionic surfactant (SDS) effect on SnO nanostructures for enhanced photocatalytic RhB dye degradation. <i>Environmental Research</i> , <b>2021</b> , 199, 111312	7.9	5
303	Exploration of electronic properties, radical scavenging activity and QSAR of oxadiazole derivatives by molecular docking and first-principles approaches. <i>Saudi Journal of Biological Sciences</i> , <b>2021</b> , 28, 7416-7421	4.7	1
302	Silver nanoparticles supported on smart polymer microgel system for highly proficient catalytic reduction of Cr+6 to Cr+3 with formic acid. <i>Applied Organometallic Chemistry</i> , <b>2021</b> , 35, e6405	3.1	5
301	Structural (monomer and dimer), wavefunctional, NCI analysis in aqueous phase, electronic and excited state properties in different solvent atmosphere of 3-((E)-[(3,4-dichlorophenyl)imino]methyl) benzene-1,2-diol. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 336, 116335	6	11
300	Phenolic and flavonoid contents in Malva sylvestris and exploration of active drugs as antioxidant and anti-COVID19 by quantum chemical and molecular docking studies. <i>Journal of Saudi Chemical Society</i> , <b>2021</b> , 25, 101277	4.3	8
299	Organic heterostructure modified carbon nitride as apprehension for Quercetin Biosensor. <i>Synthetic Metals</i> , <b>2021</b> , 278, 116813	3.6	13
298	Gold nanoparticles and polymer microgels: Last five years of their happy and successful marriage. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 336, 116270	6	11
297	A molecular amalgamation of carbon nitride polymer as emphasized photocatalytic performance. <i>International Journal of Energy Research</i> , <b>2021</b> , 45, 19921	4.5	6
296	Computational investigation, comparative approaches, molecular structural, vibrational spectral, non-covalent interaction (NCI), and electron excitations analysis of benzodiazepine derivatives. <i>Journal of Molecular Modeling</i> , <b>2021</b> , 27, 266	2	5
295	Combinatorial synthesis of tin antimony sulfide thin films for solar cell application. <i>International Journal of Energy Research</i> , <b>2021</b> , 45, 21527	4.5	0
294	Poly(styrene@N-isopropylmethacrylamide-co-methacrylic acid)@Ag hybrid particles with excellent catalytic potential. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 335, 116106	6	13
293	Flower-like CuO/NiO nanostructures decorated activated carbon nanofiber membranes for flexible, sensitive, and selective enzyme-free glucose detection. <i>Journal of Materials Science: Materials in Electronics</i> , <b>2021</b> , 32, 24775	2.1	6

292	Pyrazines with terminal donor groups for third-order nonlinear optics: effect of graphene oxide on nonlinear absorption. <i>Journal of Chemical Sciences</i> , <b>2021</b> , 133, 1	1.8	1
291	Metal incorporated aminothiazole-derived compounds: synthesis, density function theory analysis, antibacterial and antioxidant evaluation. <i>Royal Society Open Science</i> , <b>2021</b> , 8, 210910	3.3	10
290	Synthesis, characterization, anti-proliferative activity and DFT study of 1H-benzo[f]chromene-2-carbothioamide derivatives. <i>Journal of Molecular Structure</i> , <b>2021</b> , 1240, 130542	3.4	1
289	Quantum chemical analysis and molecular dynamics simulations to study the impact of electron-deficient substituents on electronic behavior of small molecule acceptors. <i>Computational and Theoretical Chemistry</i> , <b>2021</b> , 1204, 113387	2	10
288	Synthesis, spectral and quantum mechanical studies and molecular docking studies of Schiff base (E)2-hydroxy-5-(((4-(N-pyrimidin-2-yl)sulfamoyl)phenyl)imino)methyl benzoic acid from 5-formyl salicylic acid and sulfadiazine. <i>Journal of the Indian Chemical Society</i> , <b>2021</b> , 98, 100144		11
287	2D materials for bone therapy. <i>Advanced Drug Delivery Reviews</i> , <b>2021</b> , 178, 113970	18.5	3
286	Constructing anatase TiO/Amorphous NbO heterostructures to enhance photocatalytic degradation of acetaminophen and nitrogen oxide. <i>Journal of Colloid and Interface Science</i> , <b>2021</b> , 601, 346-354	9.3	9
285	Meteloxetin (1) Novel Phenolic Amino-Oxetane Cholinesterase Inhibitors from Datura metel Linn and First-Principle Investigations. <i>Arabian Journal for Science and Engineering</i> , <b>2021</b> , 46, 5681-5690	2.5	1
284	Synthesis of Copper(II) Coordination Complex, Its Molecular Docking and Computational Exploration for Novel Functional Properties: A Dual Approach. <i>ChemistrySelect</i> , <b>2021</b> , 6, 738-745	1.8	9
283	Structure and composition characterization of biocomposites filled with sol-gel bioglasses from the CaO/Bi <sub>2</sub> O <sub>3</sub> /P <sub>2</sub> O <sub>5</sub> /Ag <sub>2</sub> O systems. <i>Journal of Rubber Research (Kuala Lumpur, Malaysia)</i> , <b>2021</b> , 24, 77-92	0.9	
282	Molecular Docking, Structural Examination, Reactive Sites Identification (HOMO/LUMO, MEP) of 6-Phenylpteridine 2, 4, 7-triamine: Potential Bacterial Inhibitor. <i>Analytical Chemistry Letters</i> , <b>2021</b> , 11, 886-898	1	1
281	Spectroscopic (FT-IR, FT-Raman, UV-Visible), Quantum Mechanical Based Computational Studies and Molecular Docking Analysis of 2-Amino-3,5-dichloropyridine. <i>Analytical Chemistry Letters</i> , <b>2021</b> , 11, 848-861	1	
280	An Implicit Numerical Approach for 2D Rayleigh Stokes Problem for a Heated Generalized Second Grade Fluid with Fractional Derivative. <i>Fractal and Fractional</i> , <b>2021</b> , 5, 283	3	0
279	Wet chemical development of CuO/GO nanocomposites: its augmented antimicrobial, antioxidant, and anticancerous activity. <i>Journal of Materials Science: Materials in Medicine</i> , <b>2021</b> , 32, 151	4.5	0
278	Spectroscopic profiling, DFT computations, molecular docking and molecular dynamic simulation of biologically active 5-isoquinolinesulfonic acid. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 1-14	2.6	0
277	Synthesis and characterization of poly(N-isopropylmethacrylamide-acrylic acid) smart polymer microgels for adsorptive extraction of copper(II) and cobalt(II) from aqueous medium: kinetic and thermodynamic aspects. <i>Environmental Science and Pollution Research</i> , <b>2020</b> , 27, 28169-28182	5.1	10
276	Core-shell microgel stabilized silver nanoparticles for catalytic reduction of aryl nitro compounds. <i>Applied Organometallic Chemistry</i> , <b>2020</b> , 34, e5742	3.1	7
275	Synthesis, characterizations, crystal structures, and theoretical studies of copper(II) and nickel(II) coordination complexes. <i>Journal of Coordination Chemistry</i> , <b>2020</b> , 73, 1256-1279	1.6	7



