

Tariq Mahmood

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/566159/tariq-mahmood-publications-by-year.pdf>

Version: 2024-04-27

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

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

196
papers

2,991
citations

29
h-index

43
g-index

213
ext. papers

3,893
ext. citations

3.3
avg, IF

6.1
L-index

#	Paper	IF	Citations
196	Breast lesions classifications of mammographic images using a deep convolutional neural network-based approach.. <i>PLoS ONE</i> , 2022 , 17, e0263126	3.7	1
195	Superalkali (Li2F, Li3F) doped Al12N12 electrides with enhanced static, dynamic nonlinear optical responses and refractive indices. <i>Materials Science in Semiconductor Processing</i> , 2022 , 143, 106518	4.3	1
194	In memory of Professor Iain Wilkinson: cognitive and neuroimaging endophenotypes in a consanguineous schizophrenia multiplex Family.. <i>Psychological Medicine</i> , 2022 , 1-9	6.9	0
193	Effect of high pressure on structural, electrical, and optical properties of graphene-like zinc oxide (g-ZnO) structure. <i>Materials Science in Semiconductor Processing</i> , 2022 , 142, 106465	4.3	0
192	Remarkable nonlinear optical response of Mn@C20 (M = Na & K and n = 1 β); a DFT outcome. <i>Materials Science in Semiconductor Processing</i> , 2022 , 138, 106269	4.3	6
191	Association between the physical activity and metabolic syndrome in residents of a foot-hill area in India.. <i>Diabetes and Metabolic Syndrome: Clinical Research and Reviews</i> , 2022 , 16, 102471	8.9	0
190	Sensing behaviour of monocyclic C18 and B9N9 analogues toward chemical warfare agents (CWAs); quantum chemical approach. <i>Surfaces and Interfaces</i> , 2022 , 30, 101912	4.1	0
189	Olympicene as a high-performance sensor for lung irritants: A dispersion corrected DFT insight. <i>Materials Science in Semiconductor Processing</i> , 2022 , 144, 106620	4.3	0
188	First-principles study for electrochemical sensing of neurotoxin hydrazine derivatives via h-g-C3N4 quantum dot. <i>Surfaces and Interfaces</i> , 2022 , 30, 101913	4.1	2
187	DFT studies on electrochemical properties of halide ions doped GDY-28 nanoflake for Na-ion battery applications. <i>Materials Science in Semiconductor Processing</i> , 2022 , 145, 106651	4.3	0
186	Static, dynamic nonlinear optical (NLO) response and electride characteristics of superalkalis doped star like C6S6Li6. <i>Surfaces and Interfaces</i> , 2022 , 102044	4.1	1
185	Electrochemical sensing of heptazine graphitic C3N4 quantum dot for chemical warfare agents; a quantum chemical approach. <i>Materials Science in Semiconductor Processing</i> , 2022 , 148, 106753	4.3	1
184	Nano-porous CN as a toxic pesticide's scavenger: A quantum chemical approach. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 111, 108078	2.8	5
183	Demonstrating the Potential of Alkali Metal-Doped Cyclic COLi Organometallics as Electrides and High-Performance NLO Materials. <i>ACS Omega</i> , 2021 , 6, 29852-29861	3.9	1
182	Effective adsorption of A-series chemical warfare agents on graphdiyne nanoflake: a DFT study. <i>Journal of Molecular Modeling</i> , 2021 , 27, 117	2	13
181	DFT studies of single and multiple alkali metals doped C fullerene for electronics and nonlinear optical applications. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 105, 107867	2.8	7
180	Breast Mass Detection and Classification Using Deep Convolutional Neural Networks for Radiologist Diagnosis Assistance 2021 ,		2

