

Khurshid Ayub

List of Publications by Year in descending order

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333
papers

10,230
citations

28274

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h-index

79698

73
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341
all docs

341
docs citations

341
times ranked

3800
citing authors

#	ARTICLE	IF	CITATIONS
1	DFT Study of Polyaniline NH ₃ , CO ₂ , and CO Gas Sensors: Comparison with Recent Experimental Data. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23701-23711.	3.1	194
2	A comparative density functional theory study of guanine chemisorption on Al ₁₂ N ₁₂ , Al ₁₂ P ₁₂ , B ₁₂ N ₁₂ , and B ₁₂ P ₁₂ nano-cages. <i>Journal of Alloys and Compounds</i> , 2016, 672, 161-169.	5.5	151
3	Doping and Dedoping Processes of Polypyrrole: DFT Study with Hybrid Functionals. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17819-17830.	3.1	122
4	Are phosphide nano-cages better than nitride nano-cages? A kinetic, thermodynamic and non-linear optical properties study of alkali metal encapsulated X ₁₂ Y ₁₂ nano-cages. <i>Journal of Materials Chemistry C</i> , 2016, 4, 10919-10934.	5.5	122
5	Designing Three-dimensional (3D) Non-Fullerene Small Molecule Acceptors with Efficient Photovoltaic Parameters. <i>ChemistrySelect</i> , 2018, 3, 12797-12804.	1.5	119
6	Adsorption of Phosgene Gas on Pristine and Copper-Decorated B ₁₂ N ₁₂ Nanocages: A Comparative DFT Study. <i>ACS Omega</i> , 2020, 5, 7641-7650.	3.5	114
7	Theoretical insight of polypyrrole ammonia gas sensor. <i>Synthetic Metals</i> , 2013, 172, 14-20.	3.9	105
8	Superalkalis as a source of diffuse excess electrons in newly designed inorganic electrides with remarkable nonlinear response and deep ultraviolet transparency: A DFT study. <i>Applied Surface Science</i> , 2019, 483, 1118-1128.	6.1	105
9	Enhanced electronic and non-linear optical properties of alkali metal (Li, Na, K) doped boron nitride nano-cages. <i>Journal of Alloys and Compounds</i> , 2016, 687, 976-983.	5.5	102
10	Ni adsorption on Al ₁₂ P ₁₂ nano-cage: A DFT study. <i>Journal of Alloys and Compounds</i> , 2016, 678, 317-324.	5.5	102
11	Opto-electronic properties of non-fullerene fused-undecacyclic electron acceptors for organic solar cells. <i>Computational Materials Science</i> , 2019, 159, 150-159.	3.0	102
12	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.	3.9	102
13	Enhancement in hydrogen molecule adsorption on B ₁₂ N ₁₂ nano-cluster by decoration of nickel. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 22182-22191.	7.1	100
14	Enhancement in Photovoltaic Properties of <i>i>N</i>, <i>N</i>-diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. <i>ChemistrySelect</i>, 2020, 5, 5022-5034.</i>	1.5	95
15	Molecular and Electronic Structure Elucidation of Polypyrrole Gas Sensors. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15994-16003.	3.1	94
16	Phosphides or nitrides for better NLO properties? A detailed comparative study of alkali metal doped nano-cages. <i>Materials Research Bulletin</i> , 2017, 92, 113-122.	5.2	92
17	Nonlinear optical and electronic properties of Cr-, Ni-, and Ti- substituted C ₂₀ fullerenes: A quantum-chemical study. <i>Materials Research Bulletin</i> , 2018, 97, 399-404.	5.2	91
18	Design of Liquid Crystals with <i>œde Vries-like</i> Properties: Frustration between SmA- and SmC-Promoting Elements. <i>Journal of the American Chemical Society</i> , 2010, 132, 364-370.	13.7	88