274	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> , <b>2020</b> , 754, 137645	2.5	24
273	3D Flower-Like FeWO <sub>3</sub> /CeO <sub>2</sub> Hierarchical Architectures on rGO for Durable and High-Performance Microalgae Biophotovoltaic Fuel Cells. <i>Applied Biochemistry and Biotechnology</i> , <b>2020</b> , 192, 751-769	3.2	5
272	Highly enhanced bifunctional electrocatalytic activity of mixed copper/copper oxides on nickel foam via composition control. <i>New Journal of Chemistry</i> , <b>2020</b> , 44, 11993-12001	3.6	6
271	An experimental and computational study of pyrimidine based bis-uracil derivatives as efficient candidates for optical, nonlinear optical, and drug discovery applications. <i>Synthetic Communications</i> , <b>2020</b> , 50, 2199-2225	1.7	9
270	Natural rubber composites containing fillers of sol-gel glasses and glass-ceramics in the CaO/SiO <sub>2</sub> /B <sub>2</sub> O <sub>5</sub> system. <i>Iranian Polymer Journal (English Edition)</i> , <b>2020</b> , 29, 799-810	2.3	
269	Facile Synthesis, Spectral (IR, Mass, UV-Vis, NMR), Linear and Nonlinear Investigation of the Novel Phosphonate Compounds: A Combined Experimental and Simulation Study. <i>ChemistrySelect</i> , <b>2020</b> , 5, 2994-3006	1.8	12
268	Systematic study of catalytic degradation of nitrobenzene derivatives using core@shell composite micro particles as catalyst. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , <b>2020</b> , 594, 124646	5.1	11
267	UHPLC-QTOF-MS/MS metabolites profiling and antioxidant/antidiabetic attributes of <i>Cuscuta reflexa</i> grown on <i>Casearia tomentosa</i> : exploring phytochemicals role via molecular docking. <i>International Journal of Food Properties</i> , <b>2020</b> , 23, 918-940	3	6
266	Equilibrium, kinetics and artificial intelligence characteristic analysis for Zn (II) ion adsorption on rice husks digested with nitric acid. <i>Paddy and Water Environment</i> , <b>2020</b> , 18, 455-468	1.6	3
265	A Temperature Sensor Based on Al/p-Si/CuCdO <sub>2</sub> /Al Diode for Low Temperature Applications. <i>Journal of Electronic Materials</i> , <b>2020</b> , 49, 2317-2325	1.9	4
264	Thermal Conductivity of Multiwalled Carbon Nanotubes-Kapok Seed Oil-Based Nanofluid. <i>Chemical Engineering and Technology</i> , <b>2020</b> , 43, 1638-1647	2	2
263	Carbonic anhydrase and cholinesterase inhibitory activities of isolated flavonoids from <i>Oxalis corniculata</i> L. and their first-principles investigations. <i>Industrial Crops and Products</i> , <b>2020</b> , 148, 112285	5.9	12
262	Synthesis, Crystal Structure, and Nonlinear Optical Properties of Zn(II) Complex with 4,4',4''-Tri-tert-Butyl-2,2':6',2''-Terpyridine: A Dual Exploration. <i>Russian Journal of Inorganic Chemistry</i> , <b>2020</b> , 65, 368-377	1.5	1
261	Withdrawal Notice: Pharmacological analysis of <i>Cannabis sativa</i> L.: A potent herbal plant. <i>Mini-Reviews in Medicinal Chemistry</i> , <b>2020</b> ,	3.2	3
260	Rubber-ceramic composites applicable in flexible antennas. <i>Journal of Polymer Engineering</i> , <b>2020</b> , 40, 666-675	1.4	
259	Effect of fluorination on exciton binding energy and electronic coupling in small molecule acceptors for organic solar cells. <i>Computational and Theoretical Chemistry</i> , <b>2020</b> , 1179, 112797	2	20
258	Antidiabetic functionality of <i>Vitex negundo</i> L. leaves based on UHPLC-QTOF-MS/MS based bioactives profiling and molecular docking insights. <i>Industrial Crops and Products</i> , <b>2020</b> , 152, 112445	5.9	14
257	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> , <b>2020</b> , 43, 97-109	3.7	19

256	Characteristically Insights, Artificial Neural Network (ANN), Equilibrium, and Kinetic Studies of Pb(II) Ion Adsorption on Rice Husks Treated with Nitric Acid. <i>International Journal of Environmental Research</i> , <b>2020</b> , 14, 43-60	2.9	9
255	Experimental investigations on the regeneration of desulfurized 1-butyl-3-methylimidazolium tetrachloroferrate [Bmim][FeCl <sub>4</sub> ] and 1-butyl-3-methylimidazolium thiocyanate [Bmim][SCN] ionic liquids: A raman spectroscopic study. <i>Journal of Raman Spectroscopy</i> , <b>2020</b> , 51, 546-554	2.3	3
254	Synthesis, characterization and quantum chemical study of optoelectronic nature of ferrocene derivatives. <i>Bulletin of Materials Science</i> , <b>2020</b> , 43, 1	1.7	11
253	Polymorphs of a copper coordination compound: interlinking active sites enhance the electrocatalytic activity of the coordination polymer compared to the coordination complex. <i>CrystEngComm</i> , <b>2020</b> , 22, 425-429	3.3	5
252	Natural rubberBased composites filled with bioglasses from a CaO-SiO <sub>2</sub> -P <sub>2</sub> O <sub>5</sub> -Ag <sub>2</sub> O system. Effect of Ag <sub>2</sub> O concentration in the filler on composite properties. <i>Polymers for Advanced Technologies</i> , <b>2020</b> , 31, 574-588	3.2	2
251	Fe <sub>3</sub> O <sub>4</sub> -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> , <b>2020</b> , 13, 177	3.1	38
250	Vanadium Sulfide@Sulfur Composites as High-Performance Cathode for Advanced LithiumSulfur Batteries. <i>Energy Technology</i> , <b>2020</b> , 8, 1901163	3.5	13
249	Electron donating effect of amine groups on charge transfer and photophysical properties of 1,3-diphenyl-1H-pyrazolo[3,4-b]quinolone at molecular and solid state bulk levels. <i>Optik</i> , <b>2020</b> , 208, 164009	2.5	9
248	Statistical Assessment of Toxic and Essential Metals in the Serum of Female Patients with Lung Carcinoma from Pakistan. <i>Biological Trace Element Research</i> , <b>2020</b> , 197, 367-383	4.5	4
247	Physicochemical aspects of reduction of 3-Nitroaniline using methacrylamide based nano-hybrid catalyst. <i>Chemical Physics Letters</i> , <b>2020</b> , 759, 137992	2.5	1
246	Catalytic degradation of malachite green using a crosslinked colloidal polymeric system loaded with silver nanoparticles. <i>International Journal of Environmental Analytical Chemistry</i> , <b>2020</b> , 1-17	1.8	16
245	Silver nanoparticles stabilized in polymer hydrogels for catalytic degradation of azo dyes. <i>Ecotoxicology and Environmental Safety</i> , <b>2020</b> , 202, 110924	7	32
244	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> , <b>2020</b> , 100, 107665	2.8	15
243	Promising architectures modifying the D-πA architecture of 2,3-dipentylidithieno[3,2-f:2',3'-h]quinoxaline-based dye as efficient sensitizers in dye-sensitized solar cells: A DFT study. <i>Materials Science in Semiconductor Processing</i> , <b>2020</b> , 120, 105260	4.3	8
242	Porous Titanium Oxide Microspheres as Promising Catalyst for LithiumOxygen Batteries. <i>Energy Technology</i> , <b>2020</b> , 8, 1901257	3.5	4
241	Natural Products Database Screening for the Discovery of Naturally Occurring SARS-Cov-2 Spike Glycoprotein Blockers. <i>ChemistrySelect</i> , <b>2020</b> , 5, 13309-13317	1.8	11
240	Zirconium-Ferrite Nanoparticles As Improved Adsorbent for Co <sup>2+</sup> , Cu <sup>2+</sup> , and Zn <sup>2+</sup> : Thermodynamic and Kinetic Studies. <i>Russian Journal of Physical Chemistry A</i> , <b>2020</b> , 94, 2797-2809	0.7	0
239	Detailed spectra, electronic properties, qualitative non-covalent interaction analysis, solvatochromism, docking and molecular dynamics simulations in different solvent atmosphere of cenobamate. <i>Structural Chemistry</i> , <b>2020</b> , 31, 2475-2485	1.8	27

