

Shabbir Muhammad

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/9530925/publications.pdf>

Version: 2024-02-01

236
papers

6,188
citations

76326

40
h-index

118850

62
g-index

239
all docs

239
docs citations

239
times ranked

2869
citing authors

#	ARTICLE	IF	CITATIONS
1	Quantum Mechanical Design and Structure of the Li@B ₁₀ H ₁₄ Basket with a Remarkably Enhanced Electro-Optical Response. <i>Journal of the American Chemical Society</i> , 2009, 131, 11833-11840.	13.7	260
2	Quantum chemical design of nonlinear optical materials by sp ² -hybridized carbon nanomaterials: issues and opportunities. <i>Journal of Materials Chemistry C</i> , 2013, 1, 5439.	5.5	155
3	Designing Three-dimensional (3D) Non-Fullerene Small Molecule Acceptors with Efficient Photovoltaic Parameters. <i>ChemistrySelect</i> , 2018, 3, 12797-12804.	1.5	119
4	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells. <i>RSC Advances</i> , 2019, 9, 26402-26418.	3.6	115
5	Giant Enhancement of the Second Hyperpolarizabilities of Open-Shell Singlet Polyaromatic Diphenalenyl Diradicaloids by an External Electric Field and Donor-Acceptor Substitution. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1094-1098.	4.6	111
6	The stability and nonlinear optical properties: Encapsulation of an excess electron compound LiCN ⁻ Li within boron nitride nanotubes. <i>Journal of Materials Chemistry</i> , 2012, 22, 2196-2202.	6.7	111
7	A new type of organic-inorganic hybrid NLO-phore with large off-diagonal first hyperpolarizability tensors: a two-dimensional approach. <i>Dalton Transactions</i> , 2013, 42, 15053.	3.3	111
8	Quantum chemical study of benzimidazole derivatives to tune the second-order nonlinear optical molecular switching by proton abstraction. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4791.	2.8	106
9	An investigation on the key features of a D ⁺ -A type novel chalcone derivative for opto-electronic applications. <i>RSC Advances</i> , 2015, 5, 87320-87332.	3.6	103
10	Prediction of Remarkably Large Second-Order Nonlinear Optical Properties of Organoimido-Substituted Hexamolybdates. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3576-3587.	2.5	102
11	Investigation of Dibenzoboroles Having π -Electrons: Toward a New Type of Two-Dimensional NLO Molecular Switch?. <i>Journal of Physical Chemistry C</i> , 2009, 113, 12551-12557.	3.1	94
12	First principles study for the key electronic, optical and nonlinear optical properties of novel donor-acceptor chalcones. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 72, 58-69.	2.4	94
13	Redox and Photoisomerization Switching the Second-Order Nonlinear Optical Properties of a Tetrathiafulvalene Derivative Across Six States: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23946-23954.	3.1	83
14	Role of a singlet diradical character in carbon nanomaterials: a novel hot spot for efficient nonlinear optical materials. <i>Nanoscale</i> , 2016, 8, 17998-18020.	5.6	83
15	Mathematical modeling and optimal control of the COVID-19 dynamics. <i>Results in Physics</i> , 2021, 31, 105028.	4.1	82
16	Capturing a Synergistic Effect of a Conical Push and an Inward Pull in Fluoro Derivatives of Li@B ₁₀ H ₁₄ Basket: Toward a Higher Vertical Ionization Potential and Nonlinear Optical Response. <i>Journal of Physical Chemistry A</i> , 2011, 115, 923-931.	2.5	80
17	Sorption of cadmium from aqueous solution by surfactant-modified carbon adsorbents. <i>Chemical Engineering Journal</i> , 2009, 148, 365-370.	12.7	77
18	Tuning the push-pull configuration for efficient second-order nonlinear optical properties in some chalcone derivatives. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 68, 95-105.	2.4	77

#	ARTICLE	IF	CITATIONS
19	Benchmark study of the linear and nonlinear optical polarizabilities in proto-type NLO molecule of <i>p</i> -nitroaniline. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950030.	1.8	74
20	Boron/Nitrogen Substitution of the Central Carbon Atoms of the Biphenalenyl Diradical Dimer: A Novel C-C Bond and Large NLO Responses. <i>Chemistry - A European Journal</i> , 2011, 17, 11773-11779.	3.3	71
21	How the Number and Location of Lithium Atoms Affect the First Hyperpolarizability of Graphene. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19792-19798.	3.1	67
22	Synthesis, Crystal Structure, Hirshfeld Surface Analysis, and Computational Study of a Novel Organic Salt Obtained from Benzylamine and an Acidic Component. <i>ACS Omega</i> , 2021, 6, 22357-22366.	3.5	66
23	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
24	Halide Ion Complexes of Decaborane (B ₁₀ H ₁₄) and Their Derivatives: Noncovalent Charge Transfer Effect on Second-Order Nonlinear Optical Properties. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1417-1424.	2.5	62
25	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
26	Electro-optical, nonlinear and charge transfer properties of naphthalene based compounds: A dual approach study. <i>Optik</i> , 2017, 132, 101-110.	2.9	59
27	Exploring the new potential antiviral constituents of <i>Moringa oleifera</i> for SARS-COV-2 pathogenesis: An in silico molecular docking and dynamic studies. <i>Chemical Physics Letters</i> , 2021, 767, 138379.	2.6	58
28	Structural parameters, electronic, linear and nonlinear optical exploration of thiopyrimidine derivatives: A comparison between DFT/TDDFT and experimental study. <i>Journal of Molecular Structure</i> , 2020, 1201, 127183.	3.6	53
29	How does hybrid bridging core modification enhance the nonlinear optical properties in donor-acceptor configuration? A case study of dinitrophenol derivatives. <i>Journal of Computational Chemistry</i> , 2015, 36, 118-128.	3.3	52
30	Postharvest disease inhibition in fruit by synthesis and characterization of chitosan iron oxide nanoparticles. <i>Biocatalysis and Agricultural Biotechnology</i> , 2020, 28, 101729.	3.1	51
31	Knot-Isomers of Möbius Cyclacene: How Does the Number of Knots Influence the Structure and First Hyperpolarizability?. <i>Journal of Physical Chemistry C</i> , 2009, 113, 15380-15383.	3.1	48
32	Second-order nonlinear optical properties of dithienophenazine and TTF derivatives: A butterfly effect of dimalononitrile substitutions. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 59, 14-20.	2.4	47
33	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
34	Co ₂ YZ (Y= Cr, Nb, Ta, V and Z= Al, Ga) Heusler alloys under the effect of pressure and strain. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 104, 107841.	2.4	46
35	Single-Crystal Investigation, Hirshfeld Surface Analysis, and DFT Study of Third-Order NLO Properties of Unsymmetrical Acyl Thiourea Derivatives. <i>ACS Omega</i> , 2021, 6, 31211-31225.	3.5	46
36	Three-propeller-blade-shaped electride: remarkable alkali-metal-doped effect on the first hyperpolarizability. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 241-248.	1.4	45

