Tariq Mahmood

List of Publications by Citations

139 papers	1,984 citations	25 h-index	35 g-index
146 ext. papers	2,822 ext. citations	3.6 avg, IF	6.04 L-index

#	Paper	IF	Citations
139	Highly selective acridinium based cyanine dyes for the detection of DNA base pairs (adenine, cytosine, guanine and thymine). *Computational and Theoretical Chemistry*, **2019**, 1163, 112509	2	63
138	Synthesis, crystal structures and spectroscopic properties of triazine-based hydrazone derivatives; a comparative experimental-theoretical study. *Molecules*, **2015**, 20, 5851-74	4.8	60
137	Superalkalis as a source of diffuse excess electrons in newly designed inorganic electrides with remarkable nonlinear response and deep ultraviolet transparency: A DFT study. *Applied Surface Science*, **2019**, 483, 1118-1128	6.7	56
136	Cyclic versus straight chain oligofuran as sensor: A detailed DFT study. *Journal of Molecular Graphics and Modelling*, **2020**, 97, 107569	2.8	52
135	Synthesis, crystal structure, spectroscopic and density functional theory (DFT) study of N-[3-anthracen-9-yl-1-(4-bromo-phenyl)-allylidene]-N-benzenesulfonohydrazine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 142, 364-74	4.4	51
134	Design, synthesis and bioevaluation of tricyclic fused ring system as dual binding site acetylcholinesterase inhibitors. *Bioorganic Chemistry*, **2019**, 83, 336-347	5.1	50
133	Theoretical study on a boron phosphide nanocage doped with superalkalis: novel electrides having significant nonlinear optical response. *New Journal of Chemistry*, **2019**, 43, 5727-5736	3.6	46
132	Silver-graphene quantum dots based electrochemical sensor for trinitrotoluene and p-nitrophenol. *Journal of Molecular Liquids*, **2020**, 306, 112878	6	46
131	High sensitivity of polypyrrole sensor for uric acid over urea, acetamide and sulfonamide: A density functional theory study. *Synthetic Metals*, **2018**, 235, 49-60	3.6	45
130	Synthesis and spectroscopic and DNA-binding properties of fluorogenic acridine-containing cyanine dyes. *Journal of Organic Chemistry*, **2010**, 75, 204-7	4.2	42
129	Exceptionally high NLO response and deep ultraviolet transparency of superalkali doped macrocyclic oligofuran rings. *New Journal of Chemistry*, **2020**, 44, 2609-2618	3.6	41
128	An accurate cost effective DFT approach to study the sensing behaviour of polypyrrole towards nitrate ions in gas and aqueous phases. *Physical Chemistry Chemical Physics*, **2016**, 18, 19236-47	3.6	40
127	Design of novel superalkali doped silicon carbide nanocages with giant nonlinear optical response. *Optics and Laser Technology*, **2020**, 122, 105855	4.2	40
126	Theoretical study on novel superalkali doped graphdiyne complexes: Unique approach for the enhancement of electronic and nonlinear optical response. *Journal of Molecular Graphics and Modelling*, **2020**, 97, 107573	2.8	39
125	Theoretical study on design of novel superalkalis doped graphdiyne: A new donor□cceptor (D-□A) strategy for enhancing NLO response. *Applied Surface Science*, **2019**, 492, 255-263	6.7	39
124	A comprehensive DFT study on the sensing abilities of cyclic oligothiophenes (nCTs). *New Journal of Chemistry*, **2019**, 43, 14120-14133	3.6	36
123	Adsorption behaviour of chronic blistering agents on graphdiyne; excellent correlation among SAPT, reduced density gradient (RDG) and QTAIM analyses. *Journal of Molecular Liquids*, **2020**, 316, 113860	6	36

122	Synthesis of 2-acylated and sulfonated 4-hydroxycoumarins: In vitro urease inhibition and molecular docking studies. *Bioorganic Chemistry*, **2016**, 66, 111-6	5.1	35
121	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. *Journal of Molecular Structure*, **2016**, 1106, 430-439	3.4	33