179	Computer Vision-Based Microcalcification Detection in Digital Mammograms Using Fully Connected Depthwise Separable Convolutional Neural Network. <i>Sensors</i> , 2021 , 21,	3.8	7
178	A Recessively Inherited Risk Locus on Chromosome 13q22-31 Conferring Susceptibility to Schizophrenia. <i>Schizophrenia Bulletin</i> , 2021 , 47, 796-802	1.3	1
177	Fundus image-based cataract classification using a hybrid convolutional and recurrent neural network. <i>Visual Computer</i> , 2021 , 37, 2407-2417	2.3	4
176	Electronic, optical and elastic properties of cubic zirconia (c-ZrO ₂) under pressure: A DFT study. <i>Physica B: Condensed Matter</i> , 2021 , 604, 412462	2.8	4
175	Surface functionalization of twisted graphene CH and CH derivatives with alkalis and superalkalis for NLO response; a DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 102, 107794	2.8	12
174	Silver cluster (Ag) decorated coronene as non-enzymatic sensor for glucose and HO. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 103, 107824	2.8	4
173	Hybrid vector similarity measures based on complex hesitant fuzzy sets and their applications to pattern recognition and medical diagnosis. <i>Journal of Intelligent and Fuzzy Systems</i> , 2021 , 40, 625-646	1.6	14
172	Remarkable static and dynamic NLO response of alkali and superalkali doped macrocyclic [hexa-]thiophene complexes; a DFT approach.. <i>RSC Advances</i> , 2021 , 11, 4118-4128	3.7	16
171	Alteration impact of electronic properties of c-SrTiO ₃ on optical response due to Ca inclusion: A DFT study. <i>Physica B: Condensed Matter</i> , 2021 , 602, 412553	2.8	1
170	Electrochemical sensing behavior of graphdiyne nanoflake towards uric acid: a quantum chemical approach. <i>Journal of Molecular Modeling</i> , 2021 , 27, 244	2	1
169	An Automated In-Depth Feature Learning Algorithm for Breast Abnormality Prognosis and Robust Characterization from Mammography Images Using Deep Transfer Learning. <i>Biology</i> , 2021 , 10,	4.9	6
168	Impact of even number of alkaline earth metal doping on the NLO response of C ₂₀ nanocluster; a DFT outcome. <i>Computational and Theoretical Chemistry</i> , 2021 , 1204, 113386	2	2
167	DFT based investigations of BAWO ₄ : Electronic and optical properties. <i>Physica B: Condensed Matter</i> , 2021 , 621, 413309	2.8	0
166	First example of lanthanum as dopant on Al ₁₂ N ₁₂ and Al ₁₂ P ₁₂ nanocages for improved electronic and nonlinear optical properties with high stability. <i>Materials Science in Semiconductor Processing</i> , 2021 , 135, 106122	4.3	5
165	Sensing of toxic Lewisite (L1, L2, and L3) molecules by graphdiyne nanoflake using density functional theory calculations and quantum theory of atoms in molecule analysis. <i>Journal of Physical Organic Chemistry</i> , 2021 , 34, e4181	2.1	10
164	Energy routing algorithm based on OSPF protocol and virtual circuit switching mode in energy local area network 2020 , 1, 292		0
163	Synergic effect of pore size engineering and an applied electric field on the controlled permeation of alkali metal atoms and ions across pristine and defect-containing h-BN sheets. <i>New Journal of Chemistry</i> , 2020 , 44, 7891-7901	3.6	4
162	Remarkable second and third order nonlinear optical properties of organometallic C ₆ Li ₆ M ₃ O electriles. <i>New Journal of Chemistry</i> , 2020 , 44, 9822-9829	3.6	18

161	A computational insight of electronic and optical properties of Cd-doped BaZrO ₃ . <i>Chinese Journal of Physics</i> , 2020 , 66, 318-326	3.5	5
160	Outstanding NLO response of thermodynamically stable single and multiple alkaline earth metals doped C ₂₀ fullerene. <i>Journal of Molecular Liquids</i> , 2020 , 305, 112875	6	22
159	Theoretical study on novel superalkali doped graphdiyne complexes: Unique approach for the enhancement of electronic and nonlinear optical response. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 97, 107573	2.8	39
158	Cyclic versus straight chain oligofuran as sensor: A detailed DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 97, 107569	2.8	52
157	High selectivity of cyclic tetrapyrrole over tetrafulan and tetrathiophene toward toxic chemicals; A first-principles study. <i>Microporous and Mesoporous Materials</i> , 2020 , 299, 110126	5.3	29
156	Theoretical investigation on radical anion promoted electrocyclization in photochromes. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 97, 107550	2.8	1
155	Silver-graphene quantum dots based electrochemical sensor for trinitrotoluene and p-nitrophenol. <i>Journal of Molecular Liquids</i> , 2020 , 306, 112878	6	46
154	Introducing robustness in DBR routing protocol. <i>International Journal of Communication Networks and Distributed Systems</i> , 2020 , 24, 316	0.4	2
153	Exceptionally high NLO response and deep ultraviolet transparency of superalkali doped macrocyclic oligofuran rings. <i>New Journal of Chemistry</i> , 2020 , 44, 2609-2618	3.6	41
152	Structural, spectroscopic and nonlinear optical properties of sulfonamide derivatives; experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2020 , 1202, 127393	3.4	9
151	Benchmark approach to search of cost-effective and accurate density functional for homolytic cleavage of C-Mg bond of Grignard reagent. <i>International Journal of Quantum Chemistry</i> , 2020 , 120, e26106	2.1	1
150	Sentiment analysis on IMDB using lexicon and neural networks. <i>SN Applied Sciences</i> , 2020 , 2, 1	1.8	14
149	Alkaline earth metal decorated phosphide nanoclusters for potential applications as high performance NLO materials; A first principle study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 118, 113906	3	23
148	Design of novel inorganic alkaline earth metal doped aluminum nitride complexes (AEM@Al ₁₂ N ₁₂) with high chemical stability, improved electronic properties and large nonlinear optical response. <i>Optik</i> , 2020 , 207, 163792	2.5	13
147	Significant nonlinear optical response of alkaline earth metals doped beryllium and magnesium oxide nanocages. <i>Materials Chemistry and Physics</i> , 2020 , 242, 122507	4.4	21
146	Permeation of second row neutral elements through AlP and BP nanocages; a first-principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 101, 107748	2.8	3
145	Biomarkers in psychiatry: a clinician's viewpoint. <i>British Medical Bulletin</i> , 2020 , 135, 23-27	5.4	4
144	Feature Selection Optimization in Software Product Lines. <i>IEEE Access</i> , 2020 , 8, 160231-160250	3.5	1