#	ARTICLE	IF	CITATIONS
37	Zinc-Doped Boron Phosphide Nanocluster as Efficient Sensor for SO ₂ . Journal of Chemistry, 2020, 2020, 1-12.	1.9	45
38	Facile synthesis of lead iodide nanostructures by microwave irradiation technique and their structural, morphological, photoluminescence and dielectric studies. Journal of Molecular Structure, 2016, 1110, 83-90.	3.6	44
39	Non-noble metal single-atom catalyst of Co1/MXene (Mo2CS2) for CO oxidation. Science China Materials, 2021, 64, 651-663.	6.3	44
40	Design, characterization and nonlinear optical properties of coumarin appended chalcones: Use of a dual approach. Optik, 2018, 164, 5-15.	2.9	43
41	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
42	The substitution effect of heterocyclic rings to tune the optical and nonlinear optical properties of hybrid chalcones: A comparative study. Journal of Molecular Graphics and Modelling, 2018, 81, 25-31.	2.4	42
43	Synthesis, XRD, spectral (IR, UV-Vis, NMR) characterization and quantum chemical exploration of benzoimidazole-based hydrazones: A synergistic experimental-computational analysis. Applied Organometallic Chemistry, 2019, 33, e5182.	3.5	42
44	Experimental and density functional theory (DFT): A dual approach to study the various important properties of monohydrated l-proline cadmium chloride for nonlinear optical applications. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 143, 128-135.	3.9	41
45	First principal studies of spectroscopic (IR and Raman, UV-visible), molecular structure, linear and nonlinear optical properties of l-arginine p-nitrobenzoate monohydrate (LANB): A new non-centrosymmetric material. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 147, 84-92.	3.9	41
46	The impact of position and number of methoxy group(s) to tune the nonlinear optical properties of chalcone derivatives: a dual substitution strategy. Journal of Molecular Modeling, 2016, 22, 73.	1.8	39
47	A dual approach to study the key features of nickel (II) and copper (II) coordination complexes: Synthesis, crystal structure, optical and nonlinear properties. Inorganica Chimica Acta, 2019, 484, 148-159.	2.4	39
48	A dual approach to study the electro-optical properties of a noncentrosymmetric l-asparagine monohydrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 432-441.	3.9	37
49	Exploring the novel donor-nanotube archetype as an efficient third-order nonlinear optical material: asymmetric open-shell carbon nanotubes. Nanoscale, 2018, 10, 16499-16507.	5.6	37
50	Interplay between the Diradical Character and Third-Order Nonlinear Optical Properties in Fullerene Systems. Chemistry - A European Journal, 2013, 19, 1677-1685.	3.3	36
51	Syntheses, characterizations, crystal structures and efficient NLO applications of new organic compounds bearing 2-methoxy-4-nitrobenzeneamine moiety and copper (II) complex of (E)-N'-(3,4,5-trimethoxyphenyl)acetamide. Journal of Molecular Structure, 2021, 1218, 1271-1280.	3.4	36
52	Exploration of CH ₂ F & CF ₂ H mediated supramolecular arrangements into fluorinated terphenyls and theoretical prediction of their third-order nonlinear optical response. RSC Advances, 2021, 11, 7766-7778.	3.6	36
53	Quantum chemical design of triple hybrid organic, inorganic and organometallic materials: An efficient two-dimensional second-order nonlinear optical material. Materials Chemistry and Physics, 2018, 220, 286-292.	4.0	35
54	DFT study of superhalogen (AlF ₄) doped boron nitride for tuning their nonlinear optical properties. Optik, 2021, 231, 166464.	2.9	35

#	ARTICLE	IF	CITATIONS
55	First principles study of the n-channel thiophene based heterocyclic chalcones. <i>Optik</i> , 2017, 138, 349-358.	2.9	34
56	Exploring the impact of central core modifications among several push-pull configurations to enhance nonlinear optical response. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107665.	2.4	34
57	A theoretical investigation of intermolecular interaction of a phthalimide based "off" sensor with different halide ions: tuning its efficiency and electro-optical properties. <i>Theoretical Chemistry Accounts</i> , 2009, 122, 77-86.	1.4	33
58	A comparative study of key properties of glycine glycinium picrate (GGP) and glycinium picrate (GP): A combined experimental and quantum chemical approach. <i>Journal of Saudi Chemical Society</i> , 2018, 22, 352-362.	5.2	33
59	DFT study of the electronic and optical properties of ternary chalcogenides AlX_2Te_4 . <i>Materials Research Express</i> , 2019, 6, 116314.	1.6	33
60	Exploring the optoelectronic and third-order nonlinear optical susceptibility of cross-shaped molecules: insights from molecule to material level. <i>Journal of Molecular Modeling</i> , 2021, 27, 12.	1.8	33
61	Efficient Synthesis by Mono-Carboxy Methylation of 4,4'-Biphenol, X-ray Diffraction, Spectroscopic Characterization and Computational Study of the Crystal Packing of Ethyl 2-((4-hydroxy[1,1'-biphenyl]-4-yl)oxy)acetate. <i>ChemistrySelect</i> , 2019, 4, 9274-9284.	1.5	32
62	Photocatalytic degradation and hydrogen evolution using bismuth tungstate based nanocomposites under visible light irradiation. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 22833-22847.	7.1	32
63	The structural, electro-optical, charge transport and nonlinear optical properties of 2-[(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)methylidene]indan-1,3-dione. <i>Optik</i> , 2016, 127, 10148-10157.	2.9	31
64	Elastic and optoelectronic properties of CaTa ₂ O ₆ compounds: Cubic and orthorhombic phases. <i>Journal of Alloys and Compounds</i> , 2019, 785, 232-239.	5.5	31
65	Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties. <i>ACS Omega</i> , 2021, 6, 24602-24613.	3.5	31
66	Synthesis, crystal structure, spectroscopic, electronic and nonlinear optical properties of potent thiazole based derivatives: Joint experimental and computational insight. <i>Journal of Molecular Structure</i> , 2020, 1202, 127354.	3.6	30
67	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
68	Combined experimental and computational insights into the key features of L-alanine L-alaninium picrate monohydrate: growth, structural, electronic and nonlinear optical properties. <i>RSC Advances</i> , 2015, 5, 53988-54002.	3.6	29
69	Exploring the potential of boron-doped nanographene as efficient charge transport and nonlinear optical material: A first-principles study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 209-219.	2.4	29
70	Facile Synthesis, Spectral (IR, Mass, UV-Vis, NMR), Linear and Nonlinear Investigation of the Novel Phosphonate Compounds: A Combined Experimental and Simulation Study. <i>ChemistrySelect</i> , 2020, 5, 2994-3006.	1.5	29
71	2-Amino-6-methylpyridine based co-crystal salt formation using succinic acid: Single-crystal analysis and computational exploration. <i>Journal of Molecular Structure</i> , 2021, 1230, 129893.	3.6	29
72	Exploring the potential of novel phenolic compounds as potential therapeutic candidates against SARS-CoV-2, using quantum chemistry, molecular docking and dynamic studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2021, 43, 128079.	2.2	29

