

Khurshid Ayub

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.

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	Shedding light on the optical and nonlinear optical properties of superalkali-doped borophene.. <i>Journal of Molecular Modeling</i> , 2022 , 28, 46	2	0
317	Computational investigation of a covalent triazine framework (CTF-0) as an efficient electrochemical sensor.. <i>RSC Advances</i> , 2022 , 12, 3909-3923	3.7	3
316	Permeability of boron- and nitrogen-doped graphene nanoflakes for protium/deuterium ions.. <i>RSC Advances</i> , 2022 , 12, 3883-3891	3.7	
315	DFT investigation of adsorption of nitro-explosives over C ₂ N surface: Highly selective towards trinitro benzene. <i>Journal of Molecular Liquids</i> , 2022 , 352, 118652	6	3
314	Enhanced non-linear optical response of calix[4]pyrrole complexant based earthides in the presence of oriented external electric field. <i>Journal of Molecular Liquids</i> , 2022 , 350, 118504	6	0
313	Superalkali (Li ₂ F, Li ₃ F) doped Al ₁₂ N ₁₂ electrides with enhanced static, dynamic nonlinear optical responses and refractive indices. <i>Materials Science in Semiconductor Processing</i> , 2022 , 143, 106518	4.3	1
312	M@[12-crown-4] and M@[15-crown-5] where (M=Li, Na, and K); the very first examples of non-conventional one alkali metal-containing alkalides with remarkable static and dynamic NLO response. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022 , 140, 115170	3	1
311	Highly accurate DFT investigation for triggering the ultra-strong static and dynamic nonlinear optical properties of superalkali doped aminated graphdiyne (NH ₂ -GDY) donor-acceptor (D-EA) quantum dots. <i>Polyhedron</i> , 2022 , 215, 115695	2.7	0
310	Covalent triazine framework (CTF-0) surface as a smart sensing material for the detection of CWAs and industrial pollutants. <i>Materials Science in Semiconductor Processing</i> , 2022 , 139, 106334	4.3	4
309	Theoretical Approach to Evaluate the Gas-Sensing Performance of Graphene Nanoribbon/Oligothiophene Composites.. <i>ACS Omega</i> , 2022 , 7, 2260-2274	3.9	0
308	Superalkali-based alkalides Li ₃ O@[12-crown-4]M (where M= Li, Na, and K) with remarkable static and dynamic NLO properties; A DFT study. <i>Materials Science in Semiconductor Processing</i> , 2022 , 138, 106254	4.3	6
307	Remarkable nonlinear optical response of Mn@C ₂₀ (M = Na & K and n = 18); a DFT outcome. <i>Materials Science in Semiconductor Processing</i> , 2022 , 138, 106269	4.3	6
306	A first principles study on electrochemical sensing of highly toxic pesticides by using porous C ₄ N nanoflake. <i>Journal of Physics and Chemistry of Solids</i> , 2022 , 160, 110345	3.9	8
305	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. <i>Journal of Physics and Chemistry of Solids</i> , 2022 , 160, 110361	3.9	4
304	Silver cluster doped graphyne (GY) with outstanding non-linear optical properties.. <i>RSC Advances</i> , 2022 , 12, 5466-5482	3.7	3
303	Optimized nonlinear optical (NLO) response of silicon carbide nanosheet by alkali metals doping: a DFT insight. <i>European Physical Journal Plus</i> , 2022 , 137, 1	3.1	2
302	Quantum chemical designing of novel fullerene-free acceptor molecules for organic solar cell applications.. <i>Journal of Molecular Modeling</i> , 2022 , 28, 67	2	4

301	Ab Initio Study of Two-Dimensional Cross-Shaped Non-Fullerene Acceptors for Efficient Organic Solar Cells.. <i>ACS Omega</i> , 2022 , 7, 10638-10648	3.9	0
300	Enhancement in non-linear optical properties of carbon nitride (C ₂ N) by doping superalkali (Li ₃ O): A DFT study. <i>Computational and Theoretical Chemistry</i> , 2022 , 1211, 113654	2	1
299	First example of vinylbenzene based small photovoltaic molecules: Towards the development of efficient D- π A configured optoelectronic materials for bulk heterojunction solar cells. <i>Physica B: Condensed Matter</i> , 2022 , 633, 413769	2.8	5
298	Sensing behaviour of monocyclic C ₁₈ and B ₉ N ₉ analogues toward chemical warfare agents (CWAs); quantum chemical approach. <i>Surfaces and Interfaces</i> , 2022 , 30, 101912	4.1	0
297	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
296	Potential sensing of toxic chemical warfare agents (CWAs) by twisted nanographenes: A first principle approach.. <i>Science of the Total Environment</i> , 2022 , 153858	10.2	1
