Khurshid Ayub

List of Publications by Year
in descending order

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333	10,230	28274	79698
papers	citations	55	73
		h-index	g-index

341	341	341	3800
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Therapeutic potential of C2N as targeted drug delivery system for fluorouracil and nitrosourea to treat cancer: a theoretical study. Journal of Nanostructure in Chemistry, 2023, 13, 89-102.	9.1	16
2	Computation Assisted Design and Prediction of Alkali-Metal-Centered B12N12 Nanoclusters for Efficient H2 Adsorption: New Hydrogen Storage Materials. Journal of Cluster Science, 2023, 34, 1237-1247.	3.3	16
3	Remarkable electronic and NLO properties of bimetallic superalkali clusters: a DFT study. Journal of Nanostructure in Chemistry, 2022, 12, 529-545.	9.1	16
4	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.	4.0	34
5	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.	4.0	22
6	Superalkali-based alkalides Li3O@[12-crown-4]M (where M= Li, Na, and K) with remarkable static and dynamic NLO properties; A DFT study. Materials Science in Semiconductor Processing, 2022, 138, 106254.	4.0	35
7	Remarkable nonlinear optical response of Mn@C20 (M = Na & K and n = 1â€“6); a DFT outcome. Materials Science in Semiconductor Processing, 2022, 138, 106269.	4.0	20
8	Nano-porous C4N as a toxic pesticide's scavenger: A quantum chemical approach. Journal of Molecular Graphics and Modelling, 2022, 111, 108078.	2.4	24
9	Covalent triazine framework (CTF-0) surface as a smart sensing material for the detection of CWAs and industrial pollutants. Materials Science in Semiconductor Processing, 2022, 139, 106334.	4.0	21
10	DFT study of OLi3 and MgF3 doped boron nitride with enhanced nonlinear optical behavior. Journal of Molecular Structure, 2022, 1251, 131934.	3.6	19
11	Theoretical Approach to Evaluate the Gas-Sensing Performance of Graphene Nanoribbon/Oligothiophene Composites. ACS Omega, 2022, 7, 2260-2274.	3.5	6
12	Shedding light on the optical and nonlinear optical properties of superalkali-doped borophene. Journal of Molecular Modeling, 2022, 28, 46.	1.8	6
13	Computational investigation of a covalent triazine framework (CTF-0) as an efficient electrochemical sensor. RSC Advances, 2022, 12, 3909-3923.	3.6	28
14	Novel Starâ€Shaped Benzotriindoleâ€Based Nonfullerene Donor Materials: Toward the Development of Promising Photovoltaic Compounds for Highâ€Performance Organic Solar Cells. Energy Technology, 2022, 10, .	3.8	18
15	Permeability of boron- and nitrogen-doped graphene nanoflakes for protium/deuterium ions. RSC Advances, 2022, 12, 3883-3891.	3.6	0
16	DFT investigation of adsorption of nitro-explosives over C2N surface: Highly selective towards trinitro benzene. Journal of Molecular Liquids, 2022, 352, 118652.	4.9	32
17	Enhanced non-linear optical response of calix[4]pyrrole complexant based earthides in the presence of oriented external electric field. Journal of Molecular Liquids, 2022, 350, 118504.	4.9	14
18	Superalkali (Li2F, Li3F) doped Al12N12 electrides with enhanced static, dynamic nonlinear optical responses and refractive indices. Materials Science in Semiconductor Processing, 2022, 143, 106518.	4.0	23

