Khurshid Ayub

List of Publications by Citations

318 papers	5,907 citations	41 h-index	56 g-index
341 ext. papers	7,953 ext. citations	3.7 avg, IF	7.03 L-index

#	Paper	IF	Citations
318	DFT Study of Polyaniline NH3, CO2, and CO Gas Sensors: Comparison with Recent Experimental Data. *Journal of Physical Chemistry C*, **2013**, 117, 23701-23711	3.8	146
317	A comparative density functional theory study of guanine chemisorption on Al12N12, Al12P12, B12N12, and B12P12 nano-cages. *Journal of Alloys and Compounds*, **2016**, 672, 161-169	5.7	108
316	Doping and Dedoping Processes of Polypyrrole: DFT Study with Hybrid Functionals. *Journal of Physical Chemistry C*, **2014**, 118, 17819-17830	3.8	97
315	Theoretical insight of polypyrrole ammonia gas sensor. *Synthetic Metals*, **2013**, 172, 14-20	3.6	84
314	Are phosphide nano-cages better than nitride nano-cages? A kinetic, thermodynamic and non-linear optical properties study of alkali metal encapsulated X12Y12 nano-cages. *Journal of Materials Chemistry C*, **2016**, 4, 10919-10934	7.1	83
313	Design of liquid crystals with "de Vries-like" properties: frustration between SmA- and SmC-promoting elements. *Journal of the American Chemical Society*, **2010**, 132, 364-70	16.4	83
312	Ni adsorption on Al12P12 nano-cage: A DFT study. *Journal of Alloys and Compounds*, **2016**, 678, 317-324	5.7	80
311	Molecular and Electronic Structure Elucidation of Polypyrrole Gas Sensors. *Journal of Physical Chemistry C*, **2015**, 119, 15994-16003	3.8	77
310	Enhancement in hydrogen molecule adsorption on B12N12 nano-cluster by decoration of nickel. *International Journal of Hydrogen Energy*, **2016**, 41, 22182-22191	6.7	77
309	Enhanced electronic and non-linear optical properties of alkali metal (Li, Na, K) doped boron nitride nano-cages. *Journal of Alloys and Compounds*, **2016**, 687, 976-983	5.7	72
308	The First ZnII-Catalyzed Oxidative Amidation of Benzyl Alcohols with Amines under Solvent-Free Conditions. *European Journal of Organic Chemistry*, **2013**, 2013, 2783-2787	3.2	71
307	Adsorption of thiophene on the surfaces of X 12 Y 12 (X = Al, B, and Y = N,P) nanoclusters; A DFT study. *Journal of Molecular Liquids*, **2017**, 238, 303-309	6	68
306	Designing Three-dimensional (3D) Non-Fullerene Small Molecule Acceptors with Efficient Photovoltaic Parameters. *ChemistrySelect*, **2018**, 3, 12797-12804	1.8	66
305	Phosphides or nitrides for better NLO properties? A detailed comparative study of alkali metal doped nano-cages. *Materials Research Bulletin*, **2017**, 92, 113-122	5.1	64
304	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
303	O 3 and SO 2 sensing concept on extended surface of B 12 N 12 nanocages modified by Nickel decoration: A comprehensive DFT study. *Solid State Sciences*, **2017**, 69, 22-30	3.4	61
302	Density Functional Theory Study of Poly(o-phenylenediamine) Oligomers. *Journal of Physical Chemistry C*, **2013**, 117, 4069-4078	3.8	61