143	A Brief Survey on Breast Cancer Diagnostic With Deep Learning Schemes Using Multi-Image Modalities. <i>IEEE Access</i> , 2020 , 8, 165779-165809	3.5	19
142	Superhalogen doping: a new and effective approach to design materials with excellent static and dynamic NLO responses. <i>New Journal of Chemistry</i> , 2020 , 44, 16358-16369	3.6	17
141	Natural and semisynthetic polymers blended orodispersible films of citalopram. <i>Natural Product Research</i> , 2020 , 34, 16-25	2.3	8
140	Synthesis, crystal structures, computational studies and α -amylase inhibition of three novel 1,3,4-oxadiazole derivatives. <i>Journal of Molecular Structure</i> , 2020 , 1200, 127085	3.4	16
139	Design of novel superalkali doped silicon carbide nanocages with giant nonlinear optical response. <i>Optics and Laser Technology</i> , 2020 , 122, 105855	4.2	40
138	An efficient and improved scheme for handwritten digit recognition based on convolutional neural network. <i>SN Applied Sciences</i> , 2019 , 1, 1	1.8	20
137	Doping superalkali on Zn ₁₂ O ₁₂ nanocage constitutes a superior approach to fabricate stable and high-performance nonlinear optical materials. <i>Optics and Laser Technology</i> , 2019 , 120, 105753	4.2	30
136	Benchmark DFT studies on C-CN homolytic cleavage and screening the substitution effect on bond dissociation energy. <i>Journal of Molecular Modeling</i> , 2019 , 25, 47	2	11
135	Extended Version of Linguistic Picture Fuzzy TOPSIS Method and Its Applications in Enterprise Resource Planning Systems. <i>Mathematical Problems in Engineering</i> , 2019 , 2019, 1-8	1.1	15
134	Design, synthesis and anti-bacterial studies of piperazine derivatives against drug resistant bacteria. <i>European Journal of Medicinal Chemistry</i> , 2019 , 166, 224-231	6.8	15
133	Dexibuprofen amide derivatives as potential anticancer agents: synthesis, in silico docking, bioevaluation, and molecular dynamic simulation. <i>Drug Design, Development and Therapy</i> , 2019 , 13, 1643-1657	4.4	8
132	Synthesis and Reactivities of Triphenyl Acetamide Analogs for Potential Nonlinear Optical Material Uses. <i>Symmetry</i> , 2019 , 11, 622	2.7	4
131	Fuzzy hyperideals of hyperquantales. <i>Journal of Intelligent and Fuzzy Systems</i> , 2019 , 36, 5605-5615	1.6	2
130	Pythagorean cubic fuzzy aggregation information based on confidence levels and its application to multi-criteria decision making process. <i>Journal of Intelligent and Fuzzy Systems</i> , 2019 , 36, 5669-5683	1.6	8
129	Comparative investigation of sensor application of polypyrrole for gaseous analytes. <i>Journal of Physical Organic Chemistry</i> , 2019 , 32, e3960	2.1	24
128	Synthesis, structural properties, DFT studies, antimicrobial activities and DNA binding interactions of two newly synthesized organotin(IV) carboxylates. <i>Journal of Molecular Structure</i> , 2019 , 1191, 291-300	3.4	21
127	Halides encapsulation in aluminum/boron phosphide nanoclusters: An effective strategy for high cell voltage in Na-ion battery. <i>Materials Science in Semiconductor Processing</i> , 2019 , 97, 71-79	4.3	11
126	Theoretical study on a boron phosphide nanocage doped with superalkalis: novel electrides having significant nonlinear optical response. <i>New Journal of Chemistry</i> , 2019 , 43, 5727-5736	3.6	46