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19	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. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 140, 115170.	2.7	13
20	Highly accurate DFT investigation for triggering the ultra-strong static and dynamic nonlinear optical properties of superalkali doped aminated graphdiyne (NH2-GDY) donor-Ï€-acceptor (D-Ï€-A) quantum dots. Polyhedron, 2022, 215, 115695.	2.2	17
21	Silver cluster doped graphyne (GY) with outstanding non-linear optical properties. RSC Advances, 2022, 12, 5466-5482.	3.6	29
22	Optimized nonlinear optical (NLO) response of silicon carbide nanosheet by alkali metals doping: a DFT insight. European Physical Journal Plus, 2022, 137, 1.	2.6	23
23	Quantum chemical designing of novel fullerene-free acceptor molecules for organic solar cell applications. Journal of Molecular Modeling, 2022, 28, 67.	1.8	8
24	Ab Initio Study of Two-Dimensional Cross-Shaped Non-Fullerene Acceptors for Efficient Organic Solar Cells. ACS Omega, 2022, 7, 10638-10648.	3.5	30
25	Enhancement in non-linear optical properties of carbon nitride (C2N) by doping superalkali (Li3O): A DFT study. Computational and Theoretical Chemistry, 2022, 1211, 113654.	2.5	18
26	First example of vinylbenzene based small photovoltaic molecules: Towards the development of efficient D-Ï€-A configured optoelectronic materials for bulk heterojunction solar cells. Physica B: Condensed Matter, 2022, 633, 413769.	2.7	18
27	Sensing behaviour of monocyclic C18 and B9N9 analogues toward chemical warfare agents (CWAs); quantum chemical approach. Surfaces and Interfaces, 2022, 30, 101912.	3.0	13
28	Olympicene as a high-performance sensor for lung irritants: A dispersion corrected DFT insight. Materials Science in Semiconductor Processing, 2022, 144, 106620.	4.0	17
29	Potential sensing of toxic chemical warfare agents (CWAs) by twisted nanographenes: A first principle approach. Science of the Total Environment, 2022, 824, 153858.	8.0	41
30	Shedding light on the second order nonlinear optical responses of commercially available acidic azo dyes for laser applications. Dyes and Pigments, 2022, 202, 110284.	3.7	8
31	First-principles study for electrochemical sensing of neurotoxin hydrazine derivatives via h-g-C3N4 quantum dot. Surfaces and Interfaces, 2022, 30, 101913.	3.0	12
32	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.	4.0	5
33	Bithieno Thiophene-Based Small Molecules for Application as Donor Materials for Organic Solar Cells and Hole Transport Materials for Perovskite Solar Cells. ACS Omega, 2022, 7, 844-862.	3.5	43
34	Assessment of alkali and alkaline earth metals doped cubanes as high-performance nonlinear optical materials by first-principles study. Journal of Science: Advanced Materials and Devices, 2022, 7, 100457.	3.1	8
35	Synergistic end-capped engineering on non-fused thiophene ring-based acceptors to enhance the photovoltaic properties of organic solar cells. RSC Advances, 2022, 12, 12321-12334.	3.6	19
36	Mixed superalkalis are a better choice than pure superalkalis for B₁₂N₁₂ nanocages to design high-performance nonlinear optical materials. Dalton Transactions, 2022, 51, 8437-8453.	3.3	10