301	Synthesis, crystal structures and spectroscopic properties of triazine-based hydrazone derivatives; a comparative experimental-theoretical study. *Molecules*, **2015**, 20, 5851-74	4.8	60
300	Adsorption of pyrrole on Al12N12, Al12P12, B12N12, and B12P12 fullerene-like nano-cages; a first principles study. *Vacuum*, **2016**, 131, 135-141	3.7	60
299	Enhancement in Photovoltaic Properties of N,N-diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. *ChemistrySelect*, **2020**, 5, 5022-5034	1.8	58
298	Remarkable nonlinear optical response of alkali metal doped aluminum phosphide and boron phosphide nanoclusters. *Journal of Molecular Liquids*, **2018**, 271, 51-64	6	57
297	Designing of benzodithiophene core-based small molecular acceptors for efficient non-fullerene organic solar cells. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 244, 118873	4.4	57
296	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
295	Coordination of nickel atoms with Al12X12 (X□=□N, P) nanocages enhances H2 adsorption: A surface study by DFT. *Vacuum*, **2016**, 133, 70-80	3.7	56
294	Adsorption of Phosgene Gas on Pristine and Copper-Decorated BN Nanocages: A Comparative DFT Study. *ACS Omega*, **2020**, 5, 7641-7650	3.9	54
293	Nonlinear optical and electronic properties of Cr-, Ni-, and Ti- substituted C 20 fullerenes: A quantum-chemical study. *Materials Research Bulletin*, **2018**, 97, 399-404	5.1	54
292	Density functional theory study of palladium cluster adsorption on a graphene support.. *RSC Advances*, **2020**, 10, 20595-20607	3.7	53
291	Cyclic versus straight chain oligofuran as sensor: A detailed DFT study. *Journal of Molecular Graphics and Modelling*, **2020**, 97, 107569	2.8	52
290	Supported protic ionic liquid membrane based on 3-(trimethoxysilyl)propan-1-aminium acetate for the highly selective separation of CO2. *Journal of Membrane Science*, **2017**, 543, 301-309	9.6	52
289	Phytochemical, spectroscopic and density functional theory study of Diospyrin, and non-bonding interactions of Diospyrin with atmospheric gases. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 141, 71-9	4.4	51
288	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
287	Detailed surface study of adsorbed nickel on Al12N12 nano-cage. *Thin Solid Films*, **2016**, 612, 179-185	2.2	49
286	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
285	Silver-graphene quantum dots based electrochemical sensor for trinitrotoluene and p-nitrophenol. *Journal of Molecular Liquids*, **2020**, 306, 112878	6	46
284	Opto-electronic properties of non-fullerene fused-undecacyclic electron acceptors for organic solar cells. *Computational Materials Science*, **2019**, 159, 150-159	3.2	46

283	Theoretical study of the non linear optical properties of alkali metal (Li, Na, K) doped aluminum nitride nanocages. *RSC Advances*, **2016**, 6, 94228-94235	3.7	45
282	Density functional theory and phytochemical study of Pistagremic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 118, 210-4	4.4	45
281	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
280	Designing Novel Zn-Decorated Inorganic BP Nanoclusters with Promising Electronic Properties: A Step Forward toward Efficient CO Sensing Materials. *ACS Omega*, **2020**, 5, 15547-15556	3.9	44
279	Calculation driven synthesis of an excellent dihydropyrene negative photochrome and its photochemical properties. *Journal of the American Chemical Society*, **2011**, 133, 4040-5	16.4	43
278	Synthesis, characterisation, optical and nonlinear optical properties of thiazole and benzothiazole derivatives: a dual approach. *Molecular Simulation*, **2018**, 44, 1191-1199	2	43
277	Adsorption properties of acetylene and ethylene molecules onto pristine and nickel-decorated Al 12 N 12 nanoclusters. *Materials Chemistry and Physics*, **2017**, 194, 337-344	4.4	41
276	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
275	Transportation of hydrogen atom and molecule through X 12 Y 12 nano-cages. *International Journal of Hydrogen Energy*, **2017**, 42, 11439-11451	6.7	40
274	Designing indacenodithiophene based non-fullerene acceptors with a donor-acceptor combined bridge for organic solar cells.. *RSC Advances*, **2019**, 9, 3605-3617	3.7	40
273	Combined experimental and theoretical study of poly(aniline-co-pyrrole) oligomer. *Polymer*, **2015**, 72, 30-39	3.9	40
272	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
271	Design of novel superalkali doped silicon carbide nanocages with giant nonlinear optical response. *Optics and Laser Technology*, **2020**, 122, 105855	4.2	40
270	Density functional theory and phytochemical study of 8-hydroxyisodiospyrin. *Journal of Molecular Structure*, **2015**, 1095, 69-78	3.4	39
269	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
268	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
267	Nitrogenated holey graphene (C2N) surface as highly selective electrochemical sensor for ammonia. *Journal of Molecular Liquids*, **2019**, 296, 111929	6	39
266	Zinc-Doped Boron Phosphide Nanocluster as Efficient Sensor for SO2. *Journal of Chemistry*, **2020**, 2020, 1-12	2.3	37

