

# Shabbir Muhammad

## List of Publications by Year in descending order

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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	Insight role of TiO <sub>2</sub> to improve the photocatalytic performance of WO <sub>3</sub> nanostructures for the efficient degradation of ciprofloxacin. <i>Zeitschrift Fur Physikalische Chemie</i> , 2022, 236, 169-180.	2.8	3
2	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
3	Effect of S, Se and Te replacement on structural, optoelectronic and transport properties of SrXO <sub>4</sub> (X= S, Se, Te) for energy applications: A first principles study. <i>Journal of Solid State Chemistry</i> , 2022, 305, 122689.	2.9	4
4	A DFT+U study of the effect of transition metal replacements on optoelectronic and elastic properties of TmCu <sub>3</sub> S <sub>4</sub> (Tm = V, Ta, Nb). <i>Optik</i> , 2022, 250, 168289.	2.9	15
5	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
6	Synthesis, characterization, and computational study of copper bipyridine complex [Cu(C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> ) <sub>2</sub> ] (NO <sub>3</sub> ) <sub>2</sub> to explore its functional properties. <i>Zeitschrift Fur Naturforschung - Section C Journal of Biosciences</i> , 2022, 77, 241-251.	1.4	2
7	Theoretical Approach to Evaluate the Gas-Sensing Performance of Graphene Nanoribbon/Oligothiophene Composites. <i>ACS Omega</i> , 2022, 7, 2260-2274.	3.5	6
8	Insighting the functionally modified C <sub>60</sub> fullerenes as an efficient nonlinear optical materials: A quantum chemical study. <i>Materials Science in Semiconductor Processing</i> , 2022, 141, 106421.	4.0	17
9	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
10	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
11	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
12	Prewetting Induced Hydrophilicity to Augment Photocatalytic Activity of Nanocalcite @ Polyester Fabric. <i>Polymers</i> , 2022, 14, 295.	4.5	4
13	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
14	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
15	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
16	Identification of Halogen-Based Derivatives as Potent Inhibitors of Estrogen Receptor Alpha of Breast Cancer: An In-Silico Investigation. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 181-205.	1.7	6
17	Compositional Adjusting and Antibacterial Improvement of Hydroxyapatite/Nb <sub>2</sub> O <sub>5</sub> /Graphene Oxide for Medical Applications. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2022, 32, 2160-2172.	3.7	10
18	Identification of phytochemical inhibitors of SARS-CoV-2 protease 3CLpro 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

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19	Isolation of Thioinosine and Butenolides from a Terrestrial <i>Actinomycetes</i> sp. GSCW51 and Their <i>In Silico</i> Studies for Potential against SARS-CoV-2. <i>Chemistry and Biodiversity</i> , 2022, 19, .	2.1	3
20	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
21	Synthesis, Characterization, Biological Activity and Molecular Docking Studies of Novel Organotin(IV) Carboxylates. <i>Frontiers in Pharmacology</i> , 2022, 13, 864336.	3.5	17
22	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
23	Proposition of new stable rare-earth ternary semiconductor sulfides of type LaTlS <sub>2</sub> (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
24	In Silico Drug Designing for ala438 Deleted Ribosomal Protein S1 (RpsA) on the Basis of the Active Compound <i>Zrl</i> 15. <i>ACS Omega</i> , 2022, 7, 397-408.	3.5	22
25	TRAVELING WAVE SOLUTIONS TO A MATHEMATICAL MODEL OF FRACTIONAL ORDER (2+1)-DIMENSIONAL BREAKING SOLITON EQUATION. <i>Fractals</i> , 2022, 30, .	3.7	5
26	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
27	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
28	Insighting the optoelectronic, charge transfer and biological potential of benzo-thiadiazole and its derivatives. <i>Zeitschrift Fur Naturforschung - Section C Journal of Biosciences</i> , 2022, .	1.4	0
29	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
30	Insighting the Therapeutic Potential of Fifty (50) Shogaol Derivatives Against M <sup>pro</sup> of SARS-CoV-2. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 555-568.	1.7	4
31	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
32	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
33	Virtual screening of potential inhibitor against breast cancer-causing estrogen receptor alpha (ER $\alpha$ ): molecular docking and dynamic simulations. <i>Molecular Simulation</i> , 2022, 48, 1163-1174.	2.0	5
34	Chalcone Scaffolds Exhibiting Acetylcholinesterase Enzyme Inhibition: Mechanistic and Computational Investigations. <i>Molecules</i> , 2022, 27, 3181.	3.8	7
35	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
36	Adsorption of Industrial Gases (CH <sub>4</sub> , CO <sub>2</sub> , and CO) on Olympicene: A DFT and CCSD(T) Investigation. <i>ACS Omega</i> , 2022, 7, 18852-18860.	3.5	14