125	Isolation, characterization and DFT studies of epoxy ring containing new withanolides from <i>Withania coagulans</i> Dunal. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019 , 217, 113-121	4.4	3
124	Superalkalis as a source of diffuse excess electrons in newly designed inorganic electrides with remarkable nonlinear response and deep ultraviolet transparency: A DFT study. <i>Applied Surface Science</i> , 2019 , 483, 1118-1128	6.7	56
123	A Novel UV-Spectrophotometric Method for Simultaneous Estimation of Amlodipine and Captopril. <i>Pharmaceutical Chemistry Journal</i> , 2019 , 52, 952-958	0.9	2
122	Fabrication and in vitro characterization of fenofibric acid-loaded hyaluronic acid/polyethylene glycol polymeric composites with enhanced drug solubility and dissolution rate. <i>International Journal of Polymeric Materials and Polymeric Biomaterials</i> , 2019 , 68, 510-515	3	8
121	Synthesis of novel metal complexes of 2-((phenyl (2-(4-sulfophenyl) hydrazono) methyl) diazenyl) benzoic acid formazan dyes: Characterization, antimicrobial and optical properties studies on leather. <i>Journal of Molecular Structure</i> , 2019 , 1175, 73-89	3.4	11
120	Cellulosic and acrylic polymers based composites for controlled drug release. <i>Iranian Polymer Journal (English Edition)</i> , 2019 , 28, 769-776	2.3	2
119	A comprehensive DFT study on the sensing abilities of cyclic oligothiophenes (nCTs). <i>New Journal of Chemistry</i> , 2019 , 43, 14120-14133	3.6	36
118	Role of Pyridine Nitrogen in Palladium-Catalyzed Imine Hydrolysis: A Case Study of (E)-1-(3-bromothiophen-2-yl)-N-(4-methylpyridin-2-yl)methanimine. <i>Molecules</i> , 2019 , 24,	4.8	5
117	Preparation and in vitro characterization of polyvinylpyrrolidone-ploxamer polymeric synergy for oral drug delivery. <i>Journal of Polymer Research</i> , 2019 , 26, 1	2.7	3
116	Density functional theory study of structural, electronic and CO adsorption properties of anionic $\text{Scn}(\eta = 2\text{C}3)$ clusters. <i>Computational and Theoretical Chemistry</i> , 2019 , 1163, 112511	2	6
115	Theoretical study on design of novel superalkalis doped graphdiyne: A new donor-acceptor (D-EA) strategy for enhancing NLO response. <i>Applied Surface Science</i> , 2019 , 492, 255-263	6.7	39
114	Highly selective acridinium based cyanine dyes for the detection of DNA base pairs (adenine, cytosine, guanine and thymine). <i>Computational and Theoretical Chemistry</i> , 2019 , 1163, 112509	2	63
113	Cobalt Phosphide Ultrathin and Freestanding Sheets Prepared through Microwave Chemical Vapor Deposition: A Highly Efficient Oxygen Evolution Reaction Catalyst. <i>ChemElectroChem</i> , 2019 , 6, 5469-5478	4.3	7
112	Risk of psychosis in Yorkshire South Asians. <i>Journal of Psychiatric Intensive Care</i> , 2019 , 15, 117-121	0.3	2
111	Impact of Magnetic Field and Second-Order Slip Flow of Casson Liquid with Heat Transfer Subject to Suction/Injection and Convective Boundary Condition. <i>Journal of Magnetism</i> , 2019 , 24, 81-89	1.9	11
110	Density functional theory-supported studies of structural and electronic properties of substituted-phenol derivatives synthesized by efficient O- or C-arylation via Chan-Lam or Suzuki cross-coupling reactions. <i>Turkish Journal of Chemistry</i> , 2019 , 43, 1306-1321	1	0
109	Spherical fuzzy sets and their applications in multi-attribute decision making problems. <i>Journal of Intelligent and Fuzzy Systems</i> , 2019 , 36, 2829-2844	1.6	137
108	Assessment of mold and yeast in some bakery products of Lahore, Pakistan based on LM and SEM. <i>Microscopy Research and Technique</i> , 2019 , 82, 85-91	2.8	3