265	Transition metal doping: a new and effective approach for remarkably high nonlinear optical response in aluminum nitride nanocages. *New Journal of Chemistry*, **2018**, 42, 6976-6989	3.6	37
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263	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
262	Fine Tuning the Optoelectronic Properties of Triphenylamine Based Donor Molecules for Organic Solar Cells. *Zeitschrift Fur Physikalische Chemie*, **2017**, 231, 1127-1139	3.1	35
261	How can nickel decoration affect H 2 adsorption on B 12 P 12 nano-heterostructures?. *Journal of Molecular Liquids*, **2018**, 255, 168-175	6	35
260	Direct observation of diffuse cone behavior in de Vries smectic-A and -C phases of organosiloxane mesogens. *Physical Review Letters*, **2011**, 106, 087801	7.4	34
259	Design of donor□acceptor□donor (D□A□D) type small molecule donor materials with efficient photovoltaic parameters. *International Journal of Quantum Chemistry*, **2017**, 117, e25363	2.1	33
258	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
257	Therapeutic potential of graphitic carbon nitride as a drug delivery system for cisplatin (anticancer drug): A DFT approach. *Biophysical Chemistry*, **2020**, 267, 106461	3.5	33
256	Substitutional doping of zirconium-, molybdenum-, ruthenium-, and palladium: An effective method to improve nonlinear optical and electronic property of C20 fullerene. *Computational and Theoretical Chemistry*, **2017**, 1121, 68-75	2	32
255	Suppressing the thermal metacyclophanediene to dihydropyrene isomerization: synthesis and rearrangement of 8,16-dicyano[2.2]metacyclophane-1,9-diene and evidence supporting the proposed biradicaloid mechanism. *Journal of Organic Chemistry*, **2008**, 73, 451-6	4.2	32
254	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
253	Development of fullerene free acceptors molecules for organic solar cells: A step way forward toward efficient organic solar cells. *Computational and Theoretical Chemistry*, **2019**, 1161, 26-38	2	31
252	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
251	Exploration of adsorption behavior, electronic nature and NLO response of hydrogen adsorbed Alkali metals (Li, Na and K) encapsulated Al12N12 nanocages. *Journal of Theoretical and Computational Chemistry*, **2020**, 19, 2050031	1.8	30
250	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
249	DFT study of the therapeutic potential of phosphorene as a new drug-delivery system to treat cancer.. *RSC Advances*, **2019**, 9, 24325-24332	3.7	29
248	Designing dithienothiophene (DTT)-based donor materials with efficient photovoltaic parameters for organic solar cells. *Journal of Molecular Modeling*, **2019**, 25, 222	2	29

247	Palladium catalyzed synthesis and physical properties of indolo[2,3-b]quinoxalines. *Organic and Biomolecular Chemistry*, **2014**, 12, 6151-66	3.9	28
246	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
245	Substituents effect on thermal electrocyclic reaction of dihydroazulene-vinylheptafulvene photoswitch: a DFT study to improve the photoswitch. *Structural Chemistry*, **2013**, 24, 2115-2126	1.8	27
244	Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study. *Journal of Molecular Liquids*, **2020**, 297, 111902	6	27
243	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
242	Spirobifluorene based small molecules as an alternative to traditional fullerene acceptors for organic solar cells. *Materials Science in Semiconductor Processing*, **2019**, 94, 97-106	4.3	26
241	Spectroscopic and density functional theory studies of 5,7,3',5'-tetrahydroxyflavanone from the leaves of Olea ferruginea. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 128, 225-30	4.4	26
240	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
239	Designing alkoxy-induced based high performance near infrared sensitive small molecule acceptors for organic solar cells. *Journal of Molecular Liquids*, **2020**, 305, 112829	6	25
238	Photophysical and electrochemical properties and temperature dependent geometrical isomerism in alkyl quinacridonediimines. *New Journal of Chemistry*, **2014**, 38, 752-761	3.6	25
237	Comparative investigation of sensor application of polypyrrole for gaseous analytes. *Journal of Physical Organic Chemistry*, **2019**, 32, e3960	2.1	24
236	Tuning opto-electronic properties of alkoxy-induced based electron acceptors in infrared region for high performance organic solar cells. *Journal of Molecular Liquids*, **2020**, 298, 111963	6	24
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233	Binding affinity and permeation of X12Y12 nanoclusters for helium and neon. *Journal of Molecular Liquids*, **2017**, 244, 124-134	6	23
232	Extremely large nonlinear optical response and excellent electronic stability of true alkaline earthides based on hexaammine complexant. *Journal of Molecular Liquids*, **2020**, 297, 111899	6	23
231	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
230	Designing dithienonaphthalene based acceptor materials with promising photovoltaic parameters for organic solar cells.. *RSC Advances*, **2019**, 9, 34496-34505	3.7	23