#	ARTICLE	IF	CITATIONS
73	In-depth quantum chemical investigation of electro-optical and charge-transport properties of trans-3-(3,4-dimethoxyphenyl)-2-(4-nitrophenyl)prop-2-enenitrile. <i>Comptes Rendus Chimie</i> , 2015, 18, 1289-1296.	0.5	28
74	Synthesis, growth, structural, thermal, third order nonlinear and computational studies of organic single crystal: 2-Amino-4-picolinium 2-chloro-4-nitrobenzoate. <i>Optical Materials</i> , 2019, 96, 109341.	3.6	28
75	Advances in photo-catalysis approach for the removal of toxic personal care product in aqueous environment. <i>Environment, Development and Sustainability</i> , 2020, 22, 6029-6052.	5.0	28
76	p-type Cu ₃ BiS ₃ thin films for solar cell absorber layer via one stage thermal evaporation. <i>Applied Surface Science</i> , 2020, 505, 144597.	6.1	28
77	Computational investigation of a covalent triazine framework (CTF-0) as an efficient electrochemical sensor. <i>RSC Advances</i> , 2022, 12, 3909-3923.	3.6	28
78	Packing Effect on the Transfer Integrals and Mobility in $\hat{I}_{\pm}, \hat{I}_{\pm}^{\pm}$ -bis(dithieno[3,2-b:2 \hat{a} :3 \hat{a} -d]thiophene) (BDT) and its Heteroatom-Substituted Analogues. <i>Australian Journal of Chemistry</i> , 2011, 64, 1587.	0.9	27
79	Palladium-catalyzed synthesis of 5-(arylated) pyrimidines, their characterization, electronic communication, and non-linear optical evaluations. <i>Journal of Molecular Structure</i> , 2021, 1237, 130408.	3.6	27
80	Demonstrating the Potential of Alkali Metal-Doped Cyclic C ₆ O ₆ Li ₆ Organometallics as Electrides and High-Performance NLO Materials. <i>ACS Omega</i> , 2021, 6, 29852-29861.	3.5	26
81	The effect of anchoring groups on the electro-optical and charge injection in triphenylamine derivatives@TiO ₂ . <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550027.	1.8	25
82	Tuning of optoelectronic and charge transport properties in star shaped anthracenothiophene-pyrimidine derivatives as multifunctional materials. <i>Optik</i> , 2017, 149, 321-331.	2.9	25
83	First-principles study of nitrogen-doped nanographene as an efficient charge transport and nonlinear optical material. <i>RSC Advances</i> , 2017, 7, 36632-36643.	3.6	25
84	Effect of heteroatoms substitution on electronic, photophysical and charge transfer properties of naphtho[2,1-b:6,5-b \hat{a}]difuran analogues by density functional theory. <i>Computational and Theoretical Chemistry</i> , 2014, 1045, 123-134.	2.5	24
85	Optoelectronic properties of naphtho[2,1-b:6,5-b \hat{a}]difuran derivatives for photovoltaic application: a computational study. <i>Journal of Molecular Modeling</i> , 2016, 22, 248.	1.8	24
86	Push-pull effect on the charge transport properties in anthra[2,3-b]thiophene derivatives used as dye-sensitized and hetero-junction solar cell materials. <i>Synthetic Metals</i> , 2014, 190, 27-33.	3.9	23
87	Soft template-based bismuth doped zinc oxide nanocomposites for photocatalytic depolymerization of lignin. <i>Inorganica Chimica Acta</i> , 2020, 502, 119390.	2.4	22
88	First example of lanthanum as dopant on Al ₁₂ N ₁₂ and Al ₁₂ P ₁₂ nanocages for improved electronic and nonlinear optical properties with high stability. <i>Materials Science in Semiconductor Processing</i> , 2021, 135, 106122.	4.0	22
89	In Silico Drug Designing for ala438 Deleted Ribosomal Protein S1 (RpsA) on the Basis of the Active Compound <i>Zr</i> 15. <i>ACS Omega</i> , 2022, 7, 397-408.	3.5	22
90	Influence of push-pull configuration on the electro-optical and charge transport properties of novel naphtho-difuran derivatives: a DFT study. <i>RSC Advances</i> , 2014, 4, 48876-48887.	3.6	21