295	Shedding light on the second order nonlinear optical responses of commercially available acidic azo dyes for laser applications. <i>Dyes and Pigments</i> , 2022 , 202, 110284	4.6	0
294	First-principles study for electrochemical sensing of neurotoxin hydrazine derivatives via h-g-C ₃ N ₄ quantum dot. <i>Surfaces and Interfaces</i> , 2022 , 30, 101913	4.1	2
293	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
292	Bithieno Thiophene-Based Small Molecules for Application as Donor Materials for Organic Solar Cells and Hole Transport Materials for Perovskite Solar Cells.. <i>ACS Omega</i> , 2022 , 7, 844-862	3.9	5
291	Assessment of alkali and alkaline earth metals doped cubanes as high performance nonlinear optical materials by first-principles study. <i>Journal of Science: Advanced Materials and Devices</i> , 2022 , 100457	4.7	1
290	Synergistic end-capped engineering on non-fused thiophene ring-based acceptors to enhance the photovoltaic properties of organic solar cells.. <i>RSC Advances</i> , 2022 , 12, 12321-12334	3.7	5
289	Static, dynamic nonlinear optical (NLO) response and electrone characteristics of superalkalis doped star like C ₆ S ₆ Li ₆ . <i>Surfaces and Interfaces</i> , 2022 , 102044	4.1	1
288	Remarkable non-linear optical properties of gold cluster doped graphyne (GY): A DFT study.. <i>Journal of Molecular Graphics and Modelling</i> , 2022 , 114, 108204	2.8	0
287	Theoretical investigation of double-cubed polycationic cluster (Sb ₇ Se ₈ Cl ₂) ₃₊ for the storage of helium and neon. <i>Materials Science in Semiconductor Processing</i> , 2022 , 148, 106756	4.3	1
286	Electrochemical sensing of heptazine graphitic C ₃ N ₄ quantum dot for chemical warfare agents; a quantum chemical approach. <i>Materials Science in Semiconductor Processing</i> , 2022 , 148, 106753	4.3	1
285	Nonlinear optical response of 9,10-bis(phenylethynyl)anthracene mediated by electron donating and electron withdrawing substituents: A density functional theory approach. <i>Materials Science in Semiconductor Processing</i> , 2022 , 148, 106751	4.3	1
284	DFT study of alkali and alkaline earth metal-doped benzocryptand with remarkable NLO properties. <i>RSC Advances</i> , 2022 , 12, 16029-16045	3.7	1

283	DFT study of transition metals doped calix-4-pyrrole with excellent electronic and non-linear optical properties. <i>Computational and Theoretical Chemistry</i> , 2022 , 113767	2	1
282	Hetero-porphyrin based channel for separation of proton isotope: A density functional theory study. <i>Microporous and Mesoporous Materials</i> , 2022 , 339, 111995	5.3	0
281	Germanium-based superatom clusters as excess electron compounds with significant static and dynamic NLO response; a DFT study.. <i>RSC Advances</i> , 2021 , 12, 365-377	3.7	0
280	A Theoretical Perspective on Strategies for Modeling High Performance Nonlinear Optical Materials. <i>Frontiers in Materials</i> , 2021 , 8,	4	4
279	Novel microporous B6N6 covalent organic framework (COF) as an electrochemical sensor for the ultra-selective detection of nitroaniline isomers; a DFT outcome. <i>Surfaces and Interfaces</i> , 2021 , 27, 101587	4.1	4
278	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
277	DFT study of OLi3 and MgF3 doped boron nitride with enhanced nonlinear optical behavior. <i>Journal of Molecular Structure</i> , 2021 , 1251, 131934	3.4	1
276	Exploring the Interaction of Ionic Liquids with Al12N12 and Al12P12 Nanocages for Better Electrode-Electrolyte Materials in Super Capacitors. <i>Journal of Molecular Liquids</i> , 2021 , 117828	6	0
275	C10F as a potential anode material for alkali-ion batteries; a quantum chemical approach. <i>Computational and Theoretical Chemistry</i> , 2021 , 1206, 113470	2	0
274	Demonstrating the Potential of Alkali Metal-Doped Cyclic COLi Organometallics as Electrdes and High-Performance NLO Materials. <i>ACS Omega</i> , 2021 , 6, 29852-29861	3.9	1
273	Density functional theory, molecular docking and muscle relaxant, sedative, and analgesic studies of indanone derivatives isolated from. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 6488-6499	3.6	1