238	Exploration of adsorption behavior, electronic nature and NLO response of hydrogen adsorbed Alkali metals (Li, Na and K) encapsulated Al12N12 nanocages. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2020</b> , 19, 2050031	1.8	30
237	Exploration of electronic nature and intrinsic mobility of 10-(1,3-dithiol-2-ylidene)anthracene based organic semiconductor materials. <i>Optik</i> , <b>2020</b> , 224, 165530	2.5	9
236	Synthesis, Structure Study, First-Principles Investigations and Luminescence Properties of Europium and Terbium Complexes. <i>Journal of Fluorescence</i> , <b>2020</b> , 30, 1345-1355	2.4	1
235	Hole transport nature exploration of 4,4-Difluoro-8-(C4H3X)-4-bora-3a,4a-diaza-s-indacene (X = O, S, Se) (BODIPY) systems. <i>Molecular Simulation</i> , <b>2020</b> , 46, 1334-1339	2	5
234	Zero valent iron nanoparticles as sustainable nanocatalysts for reduction reactions. <i>Catalysis Reviews - Science and Engineering</i> , <b>2020</b> , 1-70	12.6	4
233	Design and synthesis of organic dyes with various donor groups: promising dyes for dye-sensitized solar cells. <i>Bulletin of Materials Science</i> , <b>2020</b> , 43, 1	1.7	3
232	Chemical reduction of methylene blue in the presence of nanocatalysts: a critical review. <i>Reviews in Chemical Engineering</i> , <b>2020</b> , 36, 749-770	5	45
231	Hybrid Microgels for Catalytic and Photocatalytic Removal of Nitroarenes and Organic Dyes From Aqueous Medium: A Review. <i>Critical Reviews in Analytical Chemistry</i> , <b>2020</b> , 50, 513-537	5.2	25
230	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> , <b>2020</b> , 1201, 127183	3.4	34
229	Triphenylamine-based stimuli-responsive solid state fluorescent materials. <i>New Journal of Chemistry</i> , <b>2020</b> , 44, 8680-8696	3.6	24
228	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> , <b>2020</b> , 19, 931-939	1.8	17
227	Physicochemical aspects of inorganic nanoparticles stabilized in -vinyl caprolactam based microgels for various applications.. <i>RSC Advances</i> , <b>2020</b> , 11, 978-995	3.7	3
226	High-temperature CO2 removal from CH4 using silica membrane: experimental and neural network modeling <b>2019</b> , 9, 1010-1026		15
225	Exploring the optoelectronic and charge transport properties of Pechmann dyes as efficient OLED materials. <i>Optik</i> , <b>2019</b> , 197, 163200	2.5	8
224	Linear, second and third order nonlinear optical properties of novel noncentrosymmetric donor-acceptor configure chalcone derivatives: A dual approach study. <i>Optik</i> , <b>2019</b> , 199, 163354	2.5	20
223	Synthesis, growth, structural, thermal, third order nonlinear and computational studies of organic single crystal: 2-Amino-4-picolinium 2-chloro-4-nitrobenzoate. <i>Optical Materials</i> , <b>2019</b> , 96, 109341	3.3	5
222	An investigation on thermal performance of wollastonite and bentonite reinforced intumescent fire-retardant coating for steel structures. <i>Construction and Building Materials</i> , <b>2019</b> , 228, 116734	6.7	23
221	Effect of Strontium Doping on the Band Gap of (hbox {CeO}_{2}) Nanoparticles Synthesized Using Facile Co-precipitation. <i>Arabian Journal for Science and Engineering</i> , <b>2019</b> , 44, 6295-6302	2.5	10

220	Reactive kinetics of carbon dioxide loaded aqueous blend of 2-amino-2-ethyl-1,3-propanediol and piperazine using a pressure drop method. <i>International Journal of Chemical Kinetics</i> , <b>2019</b> , 51, 291-298	1.4	11
219	Synthesis, and characterization of metal-organic frameworks -177 for static and dynamic adsorption behavior of CO <sub>2</sub> and CH <sub>4</sub> . <i>Microporous and Mesoporous Materials</i> , <b>2019</b> , 288, 109569	5.3	37
218	Mercerization effect on structure and electrical properties of cellulose: Development of a novel fast Na-ionic conductor. <i>Carbohydrate Polymers</i> , <b>2019</b> , 221, 29-36	10.3	9
217	One pot synthesis and surface modification of mesoporous iron oxide nanoparticles. <i>Nano Structures Nano Objects</i> , <b>2019</b> , 19, 100343	5.6	8
216	Electrical, mechanical and dynamic properties of ternary composites from acrylonitrile butadiene rubber and conductive fillers. <i>Bulletin of Materials Science</i> , <b>2019</b> , 42, 1	1.7	1
215	Experimental and theoretical study of planar small molecule acceptor for organic solar cells. <i>Journal of Molecular Structure</i> , <b>2019</b> , 1196, 169-175	3.4	13
214	Ruthenium oxide/tungsten oxide composite nanofibers as anode catalysts for the green energy generation of <i>Chlorella vulgaris</i> mediated biophotovoltaic cells. <i>Environmental Progress and Sustainable Energy</i> , <b>2019</b> , 38, e13262	2.5	7
213	Fundamentals and applications of acrylamide based microgels and their hybrids: a review.. <i>RSC Advances</i> , <b>2019</b> , 9, 13838-13854	3.7	9
212	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> , <b>2019</b> , 143, 898-905	8.1	22
211	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> , <b>2019</b> , 125, 1	2.6	14
210	Exploring the electronic, optical and charge transfer properties of acene-based organic semiconductor materials. <i>Bulletin of Materials Science</i> , <b>2019</b> , 42, 1	1.7	11
209	A dual approach to study the synthesis, crystal structure and nonlinear optical properties of binuclear Pd(II) complex of 3-methyl-5-(trifluoromethyl) pyrazole and its potential quantum chemical analogues. <i>Inorganica Chimica Acta</i> , <b>2019</b> , 494, 160-167	2.7	9
208	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> , <b>2019</b> , 1190, 54-67	3.4	21
207	Comparison of mono- and di-substituted triphenylamine and carbazole based sensitizers @TiO <sub>2</sub> 38 cluster for dye-sensitized solar cells applications. <i>Computational and Theoretical Chemistry</i> , <b>2019</b> , 1159, 1-6	2	25
206	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> , <b>2019</b> , 13, 102304	3.7	15
205	Exploring the Effect of Electron Withdrawing Groups on Optoelectronic Properties of Pyrazole Derivatives as Efficient Donor and Acceptor Materials for Photovoltaic Devices. <i>Zeitschrift Fur Physikalische Chemie</i> , <b>2019</b> , 233, 1625-1644	3.1	5
204	PEDOT/NiFe <sub>2</sub> O <sub>4</sub> nanocomposites on biochar as a free-standing anode for high-performance and durable microbial fuel cells. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 7743-7750	3.6	27
203	Synthesis and Antiplatelet Potential Evaluation of 1,3,4-Oxadiazoles Derivatives. <i>Zeitschrift Fur Physikalische Chemie</i> , <b>2019</b> , 233, 1741-1759	3.1	2