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19	Adsorption of thiophene on the surfaces of $X_{12}Y_{12}$ ($X = Al, B,$ and $Y = N,P$) nanoclusters; A DFT study. <i>Journal of Molecular Liquids</i> , 2017, 238, 303-309.	4.9	88
20	O ₃ and SO ₂ sensing concept on extended surface of $B_{12}N_{12}$ nanocages modified by Nickel decoration: A comprehensive DFT study. <i>Solid State Sciences</i> , 2017, 69, 22-30.	3.2	87
21	Density functional theory study of palladium cluster adsorption on a graphene support. <i>RSC Advances</i> , 2020, 10, 20595-20607.	3.6	86
22	Density Functional Theory Study of Poly(<i>o</i> -phenylenediamine) Oligomers. <i>Journal of Physical Chemistry C</i> , 2013, 117, 4069-4078.	3.1	83
23	Adsorption of pyrrole on $Al_{12}N_{12}$, $Al_{12}P_{12}$, $B_{12}N_{12}$, and $B_{12}P_{12}$ fullerene-like nano-cages; a first principles study. <i>Vacuum</i> , 2016, 131, 135-141.	3.5	83
24	Designing indacenodithiophene based non-fullerene acceptors with a donor-acceptor combined bridge for organic solar cells. <i>RSC Advances</i> , 2019, 9, 3605-3617.	3.6	83
25	Synthesis, Crystal Structures and Spectroscopic Properties of Triazine-Based Hydrazone Derivatives; A Comparative Experimental-Theoretical Study. <i>Molecules</i> , 2015, 20, 5851-5874.	3.8	80
26	Remarkable nonlinear optical response of alkali metal doped aluminum phosphide and boron phosphide nanoclusters. <i>Journal of Molecular Liquids</i> , 2018, 271, 51-64.	4.9	80
27	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.	4.9	79
28	The First Zn^{II} -Catalyzed Oxidative Amidation of Benzyl Alcohols with Amines under Solvent-Free Conditions. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 2783-2787.	2.4	78
29	Highly selective acridinium based cyanine dyes for the detection of DNA base pairs (adenine, cytosine,) <i>Tj ETQq1 1 0.784314 rgBT /Over</i>	2.5	78
30	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.	4.9	76
31	Theoretical study on a boron phosphide nanocage doped with superalkalis: novel electrides having significant nonlinear optical response. <i>New Journal of Chemistry</i> , 2019, 43, 5727-5736.	2.8	73
32	Design of novel superalkali doped silicon carbide nanocages with giant nonlinear optical response. <i>Optics and Laser Technology</i> , 2020, 122, 105855.	4.6	73
33	Therapeutic potential of graphitic carbon nitride as a drug delivery system for cisplatin (anticancer) <i>Tj ETQq1 1 0.784314 rgBT /Overlock</i>	2.8	72
34	Designing Novel Zn-Decorated Inorganic $B_{12}P_{12}$ Nanoclusters with Promising Electronic Properties: A Step Forward toward Efficient CO ₂ Sensing Materials. <i>ACS Omega</i> , 2020, 5, 15547-15556.	3.5	71
35	Nitrogenated holey graphene (C ₂ N) surface as highly selective electrochemical sensor for ammonia. <i>Journal of Molecular Liquids</i> , 2019, 296, 111929.	4.9	69
36	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.	2.4	68