272	The co-crystal of copper(II) phenanthroline chloride complex hydrate with p-aminobenzoic acid: structure, cytotoxicity, thermal analysis, and DFT calculation. <i>Monatshefte Für Chemie</i> , 2021 , 152, 323-336	1.4	3
271	DFT study of superhalogen (AlF4) doped boron nitride for tuning their nonlinear optical properties. <i>Optik</i> , 2021 , 231, 166464	2.5	12
270	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
269	Adsorption and sensor applications of C2N surface for G-series and mustard series chemical warfare agents. <i>Microporous and Mesoporous Materials</i> , 2021 , 317, 110984	5.3	4
268	Nonlinear optical response of first-row transition metal doped Al12P12 nanoclusters; a first-principles study. <i>Journal of Physics and Chemistry of Solids</i> , 2021 , 151, 109914	3.9	8
267	A New Strategy of bi-Alkali Metal Doping to Design Boron Phosphide Nanocages of High Nonlinear Optical Response with Better Thermodynamic Stability. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2021 , 31, 3062	3.2	7
266	Permeation selectivity of pristine and vacancy defected hexagonal boron membranes for alkaline earth metal and ions. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 1-12	3.6	

265	Theoretical modification of C ₂₄ fullerene with single and multiple alkaline earth metal atoms for their potential use as NLO materials. <i>Journal of Physics and Chemistry of Solids</i> , 2021 , 152, 109972	3.9	9
264	Quantum chemical study on sensing of NH ₃ , NF ₃ , NCl ₃ and NBr ₃ by using cyclic tetrapyrrole. <i>Computational and Theoretical Chemistry</i> , 2021 , 1199, 113221	2	9
263	Hydrogen adsorption on Ge ₅₂ □Ge ₉₂ □ and Sn ₉₂ □intl clusters: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2021 , 1199, 113191	2	4
262	In Silico Designing of Nanoclusters with a Late Transition Metal for NO Adsorption: An Efficient Approach toward the Development of NO Sensing Materials. <i>ACS Omega</i> , 2021 , 6, 14191-14199	3.9	15
261	Exploring Li ₄ N and Li ₄ O superalkalis as efficient dopants for the Al ₁₂ N ₁₂ nanocage to design high performance nonlinear optical materials with high thermodynamic stability. <i>Polyhedron</i> , 2021 , 200, 115145	2.7	5
260	DFT study of superhalogen-doped borophene with enhanced nonlinear optical properties. <i>Journal of Molecular Modeling</i> , 2021 , 27, 188	2	9
259	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
258	DFT study on the sensitivity of silver-graphene quantum dots for vital and harmful analytes. <i>Journal of Physics and Chemistry of Solids</i> , 2021 , 153, 110028	3.9	4
257	Designing of Inorganic Al ₁₂ N ₁₂ Nanocluster with Fe, Co, Ni, Cu and Zn Metals for Efficient Hydrogen Storage Materials. <i>Journal of Computational Biophysics and Chemistry</i> , 2021 , 20, 359-375		13
256	Cu-doped phosphorene as highly efficient single atom catalyst for CO oxidation: A DFT study. <i>Molecular Catalysis</i> , 2021 , 509, 111630	3.3	2
255	Inorganic electrides of alkali metal doped ZnO nanocage with excellent nonlinear optical response. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 106, 107935	2.8	5
254	Study of nonlinear optical properties of superhalogen and superalkali doped phosphorene. <i>Journal of Molecular Structure</i> , 2021 , 1236, 130348	3.4	5
253	Oxacarbon superalkali C ₃ X ₃ Y ₃ (X≡ O, S and Y≡ Li, Na, K) clusters as excess electron compounds for remarkable static and dynamic NLO response. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 106, 107922	2.8	9
252	A Theoretical Framework of Zinc-Decorated Inorganic MgO Nanoclusters for Efficient COCl Adsorption: A Step Forward toward the Development of COCl Sensing Materials. <i>ACS Omega</i> , 2021 , 6, 19435-19444	3.9	10
251	Unprecedented saturation limit achieved by inorganic polycationic cluster (SbTe) for light noble gases (He & Ne). <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 106, 107910	2.8	
250	Anticancer evaluation of a manganese complex on HeLa and MCF-7 cancer cells: design, deterministic solvothermal synthesis approach, Hirshfeld analysis, DNA binding, intracellular reactive oxygen species production, electrochemical characterization and density functional theory. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 1068-1081	3.6	3