202	Photosensing properties of ruthenium(II) complex-based photodiode. <i>Applied Physics A: Materials Science and Processing</i> , <b>2019</b> , 125, 1	2.6	9
201	In Vitro Antimicrobial Activity and Metal Ion Sensing by Green Synthesized Silver Nanoparticles from Fruits of Opuntia Ficus Indica Grown in the Abha Region, Saudi Arabia. <i>Arabian Journal for Science and Engineering</i> , <b>2019</b> , 44, 43-49	2.5	3
200	Metallo-Phthalocyanines Based Photocapacitors. <i>Silicon</i> , <b>2019</b> , 11, 1275-1286	2.4	2
199	Removal of Cadmium (II) from Aqueous Medium Using Vigna radiata Leave Biomass: Equilibrium Isotherms, Kinetics and Thermodynamics. <i>Zeitschrift Fur Physikalische Chemie</i> , <b>2019</b> , 233, 669-690	3.1	2
198	Extraction of Heavy Metals from Aqueous Medium by Husk Biomass: Adsorption Isotherm, Kinetic and Thermodynamic study. <i>Zeitschrift Fur Physikalische Chemie</i> , <b>2019</b> , 233, 201-223	3.1	23
197	Turn-on fluorescence sensing of hydrazine using MnO <sub>2</sub> nanotube-decorated g-C <sub>3</sub> N <sub>4</sub> nanosheets. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 13196-13204	3.6	14
196	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> , <b>2019</b> , 170, 109179	3.2	15
195	Exploration of optoelectronic and photosensitization properties of triphenylamine-based organic dye on TiO <sub>2</sub> surfaces. <i>Journal of Computational Electronics</i> , <b>2019</b> , 18, 1119-1127	1.8	9
194	Effect of extended alkyl auxiliary groups on optical and electronic properties of Benzo[2,1-b:3,4-b':5,6-c']trithiophene derivatives at bulk level: a first-principles study. <i>Materials Research Express</i> , <b>2019</b> , 6, 095102	1.7	2
193	Modeling of efficient pyrene-core substituted with electron-donating groups as hole-transporting materials in perovskite solar cells. <i>Solar Energy</i> , <b>2019</b> , 188, 898-912	6.8	11
192	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> , <b>2019</b> , 18, 1950030	1.8	32
191	Exploring the Optoelectronic and Charge Transfer Nature of Ferrocene Derivatives: A First-Principles Approach. <i>Russian Journal of Inorganic Chemistry</i> , <b>2019</b> , 64, 1249-1256	1.5	0
190	Exploring the functional properties of Trimethoxy-Phenylpyridine as efficient optical and nonlinear optical material: A quantum chemical approach. <i>Journal of Molecular Structure</i> , <b>2019</b> , 1185, 268-275	3.4	0
189	A computational approach to study the optoelectronic properties of F-BODIPY derivatives at the bulk level for photovoltaic applications. <i>Materials Research Express</i> , <b>2019</b> , 6, 125110	1.7	0
188	Aggregation-enhanced emissive mechanofluorochromic carbazole-halogen positional isomers: tunable fluorescence via conformational polymorphism and crystallization-induced fluorescence switching. <i>CrystEngComm</i> , <b>2019</b> , 21, 6604-6612	3.3	9
187	Structural, spectroscopic and first-principles studies of new aminocoumarin derivatives. <i>Acta Crystallographica Section C, Structural Chemistry</i> , <b>2019</b> , 75, 1617-1627	0.8	1
186	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> , <b>2019</b> , 484, 148-159	3.7	27
185	The crystal structure of 2-((3-methylthiophen-2-yl)methylene)malononitrile, C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , <b>2019</b> , 234, 327-328	0.2	



184	AIE based On-off fluorescence probe for the detection of Cu <sup>2+</sup> ions in aqueous media. <i>Inorganic Chemistry Communication</i> , <b>2019</b> , 99, 11-15	3.1	11
183	Catalytic reduction of toxic dyes in the presence of silver nanoparticles impregnated core-shell composite microgels. <i>Journal of Cleaner Production</i> , <b>2019</b> , 211, 855-864	10.3	59
182	Synthesis and characterization of magnetic nanoparticles/dialdehyde cellulose composite as a flame retardant. <i>Materials Research Express</i> , <b>2019</b> , 6, 025312	1.7	8
181	A systematic study of the effects of thionation in naphthalene dimide derivatives to tune their nonlinear optical properties. <i>Journal of Molecular Graphics and Modelling</i> , <b>2019</b> , 87, 68-75	2.8	10
180	Anthracene Based AIE Active Probe for Colorimetric and Fluorimetric Detection of Cu <sup>2+</sup> Ions. <i>Zeitschrift Fur Physikalische Chemie</i> , <b>2019</b> , 233, 895-911	3.1	1
179	Exploring the effect of halogens on semiconducting nature of boron doped molecular precursor graphene nanoribbons at molecular and bulk level. <i>Optik</i> , <b>2019</b> , 179, 526-534	2.5	12
178	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> , <b>2019</b> , 277, 522-531	6	61
177	Structural, electronic and optical properties of furan based materials at bulk level for photovoltaic applications: A first-principles study. <i>Computational and Theoretical Chemistry</i> , <b>2019</b> , 1147, 20-28	2	6
176	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> , <b>2019</b> , 40, 2027-2036	2.6	49
175	Shedding light on molecular structure, spectroscopic, nonlinear optical and dielectric properties of bis(thiourea) silver(I) nitrate single crystal: A dual approach. <i>Arabian Journal of Chemistry</i> , <b>2019</b> , 12, 4612-4626	5.0	12
174	Exploring the Photovoltaic Properties of Metal Bipyridine Complexes (Metal = Fe, Zn, Cr, and Ru) by Density Functional Theory. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , <b>2018</b> , 73, 337-344	1.4	10
173	Design, characterization and nonlinear optical properties of coumarin appended chalcones: Use of a dual approach. <i>Optik</i> , <b>2018</b> , 164, 5-15	2.5	35
172	Modified solvothermal synthesis of cobalt ferrite (CoFe <sub>2</sub> O <sub>4</sub> ) magnetic nanoparticles photocatalysts for degradation of methylene blue with H <sub>2</sub> O <sub>2</sub> /visible light. <i>Results in Physics</i> , <b>2018</b> , 8, 1046-1053	3.7	115
171	Graphene Oxide/Poly(3-hexylthiophene) Nanocomposite Thin-Film Phototransistor for Logic Circuit Applications. <i>Journal of Electronic Materials</i> , <b>2018</b> , 47, 2461-2467	1.9	10
170	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> , <b>2018</b> , 81, 25-31	2.8	34
169	Advancement in Multi-Functional Poly(styrene)-Poly(N-isopropylacrylamide) Based CoreShell Microgels and their Applications. <i>Polymer Reviews</i> , <b>2018</b> , 58, 288-325	14	35
168	Designing of Efficient Acceptors for Organic Solar Cells: Molecular Modelling at DFT Level. <i>Journal of Cluster Science</i> , <b>2018</b> , 29, 359-365	3	30
167	Bismuth Borate Glass Based Nuclear Materials. <i>Silicon</i> , <b>2018</b> , 10, 1195-1201	2.4	7