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37	Static, dynamic nonlinear optical (NLO) response and electride characteristics of superalkalis doped star like C6S6Li6. Surfaces and Interfaces, 2022, 31, 102044.	3.0	9
38	Nonfullerene Near-Infrared Sensitive Acceptors â€œOctacyclic Naphtho[1,2-b:5,6-b] Dithiophene Coreâ€•for Organic Solar Cell Applications: In Silico Molecular Engineering. ACS Omega, 2022, 7, 16716-16727.	3.5	8
39	Remarkable non-linear optical properties of gold cluster doped graphyne (GY): A DFT study. Journal of Molecular Graphics and Modelling, 2022, 114, 108204.	2.4	9
40	Theoretical investigation of double-cubed polycationic cluster (Sb7Se8Cl2)3+ for the storage of helium and neon. Materials Science in Semiconductor Processing, 2022, 148, 106756.	4.0	3
41	Electrochemical sensing of heptazine graphitic C3N4 quantum dot for chemical warfare agents; a quantum chemical approach. Materials Science in Semiconductor Processing, 2022, 148, 106753.	4.0	18
42	Nonlinear optical response of 9,10-bis(phenylethynyl)anthracene mediated by electron donating and electron withdrawing substituents: A density functional theory approach. Materials Science in Semiconductor Processing, 2022, 148, 106751.	4.0	8
43	DFT study of alkali and alkaline earth metal-doped benzocryptand with remarkable NLO properties. RSC Advances, 2022, 12, 16029-16045.	3.6	17
44	Adsorption of Industrial Gases (CH₄, CO₂, and CO) on Olympicene: A DFT and CCSD(T) Investigation. ACS Omega, 2022, 7, 18852-18860.	3.5	14
45	Enhancement of NLO properties of supersalt (Al(BH4)3)-doped graphene: a DFT study. Journal of Molecular Modeling, 2022, 28, .	1.8	4
46	Ab initio study for superior sensitivity of graphyne nanoflake towards nitrogen halides over ammonia. Journal of Molecular Modeling, 2022, 28, .	1.8	5
47	DFT study of transition metals doped calix-4-pyrrole with excellent electronic and non-linear optical properties. Computational and Theoretical Chemistry, 2022, 1214, 113767.	2.5	29
48	Hetero-porphyrin based channel for separation of proton isotope: A density functional theory study. Microporous and Mesoporous Materials, 2022, 339, 111995.	4.4	1
49	Alkaline earth metals doped C2N with enhanced non-linear optical properties. Optik, 2022, 265, 169514.	2.9	3
50	Enhanced non-linear optical response of alkali metal-doped nitrogenated holey graphene (C2N). Journal of Molecular Structure, 2022, 1267, 133580.	3.6	3
51	Lanthanum doped corannulenes with enhanced static and dynamic nonlinear optical properties: A first principle study. Physica B: Condensed Matter, 2022, 641, 414088.	2.7	8
52	Benchmark Density Functional Theory Approach for the Calculation of Bond Dissociation Energies of the Mâ€“O₂ Bond: A Key Step in Water Splitting Reactions. ACS Omega, 2022, 7, 20800-20808.	3.5	9
53	Theoretical investigation of lithium-based clusters Lin (where nâ€‰=â€‰3, 5, 7) with remarkable electronic and frequency-dependent NLO properties. European Physical Journal Plus, 2022, 137, .	2.6	2
54	Superhalogen doping of aromatic heterocycles; effective approach for the enhancement of static and dynamic NLO response. Vacuum, 2022, 203, 111301.	3.5	4

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55	Density functional theory, molecular docking and inÂvivo muscle relaxant, sedative, and analgesic studies of indanone derivatives isolated from Heterophragma adenophyllum. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6488-6499.	3.5	3
56	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. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1068-1081.	3.5	6
57	Enhanced linear and nonlinear optical response of superhalogen (Al7) doped graphitic carbon nitride (g-C3N4). Optik, 2021, 226, 165923.	2.9	46
58	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.	4.0	18
59	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.	3.9	102
60	Exploring the twisted molecular configurations for tuning their optical and nonlinear optical response properties: A quantum chemical approach. Journal of Molecular Graphics and Modelling, 2021, 102, 107766.	2.4	14
61	Surface functionalization of twisted graphene C32H15 and C104H52 derivatives with alkalis and superalkalis for NLO response; a DFT study. Journal of Molecular Graphics and Modelling, 2021, 102, 107794.	2.4	34
62	Efficient Cu Decorated Inorganic B₁₂P₁₂Nanoclusters for Sensing Toxic COCl₂Gas: A Detailed DFT Study. Journal of Computational Biophysics and Chemistry, 2021, 20, 85-97.	1.7	36
63	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.	4.6	34
64	Theoretical investigation of superalkali clusters M2OCN and M2NCO (where M=Li, Na, K) as excess electron system with significant static and dynamic nonlinear optical response. Optik, 2021, 227, 166037.	2.9	15
65	Silver cluster (Ag6) decorated coronene as non-enzymatic sensor for glucose and H2O2. Journal of Molecular Graphics and Modelling, 2021, 103, 107824.	2.4	16
66	Endohedral metallofullerene electrides of Ca₁₂O₁₂ with remarkable nonlinear optical response. RSC Advances, 2021, 11, 1569-1580.	3.6	28
67	Remarkable static and dynamic NLO response of alkali and superalkali doped macrocyclic [hexa-]thiophene complexes; a DFT approach. RSC Advances, 2021, 11, 4118-4128.	3.6	35
68	DFT study of superhalogen and superalkali doped graphitic carbon nitride and its non-linear optical properties. RSC Advances, 2021, 11, 7779-7789.	3.6	39
69	Electronic structure of polypyrrole composited with a low percentage of graphene nanofiller. Physical Chemistry Chemical Physics, 2021, 23, 8557-8570.	2.8	8
70	Storage and permeation of hydrogen molecule, atom and ions (H+ and Hâ¯) through silicon carbide nanotube; a DFT approach. International Journal of Hydrogen Energy, 2021, 46, 9163-9173.	7.1	13
71	The co-crystal of copper(II) phenanthroline chloride complex hydrate with p-aminobenzoic acid: structure, cytotoxicity, thermal analysis, and DFT calculation. Monatshefte FÃ¼r Chemie, 2021, 152, 323-336.	1.8	7
72	DFT study of superhalogen (AlF4) doped boron nitride for tuning their nonlinear optical properties. Optik, 2021, 231, 166464.	2.9	35