107	Effect of magnesium on structural and optical properties of CaTiO ₃ : A DFT study. <i>Physica B: Condensed Matter</i> , 2019 , 568, 88-91	2.8	10
106	Design, synthesis and bioevaluation of tricyclic fused ring system as dual binding site acetylcholinesterase inhibitors. <i>Bioorganic Chemistry</i> , 2019 , 83, 336-347	5.1	50
105	Numerical treatment for Darcy-Borchheimer flow of nanofluid due to a rotating disk with slip effects. <i>Canadian Journal of Physics</i> , 2019 , 97, 856-863	1.1	10
104	Silymarin-laden PVP-PEG polymeric composite for enhanced aqueous solubility and dissolution rate: Preparation and in vitro characterization. <i>Journal of Pharmaceutical Analysis</i> , 2019 , 9, 34-39	14	21
103	Isolation, spectroscopic and density functional theory of two withanolide glycosides. <i>Journal of Molecular Structure</i> , 2019 , 1177, 449-456	3.4	7
102	Comparative efficacy of two anti-aging products containing retinyl palmitate in healthy human volunteers. <i>Journal of Cosmetic Dermatology</i> , 2018 , 17, 454-460	2.5	2
101	Palladium(0) catalyzed Suzuki cross-coupling reaction of 2,5-dibromo-3-methylthiophene: selectivity, characterization, DFT studies and their biological evaluations. <i>Chemistry Central Journal</i> , 2018 , 12, 49		17
100	Visible light photocatalytic degradation of crystal violet dye and electrochemical detection of ascorbic acid & glucose using BaWO ₄ nanorods. <i>Materials Research Bulletin</i> , 2018 , 104, 38-43	5.1	19
99	Facile synthesis of N- (4-bromophenyl)-1- (3-bromothiophen-2-yl)methanimine derivatives via Suzuki cross-coupling reaction: their characterization and DFT studies. <i>Chemistry Central Journal</i> , 2018 , 12, 84		10
98	Synthesis, quantum chemical, in vitro acetyl cholinesterase inhibition and molecular docking studies of four new coumarin based pyrazolythiazole nuclei. <i>Journal of Molecular Structure</i> , 2018 , 1168, 175-186	3.4	11
97	Accurate theoretical method for homolytic cleavage of C Sn bond: A benchmark approach. <i>Computational and Theoretical Chemistry</i> , 2018 , 1140, 134-144	2	4
96	Scorpion Venom Peptides as a Potential Source for Human Drug Candidates. <i>Protein and Peptide Letters</i> , 2018 , 25, 702-708	1.9	14
95	New Perspectives on the Efficacy of Gallic Acid in Cosmetics & Nanocosmeceuticals. <i>Current Pharmaceutical Design</i> , 2018 , 24, 5181-5187	3.3	25
94	Enhancing food security in arid areas of Pakistan through newly developed drought tolerant and short duration mustard (<i>Brassica juncea</i> L.) Canola. <i>Genetika</i> , 2018 , 50, 21-31	0.6	0
93	Multivariate analysis for adaptability and yield stability of rapeseed (<i>Brassica napus</i> L.) strains in different agro-climatic zones. <i>Genetika</i> , 2018 , 50, 369-378	0.6	1
92	Selective arylation of phenol protected propyl bromide via Pd-catalysed Suzuki coupling reaction: synthesis, mechanistic studies by DFT calculations and Their Pharmacological Aspects". <i>Acta Poloniae Pharmaceutica</i> , 2018 , 75, 911-919	1.3	2
91	Copper-doped Al ₁₂ N ₁₂ nano-cages: potential candidates for nonlinear optical materials. <i>Applied Physics A: Materials Science and Processing</i> , 2018 , 124, 1	2.6	21
90	High sensitivity of polypyrrole sensor for uric acid over urea, acetamide and sulfonamide: A density functional theory study. <i>Synthetic Metals</i> , 2018 , 235, 49-60	3.6	45

89	Synthesis, crystal structures, computational studies and antimicrobial activity of new designed bis((5-aryl-1,3,4-oxadiazol-2-yl)thio)alkanes. <i>Journal of Molecular Structure</i> , 2018 , 1155, 403-413	3-4	24
88	Impact of processing methods on the dissolution of artemether from two non-ordered mesoporous silicas. <i>European Journal of Pharmaceutical Sciences</i> , 2018 , 112, 139-145	5-1	11
87	Carbonic anhydrase inhibition of Schiff base derivative of imino-methyl-naphthalen-2-ol: Synthesis, structure elucidation, molecular docking, dynamic simulation and density functional theory calculations. <i>Journal of Molecular Structure</i> , 2018 , 1156, 193-200	3-4	13
86	Influence of polymer ratio and surfactants on controlled drug release from cellulosic microsponges. <i>International Journal of Biological Macromolecules</i> , 2018 , 109, 963-970	7-9	19
85	(M, N)-Double framed soft ideals of Abel Grassmann \bar{B} groupoids. <i>Journal of Intelligent and Fuzzy Systems</i> , 2018 , 35, 6313-6327	1-6	2
84	Synthesis of 3,4-Biaryl-2,5-Dichlorothiophene through Suzuki Cross-Coupling and Theoretical Exploration of Their Potential Applications as Nonlinear Optical Materials. <i>Symmetry</i> , 2018 , 10, 766	2-7	2
83	Sensor applications of polypyrrole for oxynitrogen analytes: a DFT study. <i>Journal of Molecular Modeling</i> , 2018 , 24, 308	2	21
82	First principles investigation of electronic and optical properties of AgAlO ₂ . <i>Chinese Journal of Physics</i> , 2018 , 56, 2186-2190	3-5	7
81	Theoretical insight into structural and electronic properties of cationic Sc ⁿ⁺ (n=2-13): A benchmark study. <i>Solid State Sciences</i> , 2018 , 86, 60-68	3-4	2
80	Detailed Mechanistic Study of Radical Mediated Chemoselective Phosphination of Aryl Halide. <i>ChemistrySelect</i> , 2018 , 3, 11302-11308	1-8	1
79	Benchmark study of structural and vibrational properties of scandium clusters. <i>Journal of Molecular Structure</i> , 2017 , 1142, 139-147	3-4	3
78	Synthesis, molecular structure, quantum mechanical studies and urease inhibition assay of two new isatin derived sulfonylhydrazides. <i>Journal of Molecular Structure</i> , 2017 , 1133, 80-89	3-4	20
77	Study of the structural and electronic properties of FeO at the LDA and GGA level. <i>Chinese Journal of Physics</i> , 2017 , 55, 1135-1141	3-5	5
76	DFT study of acceleration of electrocyclization in photochromes under radical cationic conditions: Comparison with recent experimental data. <i>Tetrahedron</i> , 2017 , 73, 3521-3528	2-4	16
75	An accurate comparative theoretical study of the interaction of furan, pyrrole, and thiophene with various gaseous analytes. <i>Journal of Molecular Modeling</i> , 2017 , 23, 295	2	31
74	Role of dispersion corrected hybrid GGA class in accurately calculating the bond dissociation energy of carbon halogen bond: A benchmark study. <i>Journal of Molecular Structure</i> , 2017 , 1150, 447-458	3-4	13
73	Thiobiuret based Ni(II) and Co(III) complexes: Synthesis, molecular structures and DFT studies. <i>Journal of Molecular Structure</i> , 2017 , 1148, 388-396	3-4	19
72	Elastic, electronic and optical properties of anatase TiO ₂ under pressure: A DFT approach. <i>Chinese Journal of Physics</i> , 2017 , 55, 1252-1263	3-5	10