166	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> , <b>2018</b> , 137, 1	1.9	34
165	Engineering of responsive polymer based nano-reactors for facile mass transport and enhanced catalytic degradation of 4-nitrophenol. <i>Journal of Environmental Sciences</i> , <b>2018</b> , 72, 43-52	6.4	30
164	A systematic study for removal of heavy metals from aqueous media using Sorghum bicolor: an efficient biosorbent. <i>Water Science and Technology</i> , <b>2018</b> , 77, 2355-2368	2.2	12
163	AIE active multianalyte fluorescent probe for the detection of Cu, Ni and Hg ions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2018</b> , 201, 54-60	4.4	24
162	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> , <b>2018</b> , 48, 503-516	5.2	66
161	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> , <b>2018</b> , 187, 296-307	10.3	127
160	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> , <b>2018</b> , 35, 1099-1107	2.8	20
159	Exploring the optoelectronic and charge transfer performance of diaza[5]helicenes at molecular and bulk level. <i>Organic Electronics</i> , <b>2018</b> , 57, 211-220	3.5	35
158	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> , <b>2018</b> , 22, 352-362	4.3	26
157	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> , <b>2018</b> , 30, 75-82	3.6	15
156	How methoxy groups change nature of the thiophene based heterocyclic chalcones from p-channel to ambipolar transport semiconducting materials. <i>Journal of King Saud University - Science</i> , <b>2018</b> , 30, 458-465	3.6	5
155	Optical, Electrical and Photoresponse Properties of Si-based Diodes with NiO-doped TiO <sub>2</sub> Film Prepared by Sol-gel Method. <i>Silicon</i> , <b>2018</b> , 10, 913-920	2.4	13
154	Antiplatelet activity, molecular docking and QSAR study of novel N <sup>?</sup> -arylmethylidene-3-methyl-1-phenyl-6-p-chlorophenyl-1H-pyrazolo[3,4-b]pyridine-4-carbohydrazides. <i>Medicinal Chemistry Research</i> , <b>2018</b> , 27, 388-405	2.2	8
153	Photodiode based on Pb <sub>0.9</sub> Cd <sub>0.1</sub> S ternary alloy semiconductor for solar tracking systems. <i>Journal of Materials Science: Materials in Electronics</i> , <b>2018</b> , 29, 16880-16893	2.1	7
152	Structural, Electronic and Nonlinear Optical Properties of Novel Derivatives of 9,12-Diiodo-1,2-dicarba-closo-dodecaborane: Density Functional Theory Approach. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , <b>2018</b> , 73, 1037-1045	1.4	3
151	Poly(N-isopropylmethacrylamide-acrylic acid) microgels as adsorbent for removal of toxic dyes from aqueous medium. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 268, 229-238	6	22
150	Investigating the coumarin capability in chalcogenide 20TlSe-80PrSe system based photovoltaics. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2018</b> , 202, 123-130	4.4	1
149	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> , <b>2018</b> , 219, 1800211	2.6	30

148	Quantum chemical investigation on molecular structure, vibrational, photophysical and nonlinear optical properties of l-threoninium picrate: an admirable contender for nonlinear applications. <i>Journal of Computational Electronics</i> , <b>2018</b> , 17, 1421-1433	1.8	13
147	Theoretical Study on Open-Shell Singlet Character and Second Hyperpolarizabilities in Cofacial Stacked Dimers Composed of Weak Open-Shell Antiaromatic Porphyrins. <i>ChemPhysChem</i> , <b>2018</b> , 19, 2863-2871	3.2	4
146	Electronic and optoelectronic properties of Al/coumarin doped Pr <sub>2</sub> Se <sub>3</sub> /In <sub>2</sub> Se <sub>3</sub> /p-Si devices. <i>Journal of Materials Science: Materials in Electronics</i> , <b>2018</b> , 29, 12561-12572	2.1	20
145	Exploring the novel donor-nanotube archetype as an efficient third-order nonlinear optical material: asymmetric open-shell carbon nanotubes. <i>Nanoscale</i> , <b>2018</b> , 10, 16499-16507	7.7	26
144	Synthesis, characterization of two new bicyclic oxazolidines and investigation of their optoelectronic properties using density functional theory. <i>Journal of the National Science Foundation of Sri Lanka</i> , <b>2018</b> , 46, 197	1.6	2
143	Exploration of donor effect on electron injection and photovoltaic properties of chalcone derivatives. <i>Materials Science-Poland</i> , <b>2018</b> , 36, 276-282	0.6	
142	Key optoelectronic properties of Diiodo-bis(carbamide)-zinc(II): An experimental and computational investigation. <i>Journal of Molecular Structure</i> , <b>2018</b> , 1156, 146-155	3.4	4
141	Colorimetric optical chemosensor of toxic metal ion (Hg <sup>2+</sup> ) and biological activity using green synthesized AgNPs. <i>Green Chemistry Letters and Reviews</i> , <b>2018</b> , 11, 484-491	4.7	14
140	Theoretical study of triphenylamine-based organic dyes with mono-, di-, and tri-anchoring groups for dye-sensitized solar cells. <i>Organic Electronics</i> , <b>2018</b> , 63, 328-342	3.5	35
139	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> , <b>2018</b> , 132, 89-97	4.6	31
138	Tuning the optoelectronic and charge transport properties of 2,5-di(pyrimidin-5-yl)thieno[3,2-b]thiophene by oligocene end cores substitution. <i>Results in Physics</i> , <b>2018</b> , 11, 599-604	3.7	12
137	Rational design of diketopyrrolopyrrole-based multifunctional materials for organic light-emitting diodes and organic solar cells. <i>Theoretical Chemistry Accounts</i> , <b>2018</b> , 137, 1	1.9	5
136	Cadmium Oxide: Titanium Dioxide Composite Based Photosensitive Diode. <i>Journal of Electronic Materials</i> , <b>2018</b> , 47, 7159-7169	1.9	17
135	Computational study and in vitro evaluation of the anti-proliferative activity of novel naproxen derivatives. <i>Journal of King Saud University - Science</i> , <b>2017</b> , 29, 311-319	3.6	16
134	Composite CuFeSnO/p-type silicon photodiodes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2017</b> , 180, 110-118	4.4	13
133	AIE active turn-off fluorescent probe for the detection of Cu ions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2017</b> , 183, 84-89	4.4	18
132	Flexible and small wearable antenna for wireless body area network applications. <i>Journal of Electromagnetic Waves and Applications</i> , <b>2017</b> , 31, 1063-1082	1.3	24
131	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> , <b>2017</b> , 75, 209-219	2.8	26