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37	Coordination of nickel atoms with Al ₁₂ X ₁₂ (X=ÅN, P) nanocages enhances H ₂ adsorption: A surface study by DFT. <i>Vacuum</i> , 2016, 133, 70-80.	3.5	67
38	Fine Tuning the Optoelectronic Properties of Triphenylamine Based Donor Molecules for Organic Solar Cells. <i>Zeitschrift Fur Physikalische Chemie</i> , 2017, 231, 1127-1139.	2.8	67
39	High sensitivity of polypyrrole sensor for uric acid over urea, acetamide and sulfonamide: A density functional theory study. <i>Synthetic Metals</i> , 2018, 235, 49-60.	3.9	66
40	Theoretical study on design of novel superalkalis doped graphdiyne: A new donor-acceptor (D-A) strategy for enhancing NLO response. <i>Applied Surface Science</i> , 2019, 492, 255-263.	6.1	66
41	Cyclic versus straight chain oligofuran as sensor: A detailed DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107569.	2.4	66
42	Supported protic ionic liquid membrane based on 3-(trimethoxysilyl)propan-1-aminium acetate for the highly selective separation of CO ₂ . <i>Journal of Membrane Science</i> , 2017, 543, 301-309.	8.2	65
43	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.	2.5	65
44	Silver-graphene quantum dots based electrochemical sensor for trinitrotoluene and p-nitrophenol. <i>Journal of Molecular Liquids</i> , 2020, 306, 112878.	4.9	65
45	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.	4.6	64
46	Synthesis, crystal structure, spectroscopic and density functional theory (DFT) study of N-[3-anthracen-9-yl-1-(4-bromo-phenyl)-allylidene]-N-benzenesulfonylhydrazine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 142, 364-374.	3.9	63
47	Theoretical study of the non linear optical properties of alkali metal (Li, Na, K) doped aluminum nitride nanocages. <i>RSC Advances</i> , 2016, 6, 94228-94235.	3.6	62
48	Synthesis, characterisation, optical and nonlinear optical properties of thiazole and benzothiazole derivatives: a dual approach. <i>Molecular Simulation</i> , 2018, 44, 1191-1199.	2.0	62
49	Transition metal doping: a new and effective approach for remarkably high nonlinear optical response in aluminum nitride nanocages. <i>New Journal of Chemistry</i> , 2018, 42, 6976-6989.	2.8	61
50	Phytochemical, spectroscopic and density functional theory study of Diospyrin, and non-bonding interactions of Diospyrin with atmospheric gases. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 141, 71-79.	3.9	60
51	DFT study of the therapeutic potential of phosphorene as a new drug-delivery system to treat cancer. <i>RSC Advances</i> , 2019, 9, 24325-24332.	3.6	58
52	Designing dithienothiophene (DTT)-based donor materials with efficient photovoltaic parameters for organic solar cells. <i>Journal of Molecular Modeling</i> , 2019, 25, 222.	1.8	58
53	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.	4.0	58
54	Tuning opto-electronic properties of alkoxy-induced based electron acceptors in infrared region for high performance organic solar cells. <i>Journal of Molecular Liquids</i> , 2020, 298, 111963.	4.9	58

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55	Exceptionally high NLO response and deep ultraviolet transparency of superalkali doped macrocyclic oligofuran rings. <i>New Journal of Chemistry</i> , 2020, 44, 2609-2618.	2.8	58
56	Density functional theory and phytochemical study of Pistagremic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 118, 210-214.	3.9	55
57	Detailed surface study of adsorbed nickel on Al ₁₂ N ₁₂ nano-cage. <i>Thin Solid Films</i> , 2016, 612, 179-185.	1.8	55
58	Adsorption properties of acetylene and ethylene molecules onto pristine and nickel-decorated Al ₁₂ N ₁₂ nanoclusters. <i>Materials Chemistry and Physics</i> , 2017, 194, 337-344.	4.0	55
59	Design of donor-acceptor-donor (D-A-D) type small molecule donor materials with efficient photovoltaic parameters. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25363.	2.0	54
60	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.	4.9	54
61	Density functional theory and phytochemical study of 8-hydroxyisodiospyrin. <i>Journal of Molecular Structure</i> , 2015, 1095, 69-78.	3.6	53
62	Transportation of hydrogen atom and molecule through X ₁₂ Y ₁₂ nano-cages. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 11439-11451.	7.1	53
63	Designing dithienonaphthalene based acceptor materials with promising photovoltaic parameters for organic solar cells. <i>RSC Advances</i> , 2019, 9, 34496-34505.	3.6	52
64	A comparative study of DFT calculated and experimental UV/Visible spectra for thirty carboline and carbazole based compounds. <i>Journal of Molecular Structure</i> , 2017, 1149, 282-298.	3.6	51
65	Calculation Driven Synthesis of an Excellent Dihydropyrene Negative Photochrome and its Photochemical Properties. <i>Journal of the American Chemical Society</i> , 2011, 133, 4040-4045.	13.7	50
66	How can nickel decoration affect H ₂ adsorption on B ₁₂ P ₁₂ nano-heterostructures?. <i>Journal of Molecular Liquids</i> , 2018, 255, 168-175.	4.9	50
67	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, 46, 37814-37823.	7.1	49
68	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.	4.4	48
69	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.	4.9	48
70	An accurate cost effective DFT approach to study the sensing behaviour of polypyrrole towards nitrate ions in gas and aqueous phases. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 19236-19247.	2.8	47
71	Designing of non-fullerene 3D star-shaped acceptors for organic solar cells. <i>Journal of Molecular Modeling</i> , 2019, 25, 129.	1.8	47
72	Combined experimental and theoretical study of poly(aniline-co-pyrrole) oligomer. <i>Polymer</i> , 2015, 72, 30-39.	3.8	46