249	Enhanced linear and nonlinear optical response of superhalogen (Al ₇) doped graphitic carbon nitride (g-C ₃ N ₄). <i>Optik</i> , 2021 , 226, 165923	2.5	16
248	Theoretical investigation of halides encapsulated Na@B ₄₀ nanocages for potential applications as anodes for sodium ion batteries. <i>Materials Science in Semiconductor Processing</i> , 2021 , 121, 105437	4.3	10

247	Designing of benzodithiophene core-based small molecular acceptors for efficient non-fullerene organic solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021 , 244, 118873	4.4	57
246	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> , 2021 , 102, 107766	2.8	5
245	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
244	Efficient Cu Decorated Inorganic B12P12 Nanoclusters for Sensing Toxic COCl ₂ Gas: A Detailed DFT Study. <i>Journal of Computational Biophysics and Chemistry</i> , 2021 , 20, 85-97		21
243	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. <i>Optics and Laser Technology</i> , 2021 , 134, 106570	4.2	11
242	Theoretical investigation of superalkali clusters M ₂ OCN and M ₂ NCO (where M=Li, Na, K) as excess electron system with significant static and dynamic nonlinear optical response. <i>Optik</i> , 2021 , 227, 166037	2.5	7
241	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
240	Endohedral metallofullerene electrides of CaO with remarkable nonlinear optical response.. <i>RSC Advances</i> , 2021 , 11, 1569-1580	3.7	9
239	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
238	DFT study of superhalogen and superalkali doped graphitic carbon nitride and its non-linear optical properties.. <i>RSC Advances</i> , 2021 , 11, 7779-7789	3.7	18
237	Electronic structure of polypyrrole composited with a low percentage of graphene nanofiller. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 8557-8570	3.6	1
236	Storage and permeation of hydrogen molecule, atom and ions (H ⁺ and H ⁺) through silicon carbide nanotube; a DFT approach. <i>International Journal of Hydrogen Energy</i> , 2021 , 46, 9163-9173	6.7	3
235	Regio- and stereoselective functionalization of alkenes with emphasis on mechanistic insight and sustainability concerns. <i>Journal of Saudi Chemical Society</i> , 2021 , 25, 101260	4.3	9
234	Influence of bi-alkali metals doping over Al ₁₂ N ₁₂ nanocage on stability and optoelectronic properties: A DFT investigation. <i>Radiation Physics and Chemistry</i> , 2021 , 184, 109457	2.5	5
233	Facile synthesis, DNA binding, Urease inhibition, anti-oxidant, molecular docking and DFT studies of 3-(3-Bromo-phenyl)-1-(2-trifluoromethyl-phenyl)-propenone and 3-(3-Bromo-5-chloro-phenyl)-1-(2-trifluoromethyl-phenyl)-propenone. <i>Journal of Molecular Liquids</i> , 2021 , 336, 116302	6	8
232	Theoretical and experimental investigation of CO ₂ capture through choline chloride based supported deep eutectic liquid membranes. <i>Journal of Molecular Liquids</i> , 2021 , 335, 116234	6	5
231	Electrochemical sensing behavior of graphdiyne nanoflake towards uric acid: a quantum chemical approach. <i>Journal of Molecular Modeling</i> , 2021 , 27, 244	2	1
230	Therapeutic potential of graphyne as a new drug-delivery system for daunorubicin to treat cancer: A DFT study. <i>Journal of Molecular Liquids</i> , 2021 , 336, 116327	6	15

229	Tuning the optoelectronic properties of superalkali doped phosphorene. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 107, 107973	2.8	4
228	High performance SACs for HER process using late first-row transition metals anchored on graphyne support: A DFT insight. <i>International Journal of Hydrogen Energy</i> , 2021 ,	6.7	4
227	Second-order NLO properties and two-state switching effects of transition metal redox complexes of iron and cobalt: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 107, 107975	2.8	2
226	Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties. <i>ACS Omega</i> , 2021 , 6, 24602-24613	3.9	8
225	Turning diamondoids into nonlinear optical materials by alkali metal Substitution: A DFT investigation. <i>Optics and Laser Technology</i> , 2021 , 142, 107231	4.2	8
224	Impact of even number of alkaline earth metal doping on the NLO response of C20 nanocluster; a DFT outcome. <i>Computational and Theoretical Chemistry</i> , 2021 , 1204, 113386	2	2