130	Computational study of structural, optoelectronic and nonlinear optical properties of dynamic solid-state chalcone derivatives. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 75, 355-364	2.8	11
129	First principles study of the n-channel thiophene based heterocyclic chalcones. <i>Optik</i> , <b>2017</b> , 138, 349-358.	5.5	32
128	Photophysics of Dihydroquinazolinone Derivatives: Experimental and Theoretical Studies. <i>Journal of Fluorescence</i> , <b>2017</b> , 27, 1161-1170	2.4	3
127	Electro-optical, nonlinear and charge transfer properties of naphthalene based compounds: A dual approach study. <i>Optik</i> , <b>2017</b> , 132, 101-110	2.5	51
126	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> , <b>2017</b> , 72, 58-69	2.8	57
125	Tuning of optoelectronic and charge transport properties in star shaped anthracenothiophene-pyrimidine derivatives as multifunctional materials. <i>Optik</i> , <b>2017</b> , 149, 321-331	2.5	17
124	Radical scavenging activity of some natural tropolones by density functional theory. <i>Bulletin of the Chemical Society of Ethiopia</i> , <b>2017</b> , 31, 149	1.2	
123	Dye based photodiodes for solar energy applications. <i>Applied Physics A: Materials Science and Processing</i> , <b>2017</b> , 123, 1	2.6	10
122	A comparative analysis of the optical and nonlinear optical properties of cross-shaped chromophores: Quantum chemical approach. <i>Optik</i> , <b>2017</b> , 147, 439-445	2.5	14
121	Synthesis, antihyperglycemic activity and computational studies of antioxidant chalcones and flavanones derived from 2,5 dihydroxyacetophenone. <i>Journal of Molecular Structure</i> , <b>2017</b> , 1148, 512-520	3.4	17
120	First-principles study of nitrogen-doped nanographene as an efficient charge transport and nonlinear optical material. <i>RSC Advances</i> , <b>2017</b> , 7, 36632-36643	3.7	21
119	Exploring the charge transfer nature and electro-optical properties of anthracene based sensitizers @TiO <sub>2</sub> cluster. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , <b>2017</b> , 80, 239-246	5.3	14
118	Molecular design of organic small molecules based on diindoleimide with fused aromatic heterocycles as donors for organic solar cells. <i>RSC Advances</i> , <b>2017</b> , 7, 39899-39905	3.7	25
117	An unexpected reactivity during periodate oxidation of chitosan and the affinity of its 2, 3-di-aldehyde toward sulfa drugs. <i>Carbohydrate Polymers</i> , <b>2017</b> , 175, 565-574	10.3	28
116	Exploring the possible existence of oxygen-bridged planarized 4-aminopyridine: promising structure, charge transport and nonlinear optical properties. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 7102-7109	7.1	11
115	Quinazolinone derivative: Model compound for determination of dipole moment, solvatochromism and metal ion sensing. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2017</b> , 171, 97-103	4.4	11
114	Synthesis, characterization and density functional theory investigations of the N,N-diacylaniline derivatives. <i>Arabian Journal of Chemistry</i> , <b>2017</b> , 10, S1847-S1854	5.9	
113	Effect of donor and acceptor groups on radical scavenging activity of phenol by density functional theory. <i>Arabian Journal of Chemistry</i> , <b>2017</b> , 10, S1703-S1710	5.9	28

112	Density functional theory investigations of radical scavenging activity of 3?-Methyl-quercetin. <i>Journal of Saudi Chemical Society</i> , <b>2016</b> , 20, S21-S28	4.3	14
111	Role of a singlet diradical character in carbon nanomaterials: a novel hot spot for efficient nonlinear optical materials. <i>Nanoscale</i> , <b>2016</b> , 8, 17998-18020	7.7	49
110	Behavioral pattern exploration of single guest, hexadecane-1,16-diol and hexadecane in urea inclusion compounds via molecular dynamics simulation. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2016</b> , 15, 1650047	1.8	2
109	Peculiar behavior of starch 2,3-dialdehyde towards sulfanilamide and sulfathiazole. <i>Carbohydrate Polymers</i> , <b>2016</b> , 152, 624-631	10.3	16
108	A first-principles study of the linear and nonlinear optical properties of isoxazole derivatives. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2016</b> , 15, 1650060	1.8	2
107	A Combined Experimental and Computational Investigation on Spectroscopic and Photophysical Properties of a Coumarinyl Chalcone. <i>Journal of Fluorescence</i> , <b>2016</b> , 26, 1357-65	2.4	14
106	The electro-optical and charge transport study of imidazolidin derivative: Quantum chemical investigations. <i>Journal of Saudi Chemical Society</i> , <b>2016</b> , 20, 680-685	4.3	15
105	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> , <b>2016</b> , 20, 336-342	4.3	16
104	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> , <b>2016</b> , 22, 73	2	30
103	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> , <b>2016</b> , 65, 175-82	5.1	24
102	Sensing performance optimization by tuning surface morphology of organic (D-EA) dye based humidity sensor. <i>Sensors and Actuators B: Chemical</i> , <b>2016</b> , 231, 30-37	8.5	26
101	Antibacterial activities, DFT and QSAR studies of quinazolinone compounds. <i>Bulletin of the Chemical Society of Ethiopia</i> , <b>2016</b> , 30, 307	1.2	10
100	Tuning the push-pull configuration for efficient second-order nonlinear optical properties in some chalcone derivatives. <i>Journal of Molecular Graphics and Modelling</i> , <b>2016</b> , 68, 95-105	2.8	65
99	Evaluation of humidity sensing properties of TMBHPET thin film embedded with spinel cobalt ferrite nanoparticles. <i>Journal of Nanoparticle Research</i> , <b>2016</b> , 18, 1	2.3	16
98	Optoelectronic properties of naphtho[2, 1-b:6, 5-b']difuran derivatives for photovoltaic application: a computational study. <i>Journal of Molecular Modeling</i> , <b>2016</b> , 22, 248	2	18
97	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> , <b>2016</b> , 127, 10148-10157	2.5	27
96	Diradical character and nonlinear optical properties of buckyferrocenes: focusing on the use of suitably modified fullerene fragments. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 5805-16	3.6	16
95	Highly efficient donor-acceptor hydrazone dyes-inorganic Si/TiO <sub>2</sub> hybrid solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2015</b> , 145, 40-46	4.4	2

94	Synthesis and structure of 1-benzyl-5-amino-1H-tetrazole in the solid state and in solution: Combining X-ray diffraction, <sup>1</sup> H NMR, FTIR, and UV-Vis spectra and DFT calculations. <i>Comptes Rendus Chimie</i> , <b>2015</b> , 18, 422-429	2.7	11
93	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> , <b>2015</b> , 5, 53988-54002	3.7	25
92	Micellization behavior of mixtures of amphiphilic promazine hydrochloride and cationic aniline hydrochloride in aqueous and electrolyte solutions. <i>Korean Journal of Chemical Engineering</i> , <b>2015</b> , 32, 2142-2152	2.8	13
91	Effect of donor strength of extended alkyl auxiliary groups on optoelectronic and charge transport properties of novel naphtha[2,1-b:6,5-b']difuran derivatives: simple yet effective strategy. <i>Journal of Molecular Modeling</i> , <b>2015</b> , 21, 199	2	10
90	Electro-optical and charge injection investigations of the donor-acceptor triphenylamine, oligocene-thiophene-pyrimidine and cyanoacetic acid based multifunctional dyes. <i>Journal of King Saud University - Science</i> , <b>2015</b> , 27, 361-368	3.6	9
89	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> , <b>2015</b> , 149, 722-30	4.4	14
88	A new pentacoordinate polymeric copper(II) complex with 2-amino-2-methyl-1,3-propandiol: Structural investigations using XRD and DFT. <i>Journal of Structural Chemistry</i> , <b>2015</b> , 56, 92-101	0.9	7
87	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> , <b>2015</b> , 14, 1550029	1.8	14
86	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> , <b>2015</b> , 18, 1289-1296 <sup>26</sup>	3.7	26
85	The effect of anchoring groups on the electro-optical and charge injection in triphenylamine derivatives@TiO <sub>2</sub> . <i>Journal of Theoretical and Computational Chemistry</i> , <b>2015</b> , 14, 1550027	1.8	20
84	An investigation on the key features of a DA type novel chalcone derivative for opto-electronic applications. <i>RSC Advances</i> , <b>2015</b> , 5, 87320-87332	3.7	86
83	DFT investigations of the ground and excited state geometries of the benzothiazine and benisothiazol based anticancer drugs. <i>Journal of Saudi Chemical Society</i> , <b>2015</b> , 19, 318-321	4.3	17
82	Humidity dependent electrical properties of an organic material DMBHPET. <i>Measurement: Journal of the International Measurement Confederation</i> , <b>2015</b> , 61, 180-184	4.6	23
81	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> , <b>2015</b> , 36, 118-28	3.5	46
80	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> , <b>2015</b> , 137, 432-41	4.4	36
79	Fluoro-silicon (FSi) interaction as a promising force for the formation of thermodynamically stabilized Brook-type silabenzene: A quantum chemical approach. <i>Journal of Fluorine Chemistry</i> , <b>2015</b> , 176, 51-56	2.1	1
78	Computational Designing of Triphenylamine Dyes with Broad and Red-shifted Absorption Spectra for Dye-sensitized Solar Cells using Multi-Thiophene Rings in $\pi$ -Spacer. <i>Bulletin of the Korean Chemical Society</i> , <b>2015</b> , 36, 2615-2620	1.2	24
77	Heterocyclic azo dyes for dye sensitized solar cells: A quantum chemical study. <i>Computational and Theoretical Chemistry</i> , <b>2015</b> , 1066, 94-99	2	41