71	Synthesis, structural studies and biological activities of three new 2-(pentadecylthio)-5-aryl-1,3,4-oxadiazoles. <i>Journal of Molecular Structure</i> , 2017 , 1129, 50-59	3.4	26
70	Efficient Synthesis of Novel Pyridine-Based Derivatives via Suzuki Cross-Coupling Reaction of Commercially Available 5-Bromo-2-methylpyridin-3-amine: Quantum Mechanical Investigations and Biological Activities. <i>Molecules</i> , 2017 , 22,	4.8	18
69	Efficacy of Phoenix dactylifera L. (Date Palm) Creams on Healthy Skin. <i>Cosmetics</i> , 2017 , 4, 13	2.7	5
68	An accurate cost effective DFT approach to study the sensing behaviour of polypyrrole towards nitrate ions in gas and aqueous phases. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 19236-47	3.6	40
67	One-pot synthesis of tetrazole-1,2,5,6-tetrahydronicotinonitriles and cholinesterase inhibition: Probing the plausible reaction mechanism via computational studies. <i>Bioorganic Chemistry</i> , 2016 , 65, 38-47	5.1	12
66	First-principles calculation of electronic and optical properties of graphene like ZnO (G-ZnO). <i>Superlattices and Microstructures</i> , 2016 , 90, 165-169	2.8	11
65	Synthesis and structural properties of 2-((10-alkyl-10H-phenothiazin-3-yl)methylene)malononitrile derivatives; a combined experimental and theoretical insight. <i>Chemistry Central Journal</i> , 2016 , 10, 13		10
64	Power analysis approach and its application to IP-based SoC design. <i>COMPEL - the International Journal for Computation and Mathematics in Electrical and Electronic Engineering</i> , 2016 , 35,	0.7	4
63	Theoretical mechanistic investigation of zinc(II) catalyzed oxidative amidation of benzyl alcohols with amines. <i>Polyhedron</i> , 2016 , 112, 34-42	2.7	3
62	Quantum mechanical investigation on acceleration of electrocyclic reactions through transition metal catalysis. <i>Journal of Organometallic Chemistry</i> , 2016 , 808, 78-86	2.3	11
61	Pressure induced electronic and optical properties of rutile SnO ₂ by first principle calculations. <i>Superlattices and Microstructures</i> , 2016 , 90, 236-241	2.8	7
60	Click one pot synthesis, spectral analyses, crystal structures, DFT studies and brine shrimp cytotoxicity assay of two newly synthesized 1,4,5-trisubstituted 1,2,3-triazoles. <i>Journal of Molecular Structure</i> , 2016 , 1106, 430-439	3.4	33
59	One Pot Selective Arylation of 2-Bromo-5-Chloro Thiophene; Molecular Structure Investigation via Density Functional Theory (DFT), X-ray Analysis, and Their Biological Activities. <i>International Journal of Molecular Sciences</i> , 2016 , 17,	6.3	18
58	Formulation and stability of topical water in oil emulsion containing corn silk extract. <i>Tropical Journal of Pharmaceutical Research</i> , 2016 , 15, 1115	0.8	8
57	Theoretical mechanistic investigation of zinc(II) catalyzed oxidation of alcohols to aldehydes and esters. <i>RSC Advances</i> , 2016 , 6, 31876-31883	3.7	7
56	Theoretical insights into thermal cyclophanediene to dihydropyrene electrocyclic reactions; a comparative study of Woodward Hoffmann allowed and forbidden reactions. <i>Journal of Molecular Modeling</i> , 2016 , 22, 81	2	4
55	Synthesis of 2-acylated and sulfonated 4-hydroxycoumarins: In vitro urease inhibition and molecular docking studies. <i>Bioorganic Chemistry</i> , 2016 , 66, 111-6	5.1	35
54	Design of a negative refractive index material based on numerical simulation. <i>Chinese Journal of Physics</i> , 2016 , 54, 587-591	3.5	3