#	ARTICLE	IF	CITATIONS
91	Effect of S and Se replacement on electronic and thermoelectric features of BaCu ₂ GeQ ₄ (Q = S, Se) chalcogenide crystals. <i>Journal of Alloys and Compounds</i> , 2019, 790, 666-674.	5.5	21
92	Shedding light on molecular structure, spectroscopic, nonlinear optical and dielectric properties of bis(thiourea) silver(I) nitrate single crystal: A dual approach. <i>Arabian Journal of Chemistry</i> , 2019, 12, 4612-4626.	4.9	21
93	Synthesis, characterization, Hirshfeld surface analysis and computational studies of 1-methylpiperazine-1,4-dium bis(hydrogen oxalate): [C ₅ H ₁₄ N ₂](HC ₂ O ₄) ₂ . <i>Journal of Molecular Structure</i> , 2020, 1211, 128075.	3.6	21
94	Proposition of new stable rare-earth ternary semiconductor sulfides of type LaTlS ₂ (La = Er, Eu, Tb): Ab-initio study and prospects for optoelectronic, spintronic and thermoelectric applications. <i>Materials Science in Semiconductor Processing</i> , 2022, 146, 106662.	4.0	21
95	Diradical character and nonlinear optical properties of buckyferrocenes: focusing on the use of suitably modified fullerene fragments. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5805-5816.	2.8	20
96	The structural, electro-optical, charge transport and nonlinear optical properties of oxazole (4 Z) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 5 Science, 2018, 30, 75-82.	3.5	20
97	Synthesis, antioxidant, antimicrobial and antiviral docking studies of ethyl 2-(2-(arylidene)hydrazinyl)thiazole-4-carboxylates. <i>Zeitschrift Fur Naturforschung - Section C Journal of Biosciences</i> , 2021, 76, 467-480.	1.4	20
98	Catalytic Oxidation of Toluene into Benzaldehyde and Benzyl Alcohol Using Molybdenum-Incorporated Manganese Oxide Nanomaterials. <i>ACS Omega</i> , 2021, 6, 19606-19615.	3.5	20
99	A Quantum Mechanical Study of the Second-Order Nonlinear Optical Properties of Aryldiazene-Substituted Hexamolybdates: A Surprising Charge Transfer. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 5181-5188.	2.0	19
100	A comparative analysis of the optical and nonlinear optical properties of cross-shaped chromophores: Quantum chemical approach. <i>Optik</i> , 2017, 147, 439-445.	2.9	19
101	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.	2.9	19
102	A dual approach to study the synthesis, crystal structure and nonlinear optical properties of binuclear Pd(II) complex of 3-methyl-5-(trifluoromethyl) pyrazole and its potential quantum chemical analogues. <i>Inorganica Chimica Acta</i> , 2019, 494, 160-167.	2.4	19
103	Designing and Encapsulation of Inorganic Al ₁₂ N ₁₂ Nanoclusters with Be, Mg, and Ca Metals for Efficient Hydrogen Adsorption: A Step Forward Towards Hydrogen Storage Materials. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 687-705.	1.7	19
104	A DFT study on the electronic and redox properties of [X ₈ V ₁₄ O ₅₀] ⁿ⁺ (X = Si ^{IV}), Tj ETQq0 0 0 rgBT /Overlock 10 Tf 18 434-442.	1.1	18
105	Investigating the effect of acene-fusion and trifluoroacetyl substitution on the electronic and charge transport properties by density functional theory. <i>Journal of Saudi Chemical Society</i> , 2016, 20, 336-342.	5.2	18
106	Exploring the possible existence of oxygen-bridged planarized 4-aminopyridine: promising structure, charge transport and nonlinear optical properties. <i>Journal of Materials Chemistry C</i> , 2017, 5, 7102-7109.	5.5	18
107	Semiconductor based nanomaterials for harvesting green hydrogen energy under solar light irradiation. <i>International Journal of Environmental Analytical Chemistry</i> , 0, , 1-17.	3.3	18
108	Visible light responsive photocatalytic hydrogen evolution using MoS ₂ incorporated ZnO. <i>Applied Nanoscience (Switzerland)</i> , 2020, 10, 3925-3931.	3.1	18

#	ARTICLE	IF	CITATIONS
109	Effect of Nb, Ta and V replacements on electronic, optical and elastic properties of NbCu ₃ Se ₄ : A GGA+U study. <i>Journal of Solid State Chemistry</i> , 2021, 301, 122338.	2.9	18
110	Emerging Mutations in Nsp1 of SARS-CoV-2 and Their Effect on the Structural Stability. <i>Pathogens</i> , 2021, 10, 1285.	2.8	18
111	Shedding Light on the Synthesis, Crystal Structure, Characterization, and Computational Study of Optoelectronic Properties and Bioactivity of Imine derivatives. <i>ACS Omega</i> , 2022, 7, 5217-5230.	3.5	18
112	The electro-optical and charge transport study of imidazolidin derivative: Quantum chemical investigations. <i>Journal of Saudi Chemical Society</i> , 2016, 20, 680-685.	5.2	17
113	Effect of Coulomb interactions on optoelectronic and magnetic properties of novel A ₂ V ₂ O ₇ (A= Fe) Tj ETQq1 1 0.784314 rgBT /Overlock 10 TF 5	5.5	17
114	Synthesis, characterizations, crystal structures, and theoretical studies of copper(II) and nickel(II) coordination complexes. <i>Journal of Coordination Chemistry</i> , 2020, 73, 1256-1279.	2.2	17
115	An experimental and computational study of pyrimidine based bis-uracil derivatives as efficient candidates for optical, nonlinear optical, and drug discovery applications. <i>Synthetic Communications</i> , 2020, 50, 2199-2225.	2.1	17
116	Study of structural, optoelectronic and magnetic properties of Half-Heusler compounds QEuPa (Q=) Tj ETQq0 0 0 rgBT /Overlock 10 TF 5	2.9	17
117	Application of Functionalized Nanomaterials as Effective Adsorbents for the Removal of Heavy Metals from Wastewater: A Review. <i>Current Analytical Chemistry</i> , 2020, 17, 4-22.	1.2	17
118	Fabrication of direct Z-scheme MoO ₃ /Nâ€“MoS ₂ photocatalyst for synergistically enhanced H ₂ production. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 39822-39829.	7.1	17
119	Insighting the functionally modified C ₆₀ fullerenes as an efficient nonlinear optical materials: A quantum chemical study. <i>Materials Science in Semiconductor Processing</i> , 2022, 141, 106421.	4.0	17
120	Synthesis, Characterization, Biological Activity and Molecular Docking Studies of Novel Organotin(IV) Carboxylates. <i>Frontiers in Pharmacology</i> , 2022, 13, 864336.	3.5	17
121	Quantum chemical investigation of spectroscopic studies and hydrogen bonding interactions between water and methoxybenzylidene-based humidity sensor. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550029.	1.8	16
122	Computational study of structural, optoelectronic and nonlinear optical properties of dynamic solid-state chalcone derivatives. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 355-364.	2.4	16
123	Exploring the charge transfer nature and electro-optical properties of anthracene based sensitizers @TiO ₂ cluster. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2017, 80, 239-246.	5.3	16
124	Exploring the Effect of Electron Withdrawing Groups on Optoelectronic Properties of Pyrazole Derivatives as Efficient Donor and Acceptor Materials for Photovoltaic Devices. <i>Zeitschrift Fur Physikalische Chemie</i> , 2019, 233, 1625-1644.	2.8	16
125	Facile hydrothermal synthesis of highly efficient and visible light-driven Ni-doped V ₂ O ₅ photocatalyst for degradation of Rhodamine B dye. <i>Journal of Materials Science: Materials in Electronics</i> , 2020, 31, 12913-12925.	2.2	16
126	Comparative study of diradical characters and thirdâ€“order nonlinear optical properties of linear/cyclic acenes versus phenylenes. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 592-598.	2.0	15