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73	Adamanzane based alkaline earthides with excellent nonlinear optical response and ultraviolet transparency. <i>Optics and Laser Technology</i> , 2020, 129, 106298.	4.6	46
74	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.	2.9	46
75	A comprehensive DFT study on the sensing abilities of cyclic oligothiophenes (C _n CTs). <i>New Journal of Chemistry</i> , 2019, 43, 14120-14133.	2.8	45
76	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.	2.4	45
77	Zinc-Doped Boron Phosphide Nanocluster as Efficient Sensor for SO ₂ . <i>Journal of Chemistry</i> , 2020, 2020, 1-12.	1.9	45
78	Significant nonlinear optical response of alkaline earth metals doped beryllium and magnesium oxide nanocages. <i>Materials Chemistry and Physics</i> , 2020, 242, 122507.	4.0	44
79	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.	2.5	43
80	Remarkable second and third order nonlinear optical properties of organometallic C ₆ Li ₆ MO ₃ electrides. <i>New Journal of Chemistry</i> , 2020, 44, 9822-9829.	2.8	43
81	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.	4.9	43
82	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.	3.5	43
83	Click one pot synthesis, spectral analyses, crystal structures, DFT studies and brine shrimp cytotoxicity assay of two newly synthesized 1,4,5-trisubstituted 1,2,3-triazoles. <i>Journal of Molecular Structure</i> , 2016, 1106, 430-439.	3.6	42
84	Theoretical Calculations of the Optical and Electronic Properties of Dithienosilole and Dithiophene-Based Donor Materials for Organic Solar Cells. <i>ChemistrySelect</i> , 2018, 3, 1593-1601.	1.5	42
85	Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study. <i>Journal of Molecular Liquids</i> , 2020, 297, 111902.	4.9	42
86	Potential sensing of toxic chemical warfare agents (CWAs) by twisted nanographenes: A first principle approach. <i>Science of the Total Environment</i> , 2022, 824, 153858.	8.0	41
87	An accurate comparative theoretical study of the interaction of furan, pyrrole, and thiophene with various gaseous analytes. <i>Journal of Molecular Modeling</i> , 2017, 23, 295.	1.8	40
88	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	40
89	Comparative investigation of sensor application of polypyrrole for gaseous analytes. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3960.	1.9	39
90	DFT study of superhalogen and superalkali doped graphitic carbon nitride and its non-linear optical properties. <i>RSC Advances</i> , 2021, 11, 7779-7789.	3.6	39

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91	Adsorption mechanism of p-aminophenol over silver-graphene composite: A first principles study. <i>Journal of Molecular Liquids</i> , 2021, 341, 117415.	4.9	39
92	Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications. <i>Chemical Physics Letters</i> , 2021, 782, 139018.	2.6	39
93	Copper-doped Al ₁₂ N ₁₂ nano-cages: potential candidates for nonlinear optical materials. <i>Applied Physics A: Materials Science and Processing</i> , 2018, 124, 1.	2.3	38
94	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.	2.7	38
95	Isatin-derived non-fullerene acceptors for efficient organic solar cells. <i>Materials Science in Semiconductor Processing</i> , 2021, 121, 105345.	4.0	38
96	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.	4.9	38
97	Palladium catalyzed synthesis and physical properties of indolo[2,3-b]quinoxalines. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 6151-6166.	2.8	37
98	Substitutional doping of zirconium-, molybdenum-, ruthenium-, and palladium: An effective method to improve nonlinear optical and electronic property of C ₂₀ fullerene. <i>Computational and Theoretical Chemistry</i> , 2017, 1121, 68-75.	2.5	37
99	Phases of Organosiloxane Mesogens. <i>Physical Chemistry Letters</i> , 2011, 06, 087801.	7.8	36
100	Efficient Cu Decorated Inorganic B ₁₂ P ₁₂ Nanoclusters for Sensing Toxic COCl ₂ Gas: A Detailed DFT Study. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 85-97.	1.7	36
101	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. <i>Journal of Organic Chemistry</i> , 2008, 73, 451-456.	3.2	35
102	Synthesis, structural studies and biological activities of three new 2-(pentadecylthio)-5-aryl-1,3,4-oxadiazoles. <i>Journal of Molecular Structure</i> , 2017, 1129, 50-59.	3.6	35
103	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.	2.8	35
104	The C ₂ N surface as a highly selective sensor for the detection of nitrogen iodide from a mixture of NX ₃ (X = Cl, Br, I) explosives. <i>RSC Advances</i> , 2020, 10, 31997-32010.	3.6	35
105	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.	3.6	35
106	DFT study of superhalogen (AlF ₄) doped boron nitride for tuning their nonlinear optical properties. <i>Optik</i> , 2021, 231, 166464.	2.9	35
107	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.	4.0	35
108	Novel acridine-based thiosemicarbazones as 'turn-on' chemosensors for selective recognition of fluoride anion: a spectroscopic and theoretical study. <i>Royal Society Open Science</i> , 2018, 5, 180646.	2.4	34