120	An accurate comparative theoretical study of the interaction of furan, pyrrole, and thiophene with various gaseous analytes. *Journal of Molecular Modeling*, **2017**, 23, 295	2	31
119	Doping superalkali on Zn12O12 nanocage constitutes a superior approach to fabricate stable and high-performance nonlinear optical materials. *Optics and Laser Technology*, **2019**, 120, 105753	4.2	30
118	High selectivity of cyclic tetrapyrrole over tetrafuran and tetrathiophene toward toxic chemicals; A first-principles study. *Microporous and Mesoporous Materials*, **2020**, 299, 110126	5.3	29
117	High sensitivity of graphdiyne nanoflake toward detection of phosgene, thiophosgene and phosogenoxime; a first-principles study. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107658	2.8	27
116	First-principles study for exploring the adsorption behavior of G-series nerve agents on graphdyine surface. *Computational and Theoretical Chemistry*, **2020**, 1191, 113043	2	27
115	Synthesis, structural studies and biological activities of three new 2-(pentadecylthio)-5-aryl-1,3,4-oxadiazoles. *Journal of Molecular Structure*, **2017**, 1129, 50-59	3.4	26
114	Comparative investigation of sensor application of polypyrrole for gaseous analytes. *Journal of Physical Organic Chemistry*, **2019**, 32, e3960	2.1	24
113	Synthesis, crystal structures, computational studies and antimicrobial activity of new designed bis((5-aryl-1,3,4-oxadiazol-2-yl)thio)alkanes. *Journal of Molecular Structure*, **2018**, 1155, 403-413	3.4	24
112	Alkaline earth metal decorated phosphide nanoclusters for potential applications as high performance NLO materials; A first principle study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 118, 113906	3	23
111	Outstanding NLO response of thermodynamically stable single and multiple alkaline earth metals doped C20 fullerene. *Journal of Molecular Liquids*, **2020**, 305, 112875	6	22
110	Synthesis, structural properties, DFT studies, antimicrobial activities and DNA binding interactions of two newly synthesized organotin(IV) carboxylates. *Journal of Molecular Structure*, **2019**, 1191, 291-300	3.4	21
109	Significant nonlinear optical response of alkaline earth metals doped beryllium and magnesium oxide nanocages. *Materials Chemistry and Physics*, **2020**, 242, 122507	4.4	21
108	Copper-doped Al12N12 nano-cages: potential candidates for nonlinear optical materials. *Applied Physics A: Materials Science and Processing*, **2018**, 124, 1	2.6	21
107	Sensor applications of polypyrrole for oxynitrogen analytes: a DFT study. *Journal of Molecular Modeling*, **2018**, 24, 308	2	21
106	Synthesis, molecular structure, quantum mechanical studies and urease inhibition assay of two new isatin derived sulfonylhydrazides. *Journal of Molecular Structure*, **2017**, 1133, 80-89	3.4	20
105	Spectroscopic and density functional theory studies of 7-hydroxy-3-methoxyisoflavone: A new isoflavone from the seeds of Indigofera heterantha (Wall). *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 148, 375-81	4.4	20

104	Thiobiuret based Ni(II) and Co(III) complexes: Synthesis, molecular structures and DFT studies. *Journal of Molecular Structure*, **2017**, 1148, 388-396	3.4	19
103	Remarkable second and third order nonlinear optical properties of organometallic C6Li6M3O electrides. *New Journal of Chemistry*, **2020**, 44, 9822-9829	3.6	18
102	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. *Molecules*, **2017**, 22,	4.8	18
101	Synthesis, Density Functional Theory (DFT), Urease Inhibition and Antimicrobial Activities of 5-Aryl Thiophenes Bearing Sulphonylacetamide Moieties. *Molecules*, **2015**, 20, 19914-28	4.8	18