#	ARTICLE	IF	CITATIONS
127	Tuning the optoelectronic and charge transport properties of 2,5-di(pyrimidin-5-yl)thieno[3,2-b]thiophene by oligocene end cores substitution. <i>Results in Physics</i> , 2018, 11, 599-604.	4.1	15
128	Reactive kinetics of carbon dioxide loaded aqueous blend of 2-ethyl-1,3-propanediol and piperazine using a pressure drop method. <i>International Journal of Chemical Kinetics</i> , 2019, 51, 291-298.	1.6	15
129	Novel halogenated pyrido[2,3- <i>i></i>]carbazoles with enhanced aromaticity as potent anticancer and antioxidant agents: rational design and microwave assisted synthesis. <i>New Journal of Chemistry</i> , 2019, 43, 17231-17240.	2.8	15
130	Exploring the effect of halogens on semiconducting nature of boron doped molecular precursor graphene nanoribbons at molecular and bulk level. <i>Optik</i> , 2019, 179, 526-534.	2.9	15
131	Hierarchical WO ₃ @ BiVO ₄ nanostructures for improved green energy production. <i>Applied Nanoscience (Switzerland)</i> , 2020, 10, 1183-1190.	3.1	15
132	Synthesis of Copper(II) Coordination Complex, Its Molecular Docking and Computational Exploration for Novel Functional Properties: A Dual Approach. <i>ChemistrySelect</i> , 2021, 6, 738-745.	1.5	15
133	A DFT+U study of the effect of transition metal replacements on optoelectronic and elastic properties of TmCu ₃ S ₄ (Tm = V, Ta, Nb). <i>Optik</i> , 2022, 250, 168289.	2.9	15
134	Theoretical study on dithieno[3,2- <i>b</i> :2',3'- <i>d</i>]phosphole derivatives: high-efficiency blue-emitting materials with ambipolar semiconductor behavior. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 419-427.	1.4	14
135	Stimulating intra- and intermolecular charge transfer and nonlinear optical response for biphenalenyl biradicaloid dimer under an external electric field. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18699-18706.	2.8	14
136	Doping induced effect on optical and band structure properties of Sr ₂ Si ₅ N ₈ based phosphors: DFT approach. <i>Journal of Alloys and Compounds</i> , 2019, 771, 1072-1079.	5.5	14
137	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.	2.4	14
138	First-principles study of the electronic structures and optical and photocatalytic performances of van der Waals heterostructures of SiS, P and SiC monolayers. <i>RSC Advances</i> , 2021, 11, 14263-14268.	3.6	14
139	Inorganic electrides of alkali metal doped Zn ₁₂ O ₁₂ nanocage with excellent nonlinear optical response. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 106, 107935.	2.4	14
140	Influence of van der waals heterostructures of 2D materials on catalytic performance of ZnO and its applications in energy: A review. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 25413-25423.	7.1	14
141	Novel, facile and first time synthesis of zinc oxide nanoparticles using leaves extract of <i>Citrus reticulata</i> for photocatalytic and antibacterial activity. <i>Optik</i> , 2021, 243, 167495.	2.9	14
142	Structural, Elemental, Morphological and Optical Spectroscopic Studies on High Quality ~111% Grown Nanocrystalline ZnTe Thin Films: An Effect of Thickness. <i>Materials Focus</i> , 2015, 4, 202-207.	0.4	14
143	A Novel Method of Magnetic Nanoparticles Functionalized with Anti-Folate Receptor Antibody and Methotrexate for Antibody Mediated Targeted Drug Delivery. <i>Molecules</i> , 2022, 27, 261.	3.8	14
144	Exploring the inhibitory potential of novel bioactive compounds from mangrove actinomycetes against nsp10 the major activator of SARS-CoV-2 replication. <i>Chemical Papers</i> , 2022, 76, 3051-3064.	2.2	14