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73	Effective adsorption of A-series chemical warfare agents on graphdiyne nanoflake: a DFT study. Journal of Molecular Modeling, 2021, 27, 117.	1.8	26
74	Adsorption and sensor applications of C2N surface for G-series and mustard series chemical warfare agents. Microporous and Mesoporous Materials, 2021, 317, 110984.	4.4	19
75	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.	4.0	18
76	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, 3062-3076.	3.7	25
77	Permeation selectivity of pristine and vacancy defected hexagonal boron membranes for alkaline earth metal and ions. Journal of Biomolecular Structure and Dynamics, 2021, , 1-12.	3.5	0
78	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.	4.0	20
79	Quantum chemical study on sensing of NH3, NF3, NCl3 and NBr3 by using cyclic tetrapyrrole. Computational and Theoretical Chemistry, 2021, 1199, 113221.	2.5	18
80	Hydrogen adsorption on Ge52â^', Ge92â^' and Sn92â^' Zintl clusters: A DFT study. Computational and Theoretical Chemistry, 2021, 1199, 113191.	2.5	10
81	In Silico Designing of Mg₁₂O<sub>12 Nanoclusters with a Late Transition Metal for NO₂ Adsorption: An Efficient Approach toward the Development of NO₂ Sensing Materials. ACS Omega, 2021, 6, 14191-14199.	3.5	23
82	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.	2.2	12
83	DFT study of superhalogen-doped borophene with enhanced nonlinear optical properties. Journal of Molecular Modeling, 2021, 27, 188.	1.8	28
84	DFT studies of single and multiple alkali metals doped C24 fullerene for electronics and nonlinear optical applications. Journal of Molecular Graphics and Modelling, 2021, 105, 107867.	2.4	33
85	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.	4.0	16
86	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.	1.7	26
87	Cu-doped phosphorene as highly efficient single atom catalyst for CO oxidation: A DFT study. Molecular Catalysis, 2021, 509, 111630.	2.0	5
88	Inorganic electrides of alkali metal doped Zn12O12 nanocage with excellent nonlinear optical response. Journal of Molecular Graphics and Modelling, 2021, 106, 107935.	2.4	14
89	Study of nonlinear optical properties of superhalogen and superalkali doped phosphorene. Journal of Molecular Structure, 2021, 1236, 130348.	3.6	18
90	Oxacarbon superalkali C3X3Y3 (XÂ= O, S and YÂ= Li, Na, K) clusters as excess electron compounds for remarkable static and dynamic NLO response. Journal of Molecular Graphics and Modelling, 2021, 106, 107922.	2.4	19