223	Silver cluster decorated graphene nanoflakes for selective and accurate detection of nitroaniline isomers; DFT calculations. <i>Materials Science in Semiconductor Processing</i> , 2021 , 134, 106023	4.3	7
222	Zintl based superatom P7M2 (M=Li, Na, K & Be, Mg, Ca) clusters with excellent second and third-order nonlinear optical response. <i>Materials Science in Semiconductor Processing</i> , 2021 , 134, 105986 ^{4.3}	4.3	7
221	Adsorption mechanism of p- aminophenol over silver-graphene composite: A first principles study. <i>Journal of Molecular Liquids</i> , 2021 , 341, 117415	6	11
220	First example of lanthanum as dopant on Al12N12 and Al12P12 nanocages for improved electronic and nonlinear optical properties with high stability. <i>Materials Science in Semiconductor Processing</i> , 2021 , 135, 106122	4.3	5
219	Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications. <i>Chemical Physics Letters</i> , 2021 , 782, 139018	2.5	14
218	Extremely large static and dynamic nonlinear optical response of small superalkali clusters NMM' (M, M'=Li, Na, K). <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 109, 108031	2.8	7
217	Isatin-derived non-fullerene acceptors for efficient organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2021 , 121, 105345	4.3	19
216	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
215	Remarkable enhancement in sensor ability of polyaniline upon composite formation with ZnO for industrial effluents. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 101, 107724	2.8	2
214	Enhancement in Photovoltaic Properties of N,N-diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. <i>ChemistrySelect</i> , 2020 , 5, 5022-5034	1.8	58
213	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
212	Density functional theory study of palladium cluster adsorption on a graphene support.. <i>RSC Advances</i> , 2020 , 10, 20595-20607	3.7	53

211	Remarkable second and third order nonlinear optical properties of organometallic C ₆ Li ₆ M ₃ O electrides. <i>New Journal of Chemistry</i> , 2020 , 44, 9822-9829	3.6	18
210	Nonlinear optical response of sodium based superalkalis decorated graphdiyne surface: A DFT study. <i>Optik</i> , 2020 , 218, 165033	2.5	12
209	Designing Novel Zn-Decorated Inorganic BP Nanoclusters with Promising Electronic Properties: A Step Forward toward Efficient CO Sensing Materials. <i>ACS Omega</i> , 2020 , 5, 15547-15556	3.9	44
208	High sensitivity of graphdiyne nanoflake toward detection of phosgene, thiophosgene and phosgenoxime; a first-principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 100, 107658	2.8	27
207	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
206	Expanding the horizons of covalent organic frameworks to electrochemical sensors; A case study of CTF-FUM. <i>Microporous and Mesoporous Materials</i> , 2020 , 300, 110146	5.3	18
205	Designing alkoxy-induced based high performance near infrared sensitive small molecule acceptors for organic solar cells. <i>Journal of Molecular Liquids</i> , 2020 , 305, 112829	6	25
204	Adsorption of Phosgene Gas on Pristine and Copper-Decorated BN Nanocages: A Comparative DFT Study. <i>ACS Omega</i> , 2020 , 5, 7641-7650	3.9	54
203	Rational design of naphthalimide based small molecules non-fullerene acceptors for organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020 , 1187, 112916	2	9
202	Zinc-Doped Boron Phosphide Nanocluster as Efficient Sensor for SO ₂ . <i>Journal of Chemistry</i> , 2020 , 2020, 1-12	2.3	37
201	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
200	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
199	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
198	Permeation selectivity of alkali metal ions through crown ether based ion channels. <i>Journal of Molecular Liquids</i> , 2020 , 302, 112577	6	10
197	Theoretical investigation on radical anion promoted electrocyclization in photochromes. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 97, 107550	2.8	1
196	Adamantane based alkaline earthides with excellent nonlinear optical response and ultraviolet transparency. <i>Optics and Laser Technology</i> , 2020 , 129, 106298	4.2	22
195	Silver-graphene quantum dots based electrochemical sensor for trinitrotoluene and p-nitrophenol. <i>Journal of Molecular Liquids</i> , 2020 , 306, 112878	6	46