#	ARTICLE	IF	CITATIONS
145	Synthesis, single-crystal exploration, hirshfeld surface analysis, and DFT investigation of the thiosemicarbazones. <i>Journal of Molecular Structure</i> , 2022, 1262, 133088.	3.6	14
146	Adsorption of Industrial Gases (CH ₄ , CO ₂ , and CO) on Olympicene: A DFT and CCSD(T) Investigation. <i>ACS Omega</i> , 2022, 7, 18852-18860.	3.5	14
147	Shedding light on the structural, optoelectronic, and thermoelectric properties of pyrochlore oxides (La ₂ Q ₂ O ₇ (Q = Ge, Sn)) for energy applications: A first-principles investigation. <i>Journal of Solid State Chemistry</i> , 2022, 313, 123305.	2.9	14
148	Effect of donor strength of extended alkyl auxiliary groups on optoelectronic and charge transport properties of novel naphtha[2,1-b:6,5-b']difuran derivatives: simple yet effective strategy. <i>Journal of Molecular Modeling</i> , 2015, 21, 199.	1.8	13
149	Synthesis, Crystal Structures and Photoluminescent Properties of One-Dimensional Europium(III)- and Terbium(III)-Glutarate Coordination Polymers, and Their Applications for the Sensing of Fe ³⁺ and Nitroaromatics. <i>Frontiers in Chemistry</i> , 2019, 7, 728.	3.6	13
150	A systematic study of the effects of thionation in naphthalene dimide derivatives to tune their nonlinear optical properties. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 87, 68-75.	2.4	13
151	Electro-optical and charge injection investigations of the donor-acceptor triphenylamine, oligocene-thiophene-pyrimidine and cyanoacetic acid based multifunctional dyes. <i>Journal of King Saud University - Science</i> , 2015, 27, 361-368.	3.5	12
152	i-Propylammonium Lead Chloride Based Perovskite Photocatalysts for Depolymerization of Lignin Under UV Light. <i>Molecules</i> , 2020, 25, 3520.	3.8	12
153	First-principles calculations to investigate structural, electronic and optical properties of Na based fluoroperovskites NaXF ₃ (X= Sr, Zn). <i>Solid State Communications</i> , 2021, 334-335, 114396.	1.9	12
154	Copper(II) and Nickel(II) Complexes of Tridentate Hydrazide and Schiff Base Ligands Containing Phenyl and Naphthalyl Groups: Synthesis, Structural, Molecular Docking and Density Functional Study. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2020, 30, 4426-4440.	3.7	12
155	Effect of Fe doping on optoelectronic properties of CdS nanostructure: Insights from DFT calculations. <i>Physica B: Condensed Matter</i> , 2020, 583, 412056.	2.7	11
156	Synthesis and characterization of ferrocene-based thiosemicarbazones along with their computational studies for potential as inhibitors for SARS-CoV-2. <i>Journal of the Iranian Chemical Society</i> , 2022, 19, 839-846.	2.2	11
157	Specific features of structural, electronic, optical and elastic properties of the cubic calcium pyroniobate Ca ₂ Nb ₂ O ₇ crystals. <i>Physica B: Condensed Matter</i> , 2018, 545, 69-75.	2.7	10
158	Synthesis, X-ray crystal structure and spin polarized DFT study of high spin Mn based metal-organic framework. <i>Journal of Molecular Structure</i> , 2019, 1175, 439-444.	3.6	10
159	Synthesis, Thermal, Structural Analyses, and Photoluminescent Properties of a New Family of Malonate-Containing Lanthanide(III) Coordination Polymers. <i>Frontiers in Chemistry</i> , 2019, 7, 260.	3.6	10
160	A Systematic and Comparative Analysis of Four Major Classes of DFT Functionals to Compute Linear and Nonlinear Optical Properties of Benchmark Molecules. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 517-528.	1.7	10
161	Electro-optical and charge transport properties of chalcone derivatives using a dual approach from molecule to material level simulations. <i>Computational and Theoretical Chemistry</i> , 2021, 1203, 113349.	2.5	10
162	Experimental and computational study of naphthalimide derivatives: Synthesis, optical, nonlinear optical and antiviral properties. <i>Optik</i> , 2021, 246, 167748.	2.9	10

#	ARTICLE	IF	CITATIONS
163	Compositional Adjusting and Antibacterial Improvement of Hydroxyapatite/Nb ₂ O ₅ /Graphene Oxide for Medical Applications. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2022, 32, 2160-2172.	3.7	10
164	Probing the Chemical Functionalization of Single-Walled Carbon Nanotubes with Multiple Carbon Ad-Dimer Defects. <i>ChemPhysChem</i> , 2012, 13, 1232-1239.	2.1	9
165	Theoretical study on photophysical properties of novel bis(BF ₂) ² -bidipyrrins dyes: Effect of variation in monomer structure. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 440-452.	2.0	9
166	Crystal and Quantum Chemical Exploration of the Potent Monocarbonyl Curcuminoids to Unveil Their Structural and Intriguing Electronic Properties. <i>ChemistrySelect</i> , 2020, 5, 3735-3745.	1.5	9
167	Hydrothermal synthesis of an efficient and visible light responsive pure and strontium doped zinc oxide nano-hexagonal photocatalysts for photodegradation of Rhodamine B dye. <i>Applied Nanoscience (Switzerland)</i> , 2021, 11, 1045-1056.	3.1	9
168	Identification of phytochemical inhibitors of SARS-CoV-2 protease 3CL ^{pro} from selected medicinal plants as per molecular docking, bond energies and amino acid binding energies. <i>Saudi Journal of Biological Sciences</i> , 2022, 29, 103274.	3.8	9
169	Benchmark Density Functional Theory Approach for the Calculation of Bond Dissociation Energies of the M ⁺ O ₂ Bond: A Key Step in Water Splitting Reactions. <i>ACS Omega</i> , 2022, 7, 20800-20808.	3.5	9
170	Theoretical Study on Open-Shell Singlet Character and Second Hyperpolarizabilities in Cofacial π -Stacked Dimers Composed of Weak Open-Shell Antiaromatic Porphyrins. <i>ChemPhysChem</i> , 2018, 19, 2863-2871.	2.1	8
171	Electrochemical and thermal catalytic studies of Co based molybdenum oxide nanomaterials for C H bond activation. <i>Inorganica Chimica Acta</i> , 2021, 517, 120219.	2.4	8
172	Functionalized role of highly porous activated carbon in bismuth vanadate nanomaterials for boosted photocatalytic hydrogen evolution and synchronous activity in water. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 39778-39785.	7.1	8
173	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.	3.7	8
174	Symmetric vs. asymmetric: Which one is the better molecular configuration for achieving robust NLO response?. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 114, 108209.	2.4	8
175	How does the increment of hetero-cyclic conjugated moieties affect electro-optical and charge transport properties of novel naphtha-difuran derivatives? A computational approach. <i>Journal of Molecular Modeling</i> , 2014, 20, 2547.	1.8	7
176	How methoxy groups change nature of the thiophene based heterocyclic chalcones from p-channel to ambipolar transport semiconducting materials. <i>Journal of King Saud University - Science</i> , 2018, 30, 458-465.	3.5	7
177	Structural, electronic and optical properties of furan based materials at bulk level for photovoltaic applications: A first-principles study. <i>Computational and Theoretical Chemistry</i> , 2019, 1147, 20-28.	2.5	7
178	Role of rGO to improve the performance of BiVO ₄ nanostructures for efficient removal of heavy metals. <i>Applied Nanoscience (Switzerland)</i> , 2020, 10, 1421-1432.	3.1	7
179	Stacking effects in van der Waals heterostructures of blueP and Janus XYO (X = Ti, Zr, Hf; Y = S, Se) monolayers. <i>RSC Advances</i> , 2021, 11, 12189-12199.	3.6	7
180	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.	2.4	7