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91	A Theoretical Framework of Zinc-Decorated Inorganic Mg₁₂O₁₂ Nanoclusters for Efficient COCl₂ Adsorption: A Step Forward toward the Development of COCl₂ Sensing Materials. ACS Omega, 2021, 6, 19435-19444.	3.5	30
92	Unprecedented saturation limit achieved by inorganic polycationic cluster (Sb7Te8)5+ for light noble gases (He & Ne). Journal of Molecular Graphics and Modelling, 2021, 106, 107910.	2.4	0
93	Regio- and stereoselective functionalization of alkenes with emphasis on mechanistic insight and sustainability concerns. Journal of Saudi Chemical Society, 2021, 25, 101260.	5.2	20
94	Influence of bi-alkali metals doping over Al12N12 nanocage on stability and optoelectronic properties: A DFT investigation. Radiation Physics and Chemistry, 2021, 184, 109457.	2.8	15
95	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) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 577 Td (Ch	4.1	55
96	Synthesis, characterization, antimicrobial, cytotoxic, DNA-interaction, molecular docking and DFT studies of novel di- and tri-organotin(IV) carboxylates using 3-(3-nitrophenyl)2-methylpropenoic acid. Journal of Coordination Chemistry, 2021, 74, 2407-2426.	2.2	12
97	Theoretical and experimental investigation of CO2 capture through choline chloride based supported deep eutectic liquid membranes. Journal of Molecular Liquids, 2021, 335, 116234.	4.9	12
98	Electrochemical sensing behavior of graphdiyne nanoflake towards uric acid: a quantum chemical approach. Journal of Molecular Modeling, 2021, 27, 244.	1.8	4
99	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.	4.9	48
100	Mechanochemical Transformation of CF₃ Group: Synthesis of Amides and Schiff Bases. Advanced Synthesis and Catalysis, 2021, 363, 5448-5460.	4.3	16
101	Tuning the optoelectronic properties of superalkali doped phosphorene. Journal of Molecular Graphics and Modelling, 2021, 107, 107973.	2.4	10
102	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, 46, 37814-37823.	7.1	49
103	Second-order NLO properties and two-state switching effects of transition metal redox complexes of iron and cobalt: A DFT study. Journal of Molecular Graphics and Modelling, 2021, 107, 107975.	2.4	7
104	Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties. ACS Omega, 2021, 6, 24602-24613.	3.5	31
105	Turning diamondoids into nonlinear optical materials by alkali metal Substitution: A DFT investigation. Optics and Laser Technology, 2021, 142, 107231.	4.6	21
106	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.	2.5	16
107	Silver cluster decorated graphene nanoflakes for selective and accurate detection of nitroaniline isomers; DFT calculations. Materials Science in Semiconductor Processing, 2021, 134, 106023.	4.0	15
108	Zintl based superatom P7M2 (M=Li, Na, K & Be, Mg, Ca) clusters with excellent second and third-order nonlinear optical response. Materials Science in Semiconductor Processing, 2021, 134, 105986.	4.0	16