194	Electronic structure of polythiophene gas sensors for chlorinated analytes. <i>Journal of Molecular Modeling</i> , 2020 , 26, 44	2	6

193	Carbon nitride 2-D surface as a highly selective electrochemical sensor for V-series nerve agents. <i>Journal of Molecular Liquids</i> , 2020 , 311, 113357	6	20
192	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
191	Extremely large nonlinear optical response and excellent electronic stability of true alkaline earthides based on hexaammine complexant. <i>Journal of Molecular Liquids</i> , 2020 , 297, 111899	6	23
190	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, e26105	2.1	1
189	Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study. <i>Journal of Molecular Liquids</i> , 2020 , 297, 111902	6	27
188	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
187	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
186	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
185	Graphene-polyaniline composite as superior electrochemical sensor for detection of cyano explosives. <i>European Polymer Journal</i> , 2020 , 138, 109981	5.2	12
184	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
183	Therapeutic potential of graphitic carbon nitride as a drug delivery system for cisplatin (anticancer drug): A DFT approach. <i>Biophysical Chemistry</i> , 2020 , 267, 106461	3.5	33
182	First-principles study for exploring the adsorption behavior of G-series nerve agents on graphdiyne surface. <i>Computational and Theoretical Chemistry</i> , 2020 , 1191, 113043	2	27
181	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. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 101, 107759	2.8	13
180	Janus alkaline earthides with excellent NLO response from sodium and potassium as source of excess electrons; a first principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 100, 107668	2.8	13
179	Synthesis, single-crystal X-ray diffraction, and in vitro biological evaluation of sodium, cobalt, and tin complexes of o-nitro-/o-methoxyphenylacetic acid: experimental and theoretical investigation. <i>Monatshefte für Chemie</i> , 2020 , 151, 1727-1736	1.4	3
178	Polyaniline emeraldine salt as selective electrochemical sensor for HBr over HCl: a systematic density functional theory study through oligomer approach. <i>Journal of Molecular Modeling</i> , 2020 , 26, 332	2	2
177	Adsorption behaviour of chronic blistering agents on graphdiyne; excellent correlation among SAPT, reduced density gradient (RDG) and QTAIM analyses. <i>Journal of Molecular Liquids</i> , 2020 , 316, 113860	6	36
176	Exploration of adsorption behavior, electronic nature and NLO response of hydrogen adsorbed Alkali metals (Li, Na and K) encapsulated Al ₁₂ N ₁₂ nanocages. <i>Journal of Theoretical and Computational Chemistry</i> , 2020 , 19, 2050031	1.8	30

175	Selective detection and removal of picric acid by C ₂ N surface from a mixture of nitro-explosives. <i>New Journal of Chemistry</i> , 2020 , 44, 18646-18655	3.6	4
174	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
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172	Comparative study on sensing abilities of polyaniline and graphene polyaniline composite sensors toward methylamine and ammonia. <i>Polymers for Advanced Technologies</i> , 2020 , 31, 3351-3360	3.2	6
171	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
170	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
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167	Exploring the potential of novel transition metal complexes derived from ONO donor type ligand: a quantum chemical study. <i>Journal of Molecular Modeling</i> , 2019 , 25, 284	2	2
166	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
165	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
164	Designing indacenodithiophene based non-fullerene acceptors with a donor-acceptor combined bridge for organic solar cells.. <i>RSC Advances</i> , 2019 , 9, 3605-3617	3.7	40
163	Spirobifluorene based small molecules as an alternative to traditional fullerene acceptors for organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2019 , 94, 97-106	4.3	26