#	ARTICLE	IF	CITATIONS
181	Chalcone Scaffolds Exhibiting Acetylcholinesterase Enzyme Inhibition: Mechanistic and Computational Investigations. <i>Molecules</i> , 2022, 27, 3181.	3.8	7
182	Towards Rational Designing of Efficient Sensitizers Based on Thiophene and Infrared Dyes for Dye-Sensitized Solar Cells. <i>Journal of Quantum Chemistry</i> , 2014, 2014, 1-6.	0.9	6
183	Structural, Electronic and Nonlinear Optical Properties of Novel Derivatives of 9,12-Diiodo-1,2-dicarba-closo-dodecaborane: Density Functional Theory Approach. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2018, 73, 1037-1045.	1.5	6
184	Cation effect on electronic, optical and thermoelectric properties of perovskite oxynitrides: Density functional theory. <i>Materials Science in Semiconductor Processing</i> , 2020, 107, 104800.	4.0	6
185	An efficient and eco-friendly synthesis, computational assay and antimicrobial evaluation of some novel diastereoselective monocyclic cis- β -lactams. <i>Journal of Molecular Structure</i> , 2020, 1219, 128638.	3.6	6
186	Synthesis, crystal structures and, magnetic and photoluminescence properties of lanthanide-based metal-organic frameworks constructed with 2,5-dihydroxybenzene-1,4-dicarboxylic acid. <i>RSC Advances</i> , 2020, 10, 12841-12850.	3.6	6
187	SARS-CoV-2 Genome from the Khyber Pakhtunkhwa Province of Pakistan. <i>ACS Omega</i> , 2021, 6, 6588-6599.	3.5	6
188	Investigation analysis of optoelectronic and structural properties of cis- and trans- structures of azo dyes: density functional theory study. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4183.	1.9	6
189	Theoretical Approach to Evaluate the Gas-Sensing Performance of Graphene Nanoribbon/Oligothiophene Composites. <i>ACS Omega</i> , 2022, 7, 2260-2274.	3.5	6
190	Shedding light on the optical and nonlinear optical properties of superalkali-doped borophene. <i>Journal of Molecular Modeling</i> , 2022, 28, 46.	1.8	6
191	Identification of Halogen-Based Derivatives as Potent Inhibitors of Estrogen Receptor Alpha of Breast Cancer: An <i>In-Silico</i> Investigation. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 181-205.	1.7	6
192	Insighting isatin derivatives as potential antiviral agents against NSP3 of COVID-19. <i>Chemical Papers</i> , 2022, 76, 6271-6285.	2.2	6
193	Molecular structure, vibrational, optical, molecular first order hyperpolarizability analysis of {Dibromobis(l-proline)zinc(II)}: A novel nonlinear optical material. <i>Optik</i> , 2016, 127, 2852-2860.	2.9	5
194	A dual approach to study the synthesis, crystal structure, thermal, optical and nonlinear optical properties of copper (II) malonate complex $\{(C_7H_8O_2N)_2[Cu(C_3H_2O_4)_2(H_2O)_2]\}$. <i>Inorganic Chemistry Communication</i> , 2019, 107, 107450.	3.9	5
195	Role of Nano-Photocatalysts in Detoxification of Toxic Heavy Metals. <i>Current Analytical Chemistry</i> , 2021, 17, 126-137.	1.2	5
196	Dual Penta-Compound Combination Anti-Synchronization with Analysis and Application to a Novel Fractional Chaotic System. <i>Fractal and Fractional</i> , 2021, 5, 264.	3.3	5
197	TRAVELING WAVE SOLUTIONS TO A MATHEMATICAL MODEL OF FRACTIONAL ORDER (2+1)-DIMENSIONAL BREAKING SOLITON EQUATION. <i>Fractals</i> , 2022, 30, .	3.7	5
198	Insighting the systematic impact of shape, size and substitution of heteroatoms in quinoidal oligomers to tune their optoelectronic properties. <i>Optical and Quantum Electronics</i> , 2022, 54, .	3.3	5

#	ARTICLE	IF	CITATIONS
199	Virtual screening of potential inhibitor against breast cancer-causing estrogen receptor alpha (ER α): molecular docking and dynamic simulations. <i>Molecular Simulation</i> , 2022, 48, 1163-1174.	2.0	5
200	Inhibitory effect of thymoquinone from <i>Nigella sativa</i> against SARS-CoV-2 main protease. An in-silico study. <i>Brazilian Journal of Biology</i> , 2022, 84, e250667.	0.9	5
201	Diradicalology in third-order nonlinear optical systems: Second hyperpolarizabilities of acetylene-linked phenalenyl-based superpolyenes. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 585-591.	2.0	4
202	Effect of N ⁵⁺ ion irradiation on ornithine monohydrochloride single crystals: an organic nonlinear optical material. <i>Radiation Effects and Defects in Solids</i> , 2014, 169, 954-964.	1.2	4
203	Key optoelectronic properties of Diiodo-bis(carbamide)-zinc(II): An experimental and computational investigation. <i>Journal of Molecular Structure</i> , 2018, 1156, 146-155.	3.6	4
204	Metal ions doped into merocyanine form of coumarin derivatives: nonlinear optical molecular switches. <i>Journal of Molecular Modeling</i> , 2019, 25, 212.	1.8	4
205	Tuning the Photocatalytic Performance of Tungsten Oxide by Incorporating Cu ₃ V ₂ O ₈ Nanoparticles for H ₂ Evolution Under Visible Light Irradiation. <i>Journal of Electrochemical Energy Conversion and Storage</i> , 2020, 17, .	2.1	4
206	Magnetic and electrical properties of Ba ₂ Co ₂ Fe ₁₂ O ₂₂ /PANI composites prepared by insitu polymerization. <i>Physica B: Condensed Matter</i> , 2020, 597, 412410.	2.7	4
207	Optoelectronic properties of Nd ³⁺ doped CaTa ₂ O ₆ : Insights from the GGA+U calculations. <i>Optik</i> , 2021, 225, 165270.	2.9	4
208	Effect of S, Se and Te replacement on structural, optoelectronic and transport properties of SrXO ₄ (X= S, Se, Te) for energy applications: A first principles study. <i>Journal of Solid State Chemistry</i> , 2022, 305, 122689.	2.9	4
209	Identification of Marine Fungi-Based Antiviral Agents as Potential Inhibitors of SARS-CoV-2 by Molecular Docking, ADMET and Molecular Dynamic Study. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 139-153.	1.7	4
210	Prewetting Induced Hydrophilicity to Augment Photocatalytic Activity of Nanocalcite @ Polyester Fabric. <i>Polymers</i> , 2022, 14, 295.	4.5	4
211	Exploring the quinoidal oligothiophenes to their robust limit for efficient linear and nonlinear optical response properties. <i>Chemical Papers</i> , 2022, 76, 4273-4288.	2.2	4
212	Insighting the Therapeutic Potential of Fifty (50) Shogaol Derivatives Against M ^{pro} of SARS-CoV-2. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 555-568.	1.7	4
213	A first-principles study of the linear and nonlinear optical properties of isoxazole derivatives. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650060.	1.8	3
214	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.	1.8	3
215	DFT simulations of optoelectronic and elastic features of cubic samarium zirconate (Sm ₂ Zr ₂ O ₇). <i>Computational Condensed Matter</i> , 2019, 21, e00414.	2.1	3
216	Exploring the functional properties of Trimethoxy-Phenylpyridine as efficient optical and nonlinear optical material: A quantum chemical approach. <i>Journal of Molecular Structure</i> , 2019, 1185, 268-275.	3.6	3