100	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. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	18
99	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 Millettia ovalifolia. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 146, 24-32	4.4	17
98	Palladium(0) catalyzed Suzuki cross-coupling reaction of 2,5-dibromo-3-methylthiophene: selectivity, characterization, DFT studies and their biological evaluations. *Chemistry Central Journal*, **2018**, 12, 49		17
97	Superhalogen doping: a new and effective approach to design materials with excellent static and dynamic NLO responses. *New Journal of Chemistry*, **2020**, 44, 16358-16369	3.6	17
96	DFT study of acceleration of electrocyclization in photochromes under radical cationic conditions: Comparison with recent experimental data. *Tetrahedron*, **2017**, 73, 3521-3528	2.4	16
95	Selective binding of L-glutamate derivative in aqueous solvents. *Organic and Biomolecular Chemistry*, **2008**, 6, 2340-5	3.9	16
94	Synthesis, crystal structures, computational studies and □-amylase inhibition of three novel 1,3,4-oxadiazole derivatives. *Journal of Molecular Structure*, **2020**, 1200, 127085	3.4	16
93	Remarkable static and dynamic NLO response of alkali and superalkali doped macrocyclic [hexa-]thiophene complexes; a DFT approach.. *RSC Advances*, **2021**, 11, 4118-4128	3.7	16
92	Design, synthesis and anti-bacterial studies of piperazine derivatives against drug resistant bacteria. *European Journal of Medicinal Chemistry*, **2019**, 166, 224-231	6.8	15
91	Synthesis, characterization and density functional theory study of some new 2-anilinothiazoles. *Journal of Molecular Structure*, **2014**, 1072, 221-227	3.4	15
90	Two-in-one: a pH-sensitive, acridine-based, fluorescent probe binds G-quadruplexes in oncogene promoters. *MedChemComm*, **2013**, 4, 211-215	5	14
89	Role of dispersion corrected hybrid GGA class in accurately calculating the bond dissociation energy of carbon halogen bond: A benchmark study. *Journal of Molecular Structure*, **2017**, 1150, 447-458	3.4	13
88	Design of novel inorganic alkaline earth metal doped aluminum nitride complexes (AEM@Al12N12) with high chemical stability, improved electronic properties and large nonlinear optical response. *Optik*, **2020**, 207, 163792	2.5	13
87	Janus alkaline earthides with excellent NLO response from sodium and potassium as source of excess electrons; a first principles study. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107668	2.8	13

86	Effective adsorption of A-series chemical warfare agents on graphdiyne nanoflake: a DFT study. *Journal of Molecular Modeling*, **2021**, 27, 117	2	13
85	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. *Journal of Molecular Structure*, **2018**, 1156, 193-200	3.4	13
84	Nonlinear optical response of sodium based superalkalis decorated graphdiyne surface: A DFT study. *Optik*, **2020**, 218, 165033	2.5	12
83	One-pot synthesis of tetrazole-1,2,5,6-tetrahydronicotinonitriles and cholinesterase inhibition: Probing the plausible reaction mechanism via computational studies. *Bioorganic Chemistry*, **2016**, 65, 38-47	5.1	12
82	Surface functionalization of twisted graphene CH and CH derivatives with alkalis and superalkalis for NLO response; a DFT study. *Journal of Molecular Graphics and Modelling*, **2021**, 102, 107794	2.8	12
81	Benchmark DFT studies on C-CN homolytic cleavage and screening the substitution effect on bond dissociation energy. *Journal of Molecular Modeling*, **2019**, 25, 47	2	11
80	Halides encapsulation in aluminum/boron phosphide nanoclusters: An effective strategy for high cell voltage in Na-ion battery. *Materials Science in Semiconductor Processing*, **2019**, 97, 71-79	4.3	11