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109	Surface functionalization of twisted graphene C ₃₂ H ₁₅ and C ₁₀₄ H ₅₂ derivatives with alkalis and superalkalis for NLO response; a DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 102, 107794.	2.4	34
110	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.	4.6	34
111	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.	4.0	34
112	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, 225-230.	3.9	33
113	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.	3.6	33
114	DFT studies of single and multiple alkali metals doped C ₂₄ fullerene for electronics and nonlinear optical applications. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107867.	2.4	33
115	Substituents effect on thermal electrocyclic reaction of dihydroazulene-vinylheptafulvene photoswitch: a DFT study to improve the photoswitch. <i>Structural Chemistry</i> , 2013, 24, 2115-2126.	2.0	32
116	Synthesis, Density Functional Theory (DFT), Urease Inhibition and Antimicrobial Activities of 5-Aryl Thiophenes Bearing Sulphonylacetamide Moieties. <i>Molecules</i> , 2015, 20, 19914-19928.	3.8	32
117	Synthesis biological screening and molecular docking studies of some tin (IV) Schiff base adducts. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2016, 164, 65-72.	3.8	32
118	Synthesis, structural properties, DFT studies, antimicrobial activities and DNA binding interactions of two newly synthesized organotin(IV) carboxylates. <i>Journal of Molecular Structure</i> , 2019, 1191, 291-300.	3.6	32
119	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.	4.9	32
120	Photophysical and electrochemical properties and temperature dependent geometrical isomerism in alkyl quinacridonediimines. <i>New Journal of Chemistry</i> , 2014, 38, 752-761.	2.8	31
121	Binding affinity and permeation of X ₁₂ Y ₁₂ nanoclusters for helium and neon. <i>Journal of Molecular Liquids</i> , 2017, 244, 124-134.	4.9	31
122	Synthesis, crystal structures, computational studies and antimicrobial activity of new designed bis((5-aryl-1,3,4-oxadiazol-2-yl)thio)alkanes. <i>Journal of Molecular Structure</i> , 2018, 1155, 403-413.	3.6	31
123	Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties. <i>ACS Omega</i> , 2021, 6, 24602-24613.	3.5	31
124	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.	4.4	30
125	A Theoretical Framework of Zinc-Decorated Inorganic Mg ₁₂ O ₁₂ Nanoclusters for Efficient COCl ₂ Adsorption: A Step Forward toward the Development of COCl ₂ Sensing Materials. <i>ACS Omega</i> , 2021, 6, 19435-19444.	3.5	30
126	Ab Initio Study of Two-Dimensional Cross-Shaped Non-Fullerene Acceptors for Efficient Organic Solar Cells. <i>ACS Omega</i> , 2022, 7, 10638-10648.	3.5	30

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127	Sensor applications of polypyrrole for oxynitrogen analytes: a DFT study. <i>Journal of Molecular Modeling</i> , 2018, 24, 308.	1.8	29
128	Silver cluster doped graphyne (GY) with outstanding non-linear optical properties. <i>RSC Advances</i> , 2022, 12, 5466-5482.	3.6	29
129	DFT study of transition metals doped calix-4-pyrrole with excellent electronic and non-linear optical properties. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113767.	2.5	29
130	Graphene-polyaniline composite as superior electrochemical sensor for detection of cyano explosives. <i>European Polymer Journal</i> , 2020, 138, 109981.	5.4	28
131	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.	2.4	28
132	Endohedral metallofullerene electrides of $\text{Ca}_{12}\text{O}_{12}$ with remarkable nonlinear optical response. <i>RSC Advances</i> , 2021, 11, 1569-1580.	3.6	28
133	DFT study of superhalogen-doped borophene with enhanced nonlinear optical properties. <i>Journal of Molecular Modeling</i> , 2021, 27, 188.	1.8	28
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