76	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> , <b>2014</b> , 190, 27-33	3.6	20
75	DFT studies on the tetranuclear cubane complex [Ni <sub>4</sub> (ampd) <sub>4</sub> (Cl <sub>4</sub> )]·MeCN. <i>Journal of Structural Chemistry</i> , <b>2014</b> , 55, 30-37	0.9	4
74	First principle investigations to enhance the charge transfer properties by bridge elongation. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2014</b> , 13, 1450013	1.8	11
73	Spectroscopic and computational studies of 1,4-bis[[6-tertbutyl-2-benzoxazolyl]vinyl]benzene(BTBVB) laser dye. <i>Journal of Luminescence</i> , <b>2014</b> , 148, 317-324	3.8	6
72	The enhanced efficiency to 3.6% based on organic dye as donor and Si/TiO <sub>2</sub> acceptor bulk hetero-junction solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , <b>2014</b> , 292, 1-9	4.7	12
71	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> , <b>2014</b> , 1045, 123-134	2	19
70	Highly efficient renewable energy materials benzo[2,3-b]thiophene derivatives: Electronic and charge transfer properties study. <i>Optik</i> , <b>2014</b> , 125, 4825-4830	2.5	23
69	Modeling of efficient charge transfer materials of 4,6-di(thiophen-2-yl)pyrimidine derivatives: Quantum chemical investigations. <i>Computational Materials Science</i> , <b>2014</b> , 81, 488-492	3.2	32
68	DFT study of the electronic and charge transfer properties of perfluoroarene-thiophene oligomers. <i>Journal of Saudi Chemical Society</i> , <b>2014</b> , 18, 574-580	4.3	16
67	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> , <b>2014</b> , 157, 52-57 <sup>2.1</sup>		27
66	Influence of push-pull configuration on the electro-optical and charge transport properties of novel naphtho-difuran derivatives: a DFT study. <i>RSC Advances</i> , <b>2014</b> , 4, 48876-48887	3.7	14
65	How does the increment of hetero-cyclic conjugated moieties affect electro-optical and charge transport properties of novel naphtha-difuran derivatives? A computational approach. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2547	2	5
64	An electro-optical and electron injection study of benzothiazole-based squaraine dyes as efficient dye-sensitized solar cell materials: a first principles study. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2517 <sup>2</sup>		7
63	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> , <b>2014</b> , 18, 914-919	4.3	22
62	Red and yellow color aspects of compound 3-dicyclopropylmethylene-5-dicyanomethylene-4-diphenylmethylenetetrahydrofuran-2-one: Chromism effect. <i>Chinese Chemical Letters</i> , <b>2014</b> , 25, 609-612	8.1	12
61	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> , <b>2014</b> , 1031, 76-82	2	28
60	Naphthaldehyde-derived ligands: synthesis and their Ni(II) ion complexation. <i>Monatshefte Für Chemie</i> , <b>2014</b> , 145, 275-279	1.4	1
59	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> , <b>2014</b> , 6, 1727-1739	2.3	19



58	Quantum chemical investigations of electron injection in triphenylamine-dye sensitized TiO <sub>2</sub> used in dye sensitized solar cells. <i>Materials Chemistry and Physics</i> , <b>2013</b> , 142, 238-247	4.4	33
57	Chemical sensor development based on polycrystalline gold electrode embedded low-dimensional Ag <sub>2</sub> O nanoparticles. <i>Electrochimica Acta</i> , <b>2013</b> , 112, 422-430	6.7	61
56	Quantum chemical design of nonlinear optical materials by sp <sup>2</sup> -hybridized carbon nanomaterials: issues and opportunities. <i>Journal of Materials Chemistry C</i> , <b>2013</b> , 1, 5439	7.1	116
55	Facile green synthesis, optical and photocatalytic properties of zinc oxide nanosheets via microwave assisted hydrothermal technique. <i>Journal of Electroceramics</i> , <b>2013</b> , 31, 324-330	1.5	21
54	Electronic structure and absorption spectra of 6-picoline Schiff base: A DFT and XRD based approach. <i>Journal of Molecular Structure</i> , <b>2013</b> , 1050, 10-14	3.4	14
53	Synthesis, characterization, and evaluation of some novel 4(3H)-quinazolinone derivatives as anti-inflammatory and analgesic agents. <i>Medicinal Chemistry Research</i> , <b>2013</b> , 22, 440-452	2.2	27
52	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> , <b>2013</b> , 1049, 198-204	3.4	22
51	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> , <b>2013</b> , 44, 168-76	2.8	26
50	Photophysical properties, photostability and laser activity of 2,6-bis [(2-benzoxazolyl) vinyl] naphthalene (BBVN). <i>Journal of Molecular Structure</i> , <b>2013</b> , 1037, 323-331	3.4	9
49	First principles investigations of geometric, electronic and optical properties of 5-aminotetrazole derivatives. <i>Journal of Computational Electronics</i> , <b>2013</b> , 12, 437-447	1.8	6
48	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> , <b>2013</b> , 138, 468-478	4.4	23
47	Quantum chemical study of the donor-bridge-acceptor triphenylamine based sensitizers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2013</b> , 110, 60-6	4.4	67
46	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> , <b>2013</b> , 111, 223-9	4.4	30
45	Electronic, optical, and charge transfer properties of donor-bridge-acceptor hydrazone sensitizers. <i>Structural Chemistry</i> , <b>2013</b> , 24, 499-506	1.8	25
44	COMBINED EXPERIMENTAL AND COMPUTATIONAL STUDY OF THE RADICAL SCAVENGING ACTIVITY OF LUTEOLIN. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2013</b> , 12, 1350021	1.8	3
43	Synthesis, characterization and DFT study of methoxybenzylidene containing chromophores for DSSC materials. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2012</b> , 91, 239-43	4.4	37
42	Molecular design of new hydrazone dyes for dye-sensitized solar cells: Synthesis, characterization and DFT study. <i>Journal of Molecular Structure</i> , <b>2012</b> , 1019, 130-134	3.4	30
41	Donor-enhanced bridge effect on the electronic properties of triphenylamine based dyes: density functional theory investigations. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 3609-15	2	15