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37	Insighting isatin derivatives as potential antiviral agents against NSP3 of COVID-19. <i>Chemical Papers</i> , 2022, 76, 6271-6285.	2.2	6
38	Toward the Noninvasive Diagnosis of Alzheimer's Disease: Molecular Basis for the Specificity of Curcumin for Fibrillar Amyloid- $\beta$ . <i>ACS Omega</i> , 2022, 7, 22032-22038.	3.5	3
39	Benchmark Density Functional Theory Approach for the Calculation of Bond Dissociation Energies of the $\text{O}=\text{O}$ Bond: A Key Step in Water Splitting Reactions. <i>ACS Omega</i> , 2022, 7, 20800-20808.	3.5	9
40	Shedding light on the structural, optoelectronic, and thermoelectric properties of pyrochlore oxides ( $\text{La}_2\text{Q}_2\text{O}_7$ (Q = Ge, Sn)) for energy applications: A first-principles investigation. <i>Journal of Solid State Chemistry</i> , 2022, 313, 123305.	2.9	14
41	Synthesis, spectral characterization, crystal structure and computational investigation of 2-formyl-6-methoxy-3-carbethoxy quinoline as potential SARS-CoV inhibitor. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 170, 110886.	4.0	1
42	Enhanced linear and nonlinear optical response of superhalogen ( $\text{Al}_7$ ) doped graphitic carbon nitride ( $\text{g-C}_3\text{N}_4$ ). <i>Optik</i> , 2021, 226, 165923.	2.9	46
43	Optoelectronic properties of $\text{Nd}^{3+}$ doped $\text{CaTa}_2\text{O}_6$ : Insights from the GGA calculations. <i>Optik</i> , 2021, 225, 165270.	2.9	4
44	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
45	Non-noble metal single-atom catalyst of $\text{Co}_1/\text{MXene}$ ( $\text{Mo}_2\text{CS}_2$ ) for CO oxidation. <i>Science China Materials</i> , 2021, 64, 651-663.	6.3	44
46	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
47	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
48	First-principles study of the electronic structures and optical and photocatalytic performances of van der Waals heterostructures of $\text{SiS}$ , $\text{P}$ and $\text{SiC}$ monolayers. <i>RSC Advances</i> , 2021, 11, 14263-14268.	3.6	14
49	Exploration of $\text{CH}_2\text{F}$ & $\text{CF}_2\text{H}$ mediated supramolecular arrangements into fluorinated terphenyls and theoretical prediction of their third-order nonlinear optical response. <i>RSC Advances</i> , 2021, 11, 7766-7778.	3.6	36
50	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
51	Construction of $\text{Bi}_2\text{WO}_6/\text{MoSe}_2/\text{Bi}_2\text{O}_3/\text{C}_x\text{Br}_2$ heterostructures for the production of hydrogen energy and degradation of methylene blue. <i>Applied Nanoscience (Switzerland)</i> , 2021, 11, 951-959.	3.1	3
52	Role of Nano-Photocatalysts in Detoxification of Toxic Heavy Metals. <i>Current Analytical Chemistry</i> , 2021, 17, 126-137.	1.2	5
53	SARS-CoV-2 Genome from the Khyber Pakhtunkhwa Province of Pakistan. <i>ACS Omega</i> , 2021, 6, 6588-6599.	3.5	6
54	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

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55	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
56	Exploring the new potential antiviral constituents of <i>Moringa oliefera</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
57	DFT study of superhalogen (AlF <sub>4</sub> ) doped boron nitride for tuning their nonlinear optical properties. <i>Optik</i> , 2021, 231, 166464.	2.9	35
58	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
59	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
60	Co <sub>2</sub> 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
61	Mechanistic investigation of Mg <sup>2+</sup> -ion-induced ZnO nanorods for enhanced photocatalytic performance. <i>Applied Nanoscience (Switzerland)</i> , 2021, 11, 1917-1927.	3.1	0
62	Inorganic electrides of alkali metal doped Zn <sub>12</sub> O <sub>12</sub> nanocage with excellent nonlinear optical response. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 106, 107935.	2.4	14
63	Electronic band structure and optical characteristic of silver lanthanide XAgSe <sub>2</sub> (X=Eu and Er) dichalcogenides: Insight from DFT computations. <i>Inorganic Chemistry Communication</i> , 2021, 129, 108586.	3.9	2
64	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
65	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
66	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
67	First-principles calculations to investigate structural, electronic and optical properties of Na based fluoroperovskites NaXF <sub>3</sub> (X= Sr, Zn). <i>Solid State Communications</i> , 2021, 334-335, 114396.	1.9	12
68	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
69	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
70	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
71	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
72	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