162	Change in the electronic and nonlinear optical properties of Fullerene through its incorporation with Sc-, Fe-, Cu-, and Zn transition metals. <i>Applied Physics A: Materials Science and Processing</i> , 2019 , 125, 1	2.6	21
161	A combined experimental and computational study of 2,2'-(diazene-1,2-diylbis(4,1-phenylene))bis(6-(butylamino)-1H-benzo[de]isoquinoline-1,3(2H)-dione): Synthesis, optical and nonlinear optical properties. <i>Optik</i> , 2019 , 192, 162952	2.5	9
160	Development of fullerene free acceptors molecules for organic solar cells: A step way forward toward efficient organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2019 , 1161, 26-38	2	31
159	Dihydroazulene-vinylheptafulvene based photoswitchable lewis pairs for tunable H ₂ activation. <i>International Journal of Hydrogen Energy</i> , 2019 , 44, 14780-14795	6.7	3
158	Comparative investigation of sensor application of polypyrrole for gaseous analytes. <i>Journal of Physical Organic Chemistry</i> , 2019 , 32, e3960	2.1	24

157	Designing of non-fullerene 3D star-shaped acceptors for organic solar cells. <i>Journal of Molecular Modeling</i> , 2019 , 25, 129	2	17
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153	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
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151	Photo-tunable linear and nonlinear optical response of cyclophanediene-dihydropyrene photoswitches. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 88, 261-272	2.8	5
150	Antiradical, antimicrobial and enzyme inhibition evaluation of sulfonamide derived esters; synthesis, X-Ray analysis and DFT studies. <i>Journal of Molecular Structure</i> , 2019 , 1175, 379-388	3.4	18
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148	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
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137	External stimulus controlled recombination of hydrogen in photochromic dithienylethene frustrated lewis pairs. <i>International Journal of Hydrogen Energy</i> , 2019 , 44, 31141-31152	6.7	4
136	Interaction of Graphene Quantum Dots with Oligothiophene: A Comprehensive Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 29556-29570	3.8	17
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133	Isolation, spectroscopic and density functional theory of two withanolide glycosides. <i>Journal of Molecular Structure</i> , 2019 , 1177, 449-456	3.4	7
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43	Synthesis and DPPH scavenging assay of reserpine analogues, computational studies and in silico docking studies in AChE and BChE responsible for Alzheimer's disease. <i>Brazilian Journal of Pharmaceutical Sciences</i> , 2015 , 51, 53-61	1.8	4
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40	Towards thermally stable cyclophanediene-dihydropyrene photoswitches. <i>Journal of Molecular Modeling</i> , 2015 , 21, 148	2	6
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38	Dyotropic rearrangement of bridgehead substituents in closed dithienylethenes; conjugated verses non-conjugated analogues. <i>Journal of Molecular Modeling</i> , 2015 , 21, 321	2	4
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29	Syntheses of dihydropyrene-cyclophanediene negative photochromes containing internal alkenyl and alkynyl groups and comparison of their photochemical and thermochemical properties. <i>Journal of Organic Chemistry</i> , 2014 , 79, 664-78	4.2	16
28	Palladium catalyzed synthesis and physical properties of indolo[2,3-b]quinoxalines. <i>Organic and Biomolecular Chemistry</i> , 2014 , 12, 6151-66	3.9	28
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26	Spectroscopic and density functional theory studies of 5,7,3',5'-tetrahydroxyflavanone from the leaves of <i>Olea ferruginea</i> . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 128, 225-30	4.4	26
25	Density functional theory and phytochemical study of Pistagremic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 118, 210-4	4.4	45
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18	The First ZnII-Catalyzed Oxidative Amidation of Benzyl Alcohols with Amines under Solvent-Free Conditions. <i>European Journal of Organic Chemistry</i> , 2013 , 2013, 2783-2787	3.2	71
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