40	Quantum chemical study in the direction to design efficient donor-bridge-acceptor triphenylamine sensitizers with improved electron injection. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 4893-900	2	56
39	Quantum chemical approach toward rational designing of highly efficient oxadiazole based oligomers used in organic field effect transistors. <i>Journal of Computational Electronics</i> , <b>2012</b> , 11, 374-384	1.8	18
38	Synthesis, characterization and DFT study of 4H-benzo[h]chromene derivatives. <i>Journal of Molecular Structure</i> , <b>2012</b> , 1018, 171-175	3-4	30
37	Theoretical study of coumarin derivatives as chemosensors for fluoride anion. <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 986, 93-98	2	20
36	Quantum chemical investigations aimed at modeling highly efficient zinc porphyrin dye sensitized solar cells. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 4199-207	2	35
35	THEORETICAL INVESTIGATIONS OF THE CHARGE TRANSFER PROPERTIES IN OLIGOTHIOPHENE DERIVATIVES. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2012</b> , 11, 631-640	1.8	6
34	The DFT investigations of the electron injection in hydrazone-based sensitizers. <i>Theoretical Chemistry Accounts</i> , <b>2012</b> , 131, 1	1.9	41
33	Synthesis and Photooxygenation of Furo[3,2-c]coumarin Derivatives as Antibacterial and DNA Intercalating Agent. <i>Chinese Journal of Chemistry</i> , <b>2012</b> , 30, 316-320	4-9	36
32	Electronic, optical and charge transfer properties of $\pi$ -bis(dithieno[3,2-b:2',3'-d]thiophene) (BDT) and its heteroatom-substituted analogues. <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 968, 8-11	2	18
31	A study on the electronic and charge transfer properties in tin phthalocyanine (SnPc) derivatives by density functional theory. <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 977, 9-12	2	17
30	Packing Effect on the Transfer Integrals and Mobility in $\pi$ -bis(dithieno[3,2-b:2',3'-d]thiophene) (BDT) and its Heteroatom-Substituted Analogues. <i>Australian Journal of Chemistry</i> , <b>2011</b> , 64, 1587	1.2	25
29	A DFT study on the electronic and redox properties of $[X_8V_{14}O_{50}]_n$ [X = SiIV, GeIV, PV, and AsV]. <i>Canadian Journal of Chemistry</i> , <b>2010</b> , 88, 434-442	0.9	9
28	Designing of Disubstituted Derivatives of mer-Alq3: Quantum Theoretical Study. <i>Australian Journal of Chemistry</i> , <b>2010</b> , 63, 1283	1.2	11
27	Theoretical investigations of the charge transfer properties of anthracene derivatives. <i>Theoretical Chemistry Accounts</i> , <b>2010</b> , 127, 587-594	1.9	25
26	Toward rational designing of n-type materials: Theoretical investigations of mer-Alq3 derivatives. <i>Computational and Theoretical Chemistry</i> , <b>2010</b> , 956, 61-65		12
25	Energy decomposition analysis of methyl derivatives of the meridional isomer of tris(8-hydroxyquinolino)aluminum (mer-Alq3). <i>Chemical Physics</i> , <b>2009</b> , 358, 25-29	2-3	9
24	Fluorinated derivatives of mer-Alq3: energy decomposition analysis, optical properties, and charge transfer study. <i>Theoretical Chemistry Accounts</i> , <b>2009</b> , 122, 275-281	1.9	34
23	Effect of one ligand substitution on charge transfer and optical properties in mer-Alq3: a theoretical study. <i>Theoretical Chemistry Accounts</i> , <b>2009</b> , 124, 339-344	1.9	28

22	Pushpull effect on the charge transfer, and tuning of emitting color for disubstituted derivatives of mer-Alq3. <i>Chemical Physics</i> , <b>2009</b> , 364, 39-45	2.3	34
21	Theoretical investigations of the charge transfer characteristics in dichlorotitanium phthalocyanine (TiCl <sub>2</sub> Pc) and tin phthalocyanine (SnPc). <i>Chemical Physics Letters</i> , <b>2009</b> , 483, 143-146	2.5	24
20	Explaining the HOMO and LUMO distribution on individual ligands in mer-Alq3 and its CH <sub>3</sub> N substituted derivatives. <i>Computational and Theoretical Chemistry</i> , <b>2008</b> , 850, 79-83		16
19	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
18	Characteristics, properties, synthesis and advanced applications of 2D graphdiyne versus graphene. <i>Materials Chemistry Frontiers</i> ,	7.8	2
17	Investigating the Bulk Level Optoelectronic Characteristics of 10-(1,3-Dithiol-2-Ylidene)Anthracene Based Light Harvesters. <i>Polycyclic Aromatic Compounds</i> ,1-10	1.3	1
16	Structural, spectral elucidation, wavefunctional properties, natural bond orbitals, and molecular docking analysis of synthesized 1-phenyl-3(4-methoxyphenyl)-2-propenone: protease kinase inhibitor. <i>Spectroscopy Letters</i> ,1-17	1.1	1
15	Synthesis, Spectral Characterization, Electronic Structure and Biological Activity Screening of the Schiff Base 4-((4-Hydroxy-3-Methoxy-5-Nitrobenzylidene)Amino)-N-(Pyrimidin-2-yl)Benzene Sulfonamide from 5-Nitrovaniline and Sulphadiazene. <i>Polycyclic Aromatic Compounds</i> ,1-18	1.3	7
14	Molecular grafting based polymeric carbon nitride for wondrous artificial photosynthesis. <i>International Journal of Energy Research</i> ,	4.5	4
13	Nickel iron oxide electrocatalysts for electrochemical OER activity. <i>Applied Nanoscience (Switzerland)</i> ,1	3.3	
12	Schiff bases from Honone with adenine, cytosine, l-leucine biomolecules: Synthesis, structural features, electronic structure and medicinal activities. <i>Journal of Computational Biophysics and Chemistry</i> ,		2
11	Molecular conformational twist-controlled wide fluorescence tuning and white light emission in a single fluorophore via halochromism. <i>New Journal of Chemistry</i> ,	3.6	4
10	Detailed Structural Examination, Quantum Mechanical Studies of the Aromatic Compound Solarimfetol and Formation of Inclusion Compound with Cucurbituril. <i>Polycyclic Aromatic Compounds</i> ,1-13	1.3	2
9	PVP-assisted grass-like NiSe@ZnSe composite for environmental energy applications. <i>Journal of Materials Science: Materials in Electronics</i> ,1	2.1	1
8	Synthesis and characterization of ferrocene-based thiosemicarbazones along with their computational studies for potential as inhibitors for SARS-CoV-2. <i>Journal of the Iranian Chemical Society</i> ,1	2	4
7	A review on perovskite materials with solar cell prospective. <i>International Journal of Energy Research</i> ,	4.5	4
6	Concomitant Polymorphs of Aryl-Ether Amine via Catemer and Dimer Carboxylic Acid Supramolecular Interactions and Their Effect on Optical Band Gap. <i>Polycyclic Aromatic Compounds</i> ,1-10	1.3	
5	Binder-less and free-standing CoBe metal nanoparticles-decorated PVdF-HFP nanofiber membrane as an electrochemical probe for enzyme-less glucose sensors. <i>Research on Chemical Intermediates</i> ,1	2.8	2

4	Machine-Learning Analysis of Small-Molecule Donors for Fullerene Based Organic Solar Cells. <i>Energy Technology</i> ,2200019	3.5	5
3	Exploring the quinoidal oligothiophenes to their robust limit for efficient linear and nonlinear optical response properties. <i>Chemical Papers</i> ,1	1.9	0
2	Computational investigation, effects of polar and non-polar solvents on optimized structure with topological parameters (ELF, LOL, AIM, and RDG) of three glycine derivative compounds. <i>Structural Chemistry</i> ,1	1.8	0
1	Virtual screening of potential inhibitor against breast cancer-causing estrogen receptor alpha (ER $\alpha$ ) by molecular docking and dynamic simulations. <i>Molecular Simulation</i> ,1-12	2	1