79	Quantum mechanical investigation on acceleration of electrocyclic reactions through transition metal catalysis. *Journal of Organometallic Chemistry*, **2016**, 808, 78-86	2.3	11
78	Synthesis, quantum chemical, in vitro acetyl cholinesterase inhibition and molecular docking studies of four new coumarin based pyrazolylthiazole nuclei. *Journal of Molecular Structure*, **2018**, 1168, 175-186	3.4	11
77	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. *Journal of Molecular Structure*, **2019**, 1175, 73-89	3.4	11
76	First row transition metals decorated boron phosphide nanoclusters as nonlinear optical materials with high thermodynamic stability and enhanced electronic properties; A detailed quantum chemical study. *Optics and Laser Technology*, **2021**, 134, 106570	4.2	11
75	Adsorption mechanism of p- aminophenol over silver-graphene composite: A first principles study. *Journal of Molecular Liquids*, **2021**, 341, 117415	6	11
74	Synthesis and structural properties of 2-((10-alkyl-10H-phenothiazin-3-yl)methylene)malononitrile derivatives; a combined experimental and theoretical insight. *Chemistry Central Journal*, **2016**, 10, 13		10
73	Facile synthesis of N- (4-bromophenyl)-1- (3-bromothiophen-2-yl)methanimine derivatives via Suzuki cross-coupling reaction: their characterization and DFT studies. *Chemistry Central Journal*, **2018**, 12, 84		10
72	Theoretical investigation of halides encapsulated Na@B40 nanocages for potential applications as anodes for sodium ion batteries. *Materials Science in Semiconductor Processing*, **2021**, 121, 105437	4.3	10
71	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. *Journal of Physical Organic Chemistry*, **2021**, 34, e4181	2.1	10
70	Closing the ring to bring up the light: synthesis of a hexacyclic acridinium cyanine dye. *Chemistry - A European Journal*, **2012**, 18, 12349-56	4.8	9
69	Structural, spectroscopic and nonlinear optical properties of sulfonamide derivatives; experimental and theoretical study. *Journal of Molecular Structure*, **2020**, 1202, 127393	3.4	9

68	Theoretical modification of C24 fullerene with single and multiple alkaline earth metal atoms for their potential use as NLO materials. *Journal of Physics and Chemistry of Solids*, **2021**, 152, 109972	3.9	9
67	Quantum chemical study on sensing of NH3, NF3, NCl3 and NBr3 by using cyclic tetrapyrrole. *Computational and Theoretical Chemistry*, **2021**, 1199, 113221	2	9
66	Dexibuprofen amide derivatives as potential anticancer agents: synthesis, in silico docking, bioevaluation, and molecular dynamic simulation. *Drug Design, Development and Therapy*, **2019**, 13, 1643-1657	4.4	8
65	Nonlinear optical response of first-row transition metal doped Al12P12 nanoclusters; a first-principles study. *Journal of Physics and Chemistry of Solids*, **2021**, 151, 109914	3.9	8
64	Turning diamondoids into nonlinear optical materials by alkali metal Substitution: A DFT investigation. *Optics and Laser Technology*, **2021**, 142, 107231	4.2	8
63	A first principles study on electrochemical sensing of highly toxic pesticides by using porous C4N nanoflake. *Journal of Physics and Chemistry of Solids*, **2022**, 160, 110345	3.9	8
62	A New Strategy of bi-Alkali Metal Doping to Design Boron Phosphide Nanocages of High Nonlinear Optical Response with Better Thermodynamic Stability. *Journal of Inorganic and Organometallic Polymers and Materials*, **2021**, 31, 3062	3.2	7
61	DFT studies of single and multiple alkali metals doped C fullerene for electronics and nonlinear optical applications. *Journal of Molecular Graphics and Modelling*, **2021**, 105, 107867	2.8	7