53	Synthesis, crystal structures and spectroscopic properties of triazine-based hydrazone derivatives; a comparative experimental-theoretical study. <i>Molecules</i> , 2015 , 20, 5851-74	4.8	60
52	Isolation, spectroscopic and density functional theory studies of 7-(4-methoxyphenyl)-9H-furo[2,3-f]chromen-9-one: a new flavonoid from the bark of <i>Millettia ovalifolia</i> . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 146, 24-32	4.4	17
51	Spectroscopic and density functional theory studies of 7-hydroxy-3'-methoxyisoflavone: A new isoflavone from the seeds of <i>Indigofera heterantha</i> (Wall). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 148, 375-81	4.4	20
50	Bifunctional catalysts of Co ₃ O ₄ @GCN tubular nanostructured (TNS) hybrids for oxygen and hydrogen evolution reactions. <i>Nano Research</i> , 2015 , 8, 3725-3736	10	86
49	Semihypergroups characterized by (???)Fuzzy hyperideals. <i>Journal of Intelligent and Fuzzy Systems</i> , 2015 , 28, 2667-2678	1.6	6
48	Synthesis, Density Functional Theory (DFT), Urease Inhibition and Antimicrobial Activities of 5-Aryl Thiophenes Bearing Sulphonylacetamide Moieties. <i>Molecules</i> , 2015 , 20, 19914-28	4.8	18
47	Towards thermally stable cyclophanediene-dihydropyrene photoswitches. <i>Journal of Molecular Modeling</i> , 2015 , 21, 148	2	6
46	Mechanistic insight of TiCl ₄ catalyzed formal [3 + 3] cyclization of 1,3-bis(silyl enol ethers) with 1,3-dielectrophiles. <i>RSC Advances</i> , 2015 , 5, 94304-94314	3.7	6
45	Dyotropic rearrangement of bridgehead substituents in closed dithienylethenes; conjugated verses non-conjugated analogues. <i>Journal of Molecular Modeling</i> , 2015 , 21, 321	2	4
44	Synthesis, crystal structure, spectroscopic and density functional theory (DFT) study of N-[3-anthracen-9-yl-1-(4-bromo-phenyl)-allylidene]-N-benzenesulfonylhydrazine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 142, 364-74	4.4	51
43	Pharmacological importance of an ethnobotanical plant: <i>Capsicum annum</i> L. <i>Natural Product Research</i> , 2014 , 28, 1267-74	2.3	39
42	Interfacial film stabilized W/O/W nano multiple emulsions loaded with green tea and lotus extracts: systematic characterization of physicochemical properties and shelf-storage stability. <i>Journal of Nanobiotechnology</i> , 2014 , 12, 20	9.4	29
41	Synthesis, characterization and density functional theory study of some new 2-anilinothiazoles. <i>Journal of Molecular Structure</i> , 2014 , 1072, 221-227	3.4	15
40	Aromaticity of azines through dyotropic double hydrogen transfer reaction. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2304	2	4
39	Metal-catalyzed synthesis of ultralong tin dioxide nanobelts: Electrical and optical properties with oxygen vacancy-related orange emission. <i>Materials Science in Semiconductor Processing</i> , 2014 , 26, 388-394	4.3	8
38	Extraction of Pb(II) from water samples by ionic liquid-modified silica sorbents. <i>Desalination and Water Treatment</i> , 2014 , 52, 7915-7924		3
37	Topical microemulsion containing <i>Punica granatum</i> extract: its control over skin erythema and melanin in healthy Asian subjects. <i>Postepy Dermatologii I Alergologii</i> , 2014 , 31, 351-5	1.5	5
36	Fabrication and Characterization of Gliclazide Loaded Microcapsules. <i>Brazilian Archives of Biology and Technology</i> , 2014 , 57, 874-881	1.8	