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109	Adsorption mechanism of p- aminophenol over silver-graphene composite: A first principles study. Journal of Molecular Liquids, 2021, 341, 117415.	4.9	39
110	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.	4.0	22
111	Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications. Chemical Physics Letters, 2021, 782, 139018.	2.6	39
112	Extremely large static and dynamic nonlinear optical response of small superalkali clusters NM3Mâ€™ (M, Mâ€™=Li, Na, K). Journal of Molecular Graphics and Modelling, 2021, 109, 108031.	2.4	12
113	Isatin-derived non-fullerene acceptors for efficient organic solar cells. Materials Science in Semiconductor Processing, 2021, 121, 105345.	4.0	38
114	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.	1.9	18
115	Exploring the interaction of ionic liquids with Al12N12 and Al12P12 nanocages for better electrode-electrolyte materials in super capacitors. Journal of Molecular Liquids, 2021, 344, 117828.	4.9	18
116	C10F as a potential anode material for alkali-ion batteries; a quantum chemical approach. Computational and Theoretical Chemistry, 2021, 1206, 113470.	2.5	5
117	Demonstrating the Potential of Alkali Metal-Doped Cyclic C₆O₆Li₆ Organometallics as Electrides and High-Performance NLO Materials. ACS Omega, 2021, 6, 29852-29861.	3.5	26
118	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.	3.0	14
119	Germanium-based superatom clusters as excess electron compounds with significant static and dynamic NLO response; a DFT study. RSC Advances, 2021, 12, 365-377.	3.6	10
120	A Theoretical Perspective on Strategies for Modeling High Performance Nonlinear Optical Materials. Frontiers in Materials, 2021, 8, .	2.4	26
121	Synthesis, crystal structures, computational studies and Î±-amylase inhibition of three novel 1,3,4-oxadiazole derivatives. Journal of Molecular Structure, 2020, 1200, 127085.	3.6	33
122	Design of novel superalkali doped silicon carbide nanocages with giant nonlinear optical response. Optics and Laser Technology, 2020, 122, 105855.	4.6	73
123	Enhancement in the mechanical property of NBR/PVC nanocomposite by using sulfur and electron beam curing in the presence of Cloisite 30B nanoclay. Journal of Macromolecular Science - Pure and Applied Chemistry, 2020, 57, 123-130.	2.2	4
124	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.	4.9	58
125	Extremely large nonlinear optical response and excellent electronic stability of true alkaline earthides based on hexaammine complexant. Journal of Molecular Liquids, 2020, 297, 111899.	4.9	54
126	Benchmark approach to search of costâ€effective and accurate density functional for homolytic cleavage of Câ”€Mg bond of Grignard reagent. International Journal of Quantum Chemistry, 2020, 120, e26106.	2.0	4

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127	Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study. Journal of Molecular Liquids, 2020, 297, 111902.	4.9	42
128	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.	2.7	38
129	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.	2.9	27
130	Significant nonlinear optical response of alkaline earth metals doped beryllium and magnesium oxide nanocages. Materials Chemistry and Physics, 2020, 242, 122507.	4.0	44
131	Graphene-polyaniline composite as superior electrochemical sensor for detection of cyano explosives. European Polymer Journal, 2020, 138, 109981.	5.4	28
132	Permeation of second row neutral elements through Al12P12 and B12P12 nanocages; a first-principles study. Journal of Molecular Graphics and Modelling, 2020, 101, 107748.	2.4	5
133	Therapeutic potential of graphitic carbon nitride as a drug delivery system for cisplatin (anticancer) Tj ETQq1 1 0.784314 rgBT /Overlo	2.8	72
134	First-principles study for exploring the adsorption behavior of G-series nerve agents on graphdyine surface. Computational and Theoretical Chemistry, 2020, 1191, 113043.	2.5	43
135	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.	2.4	28
136	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.	2.4	27
137	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. Monatshefte FÃ¼r Chemie, 2020, 151, 1727-1736.	1.8	4
138	Polyaniline emeraldine salt as selective electrochemical sensor for HBr over HCl: a systematic density functional theory study through oligomer approach. Journal of Molecular Modeling, 2020, 26, 332.	1.8	3
139	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.	4.9	79
140	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	40
141	Selective detection and removal of picric acid by C₂N surface from a mixture of nitro-explosives. New Journal of Chemistry, 2020, 44, 18646-18655.	2.8	11
142	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.	2.8	35
143	The C₂N surface as a highly selective sensor for the detection of nitrogen iodide from a mixture of NX₃ (X = Cl, Br, I) explosives. RSC Advances, 2020, 10, 31997-32010.	3.6	35
144	Comparative study on sensing abilities of polyaniline and graphene polyaniline composite sensors toward methylamine and ammonia. Polymers for Advanced Technologies, 2020, 31, 3351-3360.	3.2	10

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145	Remarkable enhancement in sensor ability of polyaniline upon composite formation with ZnO for industrial effluents. Journal of Molecular Graphics and Modelling, 2020, 101, 107724.	2.4	3
146	Enhancement in Photovoltaic Properties of N,Nâ€diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. ChemistrySelect, 2020, 5, 5022-5034.	1.5	95
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