60	Theoretical mechanistic investigation of zinc(II) catalyzed oxidation of alcohols to aldehydes and esters. *RSC Advances*, **2016**, 6, 31876-31883	3.7	7
59	Isolation, spectroscopic and density functional theory of two withanolide glycosides. *Journal of Molecular Structure*, **2019**, 1177, 449-456	3.4	7
58	Silver cluster decorated graphene nanoflakes for selective and accurate detection of nitroaniline isomers; DFT calculations. *Materials Science in Semiconductor Processing*, **2021**, 134, 106023	4.3	7
57	Ratiometric Photoacoustic Chemical Sensor for Pd Ion. *Analytical Chemistry*, **2020**, 92, 4721-4725	7.8	6
56	Density functional theory study of structural, electronic and CO adsorption properties of anionic Scn□(n = 2□13) clusters. *Computational and Theoretical Chemistry*, **2019**, 1163, 112511	2	6
55	Towards thermally stable cyclophanediene-dihydropyrene photoswitches. *Journal of Molecular Modeling*, **2015**, 21, 148	2	6
54	Mechanistic insight of TiCl4 catalyzed formal [3 + 3] cyclization of 1,3-bis(silyl enol ethers) with 1,3-dielectrophiles. *RSC Advances*, **2015**, 5, 94304-94314	3.7	6
53	Remarkable nonlinear optical response of Mn@C20 (M = Na & K and n = 1□); a DFT outcome. *Materials Science in Semiconductor Processing*, **2022**, 138, 106269	4.3	6
52	Effect of fluorination on the adsorption properties of aromatic heterocycles toward methyl halides: A quantum chemical study. *Computational and Theoretical Chemistry*, **2021**, 1204, 113394	2	6
51	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. *Molecules*, **2019**, 24,	4.8	5

50	Nano-porous CN as a toxic pesticides scavenger: A quantum chemical approach. *Journal of Molecular Graphics and Modelling*, **2021**, 111, 108078	2.8	5
49	Exploring Li4N and Li4O superalkalis as efficient dopants for the Al12N12 nanocage to design high performance nonlinear optical materials with high thermodynamic stability. *Polyhedron*, **2021**, 200, 115145	2.7	5
48	Influence of bi-alkali metals doping over Al12N12 nanocage on stability and optoelectronic properties: A DFT investigation. *Radiation Physics and Chemistry*, **2021**, 184, 109457	2.5	5
47	Facile synthesis of 4-aryl-N-(5-methyl-1H-pyrazol-3-yl)benzamides via Suzuki Miyaura reaction: Antibacterial activity against clinically isolated NDM-1-positive bacteria and their Docking Studies. *Arabian Journal of Chemistry*, **2021**, 14, 103270	5.9	5
46	First example of lanthanum as dopant on Al12N12 and Al12P12 nanocages for improved electronic and nonlinear optical properties with high stability. *Materials Science in Semiconductor Processing*, **2021**, 135, 106122	4.3	5
45	Synthesis and Reactivities of Triphenyl Acetamide Analogs for Potential Nonlinear Optical Material Uses. *Symmetry*, **2019**, 11, 622	2.7	4
44	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. *New Journal of Chemistry*, **2020**, 44, 7891-7901	3.6	4
43	Accurate theoretical method for homolytic cleavage of C Sn bond: A benchmark approach. *Computational and Theoretical Chemistry*, **2018**, 1140, 134-144	2	4
42	Aromaticity of azines through dyotropic double hydrogen transfer reaction. *Journal of Molecular Modeling*, **2014**, 20, 2304	2	4
41	Dyotropic rearrangement of bridgehead substituents in closed dithienylethenes; conjugated verses non-conjugated analogues. *Journal of Molecular Modeling*, **2015**, 21, 321	2	4
40	A Theoretical Perspective on Strategies for Modeling High Performance Nonlinear Optical Materials. *Frontiers in Materials*, **2021**, 8,	4	4
39	Novel microporous B6N6 covalent organic framework (COF) as an electrochemical sensor for the ultra-selective detection of nitroaniline isomers; a DFT outcome. *Surfaces and Interfaces*, **2021**, 27, 101587	4.1	4