229	Outstanding NLO response of thermodynamically stable single and multiple alkaline earth metals doped C20 fullerene. *Journal of Molecular Liquids*, **2020**, 305, 112875	6	22
228	Adamanzane based alkaline earthides with excellent nonlinear optical response and ultraviolet transparency. *Optics and Laser Technology*, **2020**, 129, 106298	4.2	22
227	Theoretical Calculations of the Optical and Electronic Properties of Dithienosilole- and Dithiophene-Based Donor Materials for Organic Solar Cells. *ChemistrySelect*, **2018**, 3, 1593-1601	1.8	22
226	Novel acridine-based thiosemicarbazones as 'turn-on' chemosensors for selective recognition of fluoride anion: a spectroscopic and theoretical study. *Royal Society Open Science*, **2018**, 5, 180646	3.3	22
225	A comparative study of DFT calculated and experimental UV/Visible spectra for thirty carboline and carbazole based compounds. *Journal of Molecular Structure*, **2017**, 1149, 282-298	3.4	22
224	Change in the electronic and nonlinear optical properties of Fullerene through its incorporation with Sc-, Fe-, Cu-, and Zn transition metals. *Applied Physics A: Materials Science and Processing*, **2019**, 125, 1	2.6	21
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221	Efficient Cu Decorated Inorganic B12P12 Nanoclusters for Sensing Toxic COCl2 Gas: A Detailed DFT Study. *Journal of Computational Biophysics and Chemistry*, **2021**, 20, 85-97		21
220	Copper-doped Al12N12 nano-cages: potential candidates for nonlinear optical materials. *Applied Physics A: Materials Science and Processing*, **2018**, 124, 1	2.6	21
219	Sensor applications of polypyrrole for oxynitrogen analytes: a DFT study. *Journal of Molecular Modeling*, **2018**, 24, 308	2	21
218	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
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215	DFT study of boron trichloride adsorption on the surface of Al12N12 nanocluster. *Molecular Physics* , **2017**, 115, 879-884	1.7	19
214	Spectral and electronic properties of Π-conjugated oligomers and polymers of Poly (o-chloroaniline-co-o-toluidine) calculated with density functional theory. *Synthetic Metals*, **2015**, 205, 153-163	3.6	19
213	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
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211	Remarkable second and third order nonlinear optical properties of organometallic C6Li6M3O electrides. *New Journal of Chemistry*, **2020**, 44, 9822-9829	3.6	18
210	Expanding the horizons of covalent organic frameworks to electrochemical sensors; A case study of CTF-FUM. *Microporous and Mesoporous Materials*, **2020**, 300, 110146	5.3	18
209	Antiradical, antimicrobial and enzyme inhibition evaluation of sulfonamide derived esters; synthesis, X-Ray analysis and DFT studies. *Journal of Molecular Structure*, **2019**, 1175, 379-388	3.4	18
208	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
207	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
206	Copper complexes of bioactive ligands with superoxide dismutase activity. *Mini-Reviews in Medicinal Chemistry*, **2013**, 13, 1944-56	3.2	18
205	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
204	DFT study of superhalogen and superalkali doped graphitic carbon nitride and its non-linear optical properties.. *RSC Advances*, **2021**, 11, 7779-7789	3.7	18
203	Designing of non-fullerene 3D star-shaped acceptors for organic solar cells. *Journal of Molecular Modeling*, **2019**, 25, 129	2	17
202	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
201	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
200	Synthesis biological screening and molecular docking studies of some tin (IV) Schiff base adducts. *Journal of Photochemistry and Photobiology B: Biology*, **2016**, 164, 65-72	6.7	17
199	Interaction of Graphene Quantum Dots with Oligothiophene: A Comprehensive Theoretical Study. *Journal of Physical Chemistry C*, **2019**, 123, 29556-29570	3.8	17
198	Synthesis and Properties of 5,7-Dihydropyrido[3,2-b:5,6-b?]diindoles. *European Journal of Organic Chemistry*, **2015**, 2015, 1007-1019	3.2	17
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196	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
195	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
194	Diffusion of alkali metal atoms (Li, Na, K) on aluminum nitride and boron nitride nanocages; a density functional theory study. *Journal of Molecular Liquids*, **2018**, 259, 249-259	6	16