#	ARTICLE	IF	CITATIONS
217	Exploring the potential use of Ca[LiAl ₃ N ₄]:Eu ²⁺ as phosphor-LED material: Ab-initio calculations. <i>Materials Today Communications</i> , 2020, 25, 101302.	1.9	3
218	Synthesis, Crystal Structure, and Nonlinear Optical Properties of Zn(II) Complex with 4,4',4''-Tri-tert-Butyl-2,2':6',2''-Terpyridine: A Dual Exploration. <i>Russian Journal of Inorganic Chemistry</i> , 2020, 65, 368-377.	1.3	3
219	Construction of Bi ₂ WO ₆ /MoSe ₂ /Bi ₁₂ O ₁₇ Cl _x Br ₂ ~ ^x heterostructures for the production of hydrogen energy and degradation of methylene blue. <i>Applied Nanoscience (Switzerland)</i> , 2021, 11, 951-959.	3.1	3
220	Insighting role of activated carbon based nanostructures for complete photocatalytic degradation of hazardous pharmaceutical compound. <i>Applied Nanoscience (Switzerland)</i> , 2021, 11, 1117-1126.	3.1	3
221	Insight role of TiO ₂ to improve the photocatalytic performance of WO ₃ nanostructures for the efficient degradation of ciprofloxacin. <i>Zeitschrift Fur Physikalische Chemie</i> , 2022, 236, 169-180.	2.8	3
222	Isolation of Thioinosine and Butenolides from a Terrestrial <i>Actinomycetes</i> sp. GSCWâ€51 and Their <i>in Silico</i> Studies for Potential against SARSâ€CoVâ€2. <i>Chemistry and Biodiversity</i> , 2022, 19, .	2.1	3
223	A threefold approach including quantum chemical, molecular docking and molecular dynamic studies to explore the natural compounds from <i>Centaurea jacea</i> as the potential inhibitors for COVID-19. <i>Brazilian Journal of Biology</i> , 2021, 83, e247604.	0.9	3
224	Toward the Noninvasive Diagnosis of Alzheimerâ€™s Disease: Molecular Basis for the Specificity of Curcumin for Fibrillar Amyloid- β . <i>ACS Omega</i> , 2022, 7, 22032-22038.	3.5	3
225	Exploring the opto-electronic and charge transfer nature of F-BODIPY derivatives at molecular level: A theoretical perspective. <i>Chemical Physics</i> , 2019, 527, 110488.	1.9	2
226	Effect of extended alkyl auxiliary groups on optical and electronic properties of Benzo[2,1-b:3,4-bâ€™:5,6-câ€™ ³]trithiophene derivatives at bulk level: a first-principles study. <i>Materials Research Express</i> , 2019, 6, 095102.	1.6	2
227	A computational approach to study the optoelectronic properties of <i>F</i> -BODIPY derivatives at the bulk level for photovoltaic applications. <i>Materials Research Express</i> , 2019, 6, 125110.	1.6	2
228	Electronic band structure and optical characteristic of silver lanthanide XAgSe ₂ (X=Eu and Er) dichalcogenides: Insight from DFT computations. <i>Inorganic Chemistry Communication</i> , 2021, 129, 108586.	3.9	2
229	Synthesis, characterization, and computational study of copper bipyridine complex [Cu(C ₁₈ H ₂₄ N ₂) ₂](NO ₃) ₂ to explore its functional properties. <i>Zeitschrift Fur Naturforschung - Section C Journal of Biosciences</i> , 2022, 77, 241-251.	1.4	2
230	Thermal decomposition of syn- and anti-dihydropyrenes; functional group-dependent decomposition pathway. <i>Journal of Molecular Modeling</i> , 2019, 25, 215.	1.8	1
231	Design of Distributed Bragg Reflectors for Green Light-Emitting Devices Based on Quantum Dots as Emission Layer. <i>Energies</i> , 2022, 15, 1237.	3.1	1
232	Synthesis, spectral characterization, crystal structure and computational investigation of 2-formyl-6-methoxy-3-carbomethoxy quinoline as potential SARS-CoV inhibitor. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 170, 110886.	4.0	1
233	Mechanistic investigation of Mg ²⁺ -ion-induced ZnO nanorods for enhanced photocatalytic performance. <i>Applied Nanoscience (Switzerland)</i> , 2021, 11, 1917-1927.	3.1	0
234	Exploration of optoelectronic, nonlinear and charge transport properties of hydroquinoline derivatives by DFT approach. <i>Materials Science-Poland</i> , 2020, 38, 284-295.	1.0	0

#	ARTICLE	IF	CITATIONS
235	Emerging variants of concern in Saudi Arabian SARS-CoV-2 isolates. Journal of King Abdulaziz University, Islamic Economics, 2021, 42, 1366-1368.	1.1	0
236	Insighting the optoelectronic, charge transfer and biological potential of benzo-thiadiazole and its derivatives. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 2022, .	1.4	0