38	Selective Arylation of 2-Bromo-4-chlorophenyl-2-bromobutanoate via a Pd-Catalyzed Suzuki Cross-Coupling Reaction and Its Electronic and Non-Linear Optical (NLO) Properties via DFT Studies. *Molecules*, **2020**, 25,	4.8	4
37	Hydrogen adsorption on Ge52−Ge92− and Sn92−Zintl clusters: A DFT study. *Computational and Theoretical Chemistry*, **2021**, 1199, 113191	2	4
36	DFT study on the sensitivity of silver-graphene quantum dots for vital and harmful analytes. *Journal of Physics and Chemistry of Solids*, **2021**, 153, 110028	3.9	4
35	Theoretical insights into thermal cyclophanediene to dihydropyrene electrocyclic reactions; a comparative study of Woodward Hoffmann allowed and forbidden reactions. *Journal of Molecular Modeling*, **2016**, 22, 81	2	4
34	Silver cluster (Ag) decorated coronene as non-enzymatic sensor for glucose and HO. *Journal of Molecular Graphics and Modelling*, **2021**, 103, 107824	2.8	4
33	A New Insight into Non-covalent Interactions in 1,4-Disubstituted 1H-1,2,3-Triazole: Synthesis, X-ray structure, DFT calculations, in vitro Lipoxygenase Inhibition (LOX) and in silico Studies. *Journal of Molecular Structure*, **2021**, 1236, 130283	3.4	4

32	High performance SACs for HER process using late first-row transition metals anchored on graphyne support: A DFT insight. *International Journal of Hydrogen Energy*, **2021**,	6.7	4
31	Face specific doping of Janus all-cis-1,2,3,4,5,6-hexafluorocyclohexane with superalkalis and alkaline earth metals leads to enhanced static and dynamic NLO responses. *Journal of Physics and Chemistry of Solids*, **2022**, 160, 110361	3.9	4
30	Benchmark study of structural and vibrational properties of scandium clusters. *Journal of Molecular Structure*, **2017**, 1142, 139-147	3.4	3
29	Isolation, characterization and DFT studies of epoxy ring containing new withanolides from Withania coagulans Dunal. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 217, 113-121	4.4	3
28	Permeation of second row neutral elements through AlP and BP nanocages; a first-principles study. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107748	2.8	3
27	A DFT study on M3O (M = Li & Na) doped triphenylene and its amino-, hydroxy- and thiol-functionalized quantum dots for triggering remarkable nonlinear optical properties and ultra-deep transparency in ultraviolet region. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 134, 114905	3	3
26	A Novel UV-Spectrophotometric Method for Simultaneous Estimation of Amlodipine and Captopril. *Pharmaceutical Chemistry Journal*, **2019**, 52, 952-958	0.9	2
25	Synthesis, structural properties, enzyme inhibition and molecular docking studies of (Z)-N'-(1-allyl-2-oxoindolin-3-ylidene) methanesulfono-hydrazide and (Z)-N'-(1-allyl-2-oxoindolin-3-ylidene)-3-nitrobenzenesulfono-hydrazide. *Journal of Molecular Structure*, **2020**, 1221, 128880	3.4	2
24	Sensing of SO3, SO2, H2S, NO2 and N2O toxic gases through aza-macrocycle via DFT calculations. *Computational and Theoretical Chemistry*, **2022**, 1209, 113606	2	2
23	Synthesis of 3,4-Biaryl-2,5-Dichlorothiophene through Suzuki Cross-Coupling and Theoretical Exploration of Their Potential Applications as Nonlinear Optical Materials. *Symmetry*, **2018**, 10, 766	2.7	2
22	Theoretical insight into structural and electronic properties of cationic Scn+ (n=2-13): A benchmark study. *Solid State Sciences*, **2018**, 86, 60-68	3.4	2
21	Impact of even number of alkaline earth metal doping on the NLO response of C20 nanocluster; a DFT outcome. *Computational and Theoretical Chemistry*, **2021**, 1204, 113386	2	2