193	Permeability and storage ability of inorganic X12Y12 fullerenes for lithium atom and ion. *Chemical Physics Letters*, **2018**, 698, 51-59	2.5	16
192	Syntheses of dihydropyrene-cyclophanediene negative photochromes containing internal alkenyl and alkynyl groups and comparison of their photochemical and thermochemical properties. *Journal of Organic Chemistry*, **2014**, 79, 664-78	4.2	16
191	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
190	Enhanced linear and nonlinear optical response of superhalogen (Al7) doped graphitic carbon nitride (g-C3N4). *Optik*, **2021**, 226, 165923	2.5	16
189	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
188	Acridinedione as selective flouride ion chemosensor: a detailed spectroscopic and quantum mechanical investigation.. *RSC Advances*, **2018**, 8, 1993-2003	3.7	15
187	Synthesis, characterization and density functional theory study of some new 2-anilinothiazoles. *Journal of Molecular Structure*, **2014**, 1072, 221-227	3.4	15
186	In Silico Designing of Nanoclusters with a Late Transition Metal for NO Adsorption: An Efficient Approach toward the Development of NO Sensing Materials. *ACS Omega*, **2021**, 6, 14191-14199	3.9	15
185	Therapeutic potential of graphyne as a new drug-delivery system for daunorubicin to treat cancer: A DFT study. *Journal of Molecular Liquids*, **2021**, 336, 116327	6	15
184	Density functional theory study of geometric and electronic properties of full range of bimetallic AgnYm (n□+□m□=□10) clusters. *Journal of Alloys and Compounds*, **2017**, 705, 232-246	5.7	14
183	Nonlinear optical, IR and orbital properties of Ni doped MgO nanoclusters: A DFT investigation. *Computational and Theoretical Chemistry*, **2018**, 1138, 39-47	2	14
182	The CN surface as a highly selective sensor for the detection of nitrogen iodide from a mixture of NX (X = Cl, Br, I) explosives.. *RSC Advances*, **2020**, 10, 31997-32010	3.7	14
181	Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications. *Chemical Physics Letters*, **2021**, 782, 139018	2.5	14
180	A new rosane-type diterpenoid from Stachys parviflora and its density functional theory studies. *Natural Product Research*, **2015**, 29, 813-9	2.3	13
179	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
178	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
177	Alkaline earth metals serving as source of excess electron for alkaline earth metals to impart large second and third order nonlinear optical response; a DFT study. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107759	2.8	13
176	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

175	Effective adsorption of A-series chemical warfare agents on graphdiyne nanoflake: a DFT study. *Journal of Molecular Modeling*, **2021**, 27, 117	2	13
174	Designing of Inorganic Al12N12 Nanocluster with Fe, Co, Ni, Cu and Zn Metals for Efficient Hydrogen Storage Materials. *Journal of Computational Biophysics and Chemistry*, **2021**, 20, 359-375		13
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169	Stable ion NMR and GIAO-DFT study of novel cations from 8,16-dicyano[2.2]metacyclophanedienes and from strategically substituted/benzannelated dihydropyrenes: charge-induced tropicity modulation and pi-switching. *Journal of Organic Chemistry*, **2008**, 73, 457-66	4.2	12
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