35	Pressure based first-principles study of the electronic, elastic, optic and phonon properties of zincblende InN. <i>Physica B: Condensed Matter</i> , 2013 , 430, 67-73	2.8	9
34	Tubular graphitic-C3N4: a prospective material for energy storage and green photocatalysis. <i>Journal of Materials Chemistry A</i> , 2013 , 1, 13949	13	211
33	Two-in-one: a pH-sensitive, acridine-based, fluorescent probe binds G-quadruplexes in oncogene promoters. <i>MedChemComm</i> , 2013 , 4, 211-215	5	14
32	Facile synthesis of novel Nb3O7F nanoflowers, their optical and photocatalytic properties. <i>CrystEngComm</i> , 2013 , 15, 8146	3.3	34
31	Electronic, elastic, acoustic and optical properties of cubic TiO2: A DFT approach. <i>Physica B: Condensed Matter</i> , 2013 , 420, 74-80	2.8	14
30	Single crystalline multi-petal Cd nanoleaves prepared by thermal reduction of CdO. <i>Materials Research Bulletin</i> , 2013 , 48, 819-822	5.1	3
29	Preparation of highly pure CdSe hollow structures: Their PL and hydrogen absorption properties. <i>Materials Letters</i> , 2013 , 92, 263-266	3.3	9
28	Effect of Ni charge states on structural, electronic, magnetic, and optical properties of InN. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 5650-4	2.8	1
27	Combined topical application of lotus and green tea improves facial skin surface parameters. <i>Rejuvenation Research</i> , 2013 , 16, 91-7	2.6	21
26	Short term study of human skin irritation by single application closed patch test: assessment of four multiple emulsion formulations loaded with botanical extracts. <i>Cutaneous and Ocular Toxicology</i> , 2013 , 32, 35-40	1.8	6
25	Fabrication, physicochemical characterization and preliminary efficacy evaluation of a W/O/W multiple emulsion loaded with 5% green tea extract. <i>Brazilian Journal of Pharmaceutical Sciences</i> , 2013 , 49, 341-349	1.8	12
24	Stability of a cosmetic multiple emulsion loaded with green tea extract. <i>Scientific World Journal, The</i> , 2013 , 2013, 153695	2.2	15
23	Copper complexes of bioactive ligands with superoxide dismutase activity. <i>Mini-Reviews in Medicinal Chemistry</i> , 2013 , 13, 1944-56	3.2	18
22	High yield preparation of single crystalline Cd metal nanotubes by non-catalytic thermal decomposition route. <i>Solid State Sciences</i> , 2012 , 14, 693-697	3.4	2
21	Electronic, elastic, optical properties of rutile TiO2 under pressure: A DFT study. <i>Physica B: Condensed Matter</i> , 2012 , 407, 958-965	2.8	43
20	Synthesis of highly pure single crystalline SnSe nanostructures by thermal evaporation and condensation route. <i>Materials Chemistry and Physics</i> , 2012 , 137, 565-570	4.4	34
19	Synthesis, characterization, photoluminescence and field emission properties of novel durian-like gallium nitride microstructures. <i>Materials Chemistry and Physics</i> , 2012 , 133, 793-798	4.4	20
18	Fabrication and photovoltaic characteristics of Cu2O/TiO2 thin film heterojunction solar cell. <i>Thin Solid Films</i> , 2012 , 522, 430-434	2.2	29

17	Elastic, electronic and optical properties of cotunnite TiO ₂ from first principles calculations. <i>Physica B: Condensed Matter</i> , 2012 , 407, 4495-4501	2.8	11
16	Simultaneous growth of ZnSe cactus-like structures and novel microflowers of selenium. <i>Journal of Alloys and Compounds</i> , 2012 , 513, 620-625	5.7	7
15	Closing the ring to bring up the light: synthesis of a hexacyclic acridinium cyanine dye. <i>Chemistry - A European Journal</i> , 2012 , 18, 12349-56	4.8	9
14	Controlled growth of catalyst assisted and catalyst free CdSe micro cactuses with sharply pointed nanorods, their Photoluminescence (PL) and Photo electrochemical (PEC) properties. <i>Electrochimica Acta</i> , 2012 , 85, 122-130	6.7	2
13	Fabrication of novel SnO ₂ nanofibers bundle and their optical properties. <i>Materials Chemistry and Physics</i> , 2012 , 136, 10-14	4.4	22
12	Fabrication and electrical characterization of p-Cu ₂ O/n-ZnO heterojunction. <i>Journal of Nanoscience and Nanotechnology</i> , 2012 , 12, 1967-71	1.3	4
11	1-Methyl-4-[1-(1-phenyl-ethyl-idene)-hydrazin-2-yl-idene]-3,4-dihydro-1H-2(1 <i>H</i>),1-benzothia-zine-2,2-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o2100		
10	Sebumetric and mexametric evaluation of a fennel based cream. <i>ScienceAsia</i> , 2012 , 38, 262	1.4	3
9	Thermal evaporation and condensation synthesis of metallic Zn layered polyhedral microparticles. <i>Materials Research Bulletin</i> , 2011 , 46, 2261-2265	5.1	5
8	Large-scale synthesis of highly pure Cd metal hexagonal nanosheets. <i>Materials Letters</i> , 2011 , 65, 1896-1899	3.7	15
7	Effect of electrodeposition and annealing of ZnO on optical and photovoltaic properties of the p-Cu ₂ O/n-ZnO solar cells. <i>Electrochimica Acta</i> , 2011 , 56, 8342-8346	6.7	32
6	Structural, elastic constant, and vibrational properties of wurtzite gallium nitride: a first-principles approach. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 14502-9	2.8	9
5	2-(4-Acetamido-benzene-sulfonamido)-benzoic acid. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011 , 67, o1570		1
4	Synthesis and spectroscopic and DNA-binding properties of fluorogenic acridine-containing cyanine dyes. <i>Journal of Organic Chemistry</i> , 2010 , 75, 204-7	4.2	42
3	Selective binding of L-glutamate derivative in aqueous solvents. <i>Organic and Biomolecular Chemistry</i> , 2008 , 6, 2340-5	3.9	16
2	Silymarin-Laden PVP-Nanocontainers Prepared Via the Electro spraying Technique for Improved Aqueous Solubility and Dissolution Rate. <i>Brazilian Archives of Biology and Technology</i> , 62 ,	1.8	2
1	An intelligent fault detection approach based on reinforcement learning system in wireless sensor network. <i>Journal of Supercomputing</i> , 1	2.5	5