20	Synthesis, structural properties and potent bioactivities supported by molecular docking and DFT studies of new hydrazones derived from 5-chloroisatin and 2-thiophenecarboxaldehyde. *Journal of Molecular Structure*, **2021**, 1246, 131204	3.4	2
19	Optimized nonlinear optical (NLO) response of silicon carbide nanosheet by alkali metals doping: a DFT insight. *European Physical Journal Plus*, **2022**, 137, 1	3.1	2
18	DFT outcome for comparative analysis of Be12O12, Mg12O12 and Ca12O12 nanocages toward sensing of N2O, NO2, NO, H2S, SO2 and SO3 gases. *Computational and Theoretical Chemistry*, **2022**, 1211, 113694	2	2
17	First-principles study for electrochemical sensing of neurotoxin hydrazine derivatives via h-g-C3N4 quantum dot. *Surfaces and Interfaces*, **2022**, 30, 101913	4.1	2
16	Theoretical investigation on radical anion promoted electrocyclization in photochromes. *Journal of Molecular Graphics and Modelling*, **2020**, 97, 107550	2.8	1
15	Superalkali (Li2F, Li3F) doped Al12N12 electrides with enhanced static, dynamic nonlinear optical responses and refractive indices. *Materials Science in Semiconductor Processing*, **2022**, 143, 106518	4.3	1

14	Demonstrating the Potential of Alkali Metal-Doped Cyclic COLi Organometallics as Electrides and High-Performance NLO Materials. *ACS Omega*, **2021**, 6, 29852-29861	3.9	1
13	Benchmark approach to search of cost-effective and accurate density functional for homolytic cleavage of C-Mg bond of Grignard reagent. *International Journal of Quantum Chemistry*, **2020**, 120, e26106	2.1	1
12	Synthesis, single crystal X-ray, spectroscopic and computational (DFT) studies 2,1-benzothiazine based hydrazone derivatives. *Journal of Molecular Structure*, **2021**, 1230, 129854	3.4	1
11	Detailed Mechanistic Study of Radical Mediated Chemoselective Phosphination of Aryl Halide. *ChemistrySelect*, **2018**, 3, 11302-11308	1.8	1
10	Electrochemical sensing behavior of graphdiyne nanoflake towards uric acid: a quantum chemical approach. *Journal of Molecular Modeling*, **2021**, 27, 244	2	1
9	Potential sensing of toxic chemical warfare agents (CWAs) by twisted nanographenes: A first principle approach.. *Science of the Total Environment*, **2022**, 153858	10.2	1
8	Static, dynamic nonlinear optical (NLO) response and electride characteristics of superalkalis doped star like C6S6Li6. *Surfaces and Interfaces*, **2022**, 102044	4.1	1
7	Electrochemical sensing of heptazine graphitic C3N4 quantum dot for chemical warfare agents; a quantum chemical approach. *Materials Science in Semiconductor Processing*, **2022**, 148, 106753	4.3	1
6	Highly accurate DFT investigation for triggering the ultra-strong static and dynamic nonlinear optical properties of superalkali doped aminated graphdiyne (NH2-GDY) donor-□acceptor (D-□A) quantum dots. *Polyhedron*, **2022**, 215, 115695	2.7	0
5	Exploring the Interaction of Ionic Liquids with Al12N12 and Al12P12 Nanocages for Better Electrode-Electrolyte Materials in Super Capacitors. *Journal of Molecular Liquids*, **2021**, 117828	6	0
4	C10F as a potential anode material for alkali-ion batteries; a quantum chemical approach. *Computational and Theoretical Chemistry*, **2021**, 1206, 113470	2	0
3	Sensing behaviour of monocyclic C18 and B9N9 analogues toward chemical warfare agents (CWAs); quantum chemical approach. *Surfaces and Interfaces*, **2022**, 30, 101912	4.1	0
2	Olympicene as a high-performance sensor for lung irritants: A dispersion corrected DFT insight. *Materials Science in Semiconductor Processing*, **2022**, 144, 106620	4.3	0
1	DFT studies on electrochemical properties of halide ions doped GDY-28 nanoflake for Na-ion battery applications. *Materials Science in Semiconductor Processing*, **2022**, 145, 106651	4.3	0