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73	Effect of Nb, Ta and V replacements on electronic, optical and elastic properties of NbCu <sub>3</sub> Se <sub>4</sub> : A GGA+U study. <i>Journal of Solid State Chemistry</i> , 2021, 301, 122338.	2.9	18
74	Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties. <i>ACS Omega</i> , 2021, 6, 24602-24613.	3.5	31
75	Study of structural, optoelectronic and magnetic properties of Half-Heusler compounds QEuPa (Q=) Tj ETQq1 1 0.784314 rgBT /Over	2.9	17
76	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
77	Experimental and computational study of naphthalimide derivatives: Synthesis, optical, nonlinear optical and antiviral properties. <i>Optik</i> , 2021, 246, 167748.	2.9	10
78	First example of lanthanum as dopant on Al <sub>12</sub> N <sub>12</sub> and Al <sub>12</sub> P <sub>12</sub> nanocages for improved electronic and nonlinear optical properties with high stability. <i>Materials Science in Semiconductor Processing</i> , 2021, 135, 106122.	4.0	22
79	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
80	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
81	Emerging Mutations in Nsp1 of SARS-CoV-2 and Their Effect on the Structural Stability. <i>Pathogens</i> , 2021, 10, 1285.	2.8	18
82	Fabrication of direct Z-scheme MoO <sub>3</sub> /MoS <sub>2</sub> photocatalyst for synergistically enhanced H <sub>2</sub> production. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 39822-39829.	7.1	17
83	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
84	Designing and Encapsulation of Inorganic Al <sub>12</sub> N <sub>12</sub> 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
85	Demonstrating the Potential of Alkali Metal-Doped Cyclic C <sub>6</sub> O <sub>6</sub> Li <sub>6</sub> Organometallics as Electrides and High-Performance NLO Materials. <i>ACS Omega</i> , 2021, 6, 29852-29861.	3.5	26
86	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
87	Mathematical modeling and optimal control of the COVID-19 dynamics. <i>Results in Physics</i> , 2021, 31, 105028.	4.1	82
88	Emerging variants of concern in Saudi Arabian SARS-CoV-2 isolates. <i>Journal of King Abdulaziz University, Islamic Economics</i> , 2021, 42, 1366-1368.	1.1	0
89	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
90	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

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91	Tuning the Photocatalytic Performance of Tungsten Oxide by Incorporating Cu <sub>3</sub> V <sub>2</sub> O <sub>8</sub> Nanoparticles for H <sub>2</sub> Evolution Under Visible Light Irradiation. <i>Journal of Electrochemical Energy Conversion and Storage</i> , 2020, 17, .	2.1	4
92	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
93	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
94	Hierarchical WO <sub>3</sub> @ BiVO <sub>4</sub> nanostructures for improved green energy production. <i>Applied Nanoscience (Switzerland)</i> , 2020, 10, 1183-1190.	3.1	15
95	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
96	p-type Cu <sub>3</sub> BiS <sub>3</sub> thin films for solar cell absorber layer via one stage thermal evaporation. <i>Applied Surface Science</i> , 2020, 505, 144597.	6.1	28
97	Soft template-based bismuth doped zinc oxide nanocomposites for photocatalytic depolymerization of lignin. <i>Inorganica Chimica Acta</i> , 2020, 502, 119390.	2.4	22
98	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
99	Role of rGO to improve the performance of BiVO <sub>4</sub> nanostructures for efficient removal of heavy metals. <i>Applied Nanoscience (Switzerland)</i> , 2020, 10, 1421-1432.	3.1	7
100	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
101	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
102	Magnetic and electrical properties of Ba <sub>2</sub> Co <sub>2</sub> Fe <sub>12</sub> O <sub>22</sub> /PANI composites prepared by insitu polymerization. <i>Physica B: Condensed Matter</i> , 2020, 597, 412410.	2.7	4
103	i-Propylammonium Lead Chloride Based Perovskite Photocatalysts for Depolymerization of Lignin Under UV Light. <i>Molecules</i> , 2020, 25, 3520.	3.8	12
104	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
105	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
106	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
107	An efficient and eco-friendly synthesis, computational assay and antimicrobial evaluation of some novel diastereoselective monocyclic cis- $\beta$ -lactams. <i>Journal of Molecular Structure</i> , 2020, 1219, 128638.	3.6	6
108	Exploring the potential use of Ca[LiAl <sub>3</sub> N <sub>4</sub> ]:Eu <sup>2+</sup> as phosphor-LED material: Ab-initio calculations. <i>Materials Today Communications</i> , 2020, 25, 101302.	1.9	3



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109	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
110	Visible light responsive photocatalytic hydrogen evolution using MoS <sub>2</sub> incorporated ZnO. <i>Applied Nanoscience (Switzerland)</i> , 2020, 10, 3925-3931.	3.1	18
111	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
112	Synthesis, characterization, Hirshfeld surface analysis and computational studies of 1-methylpiperazine-1,4-dium bis(hydrogen oxalate): [C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> ](HC <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> . <i>Journal of Molecular Structure</i> , 2020, 1211, 128075.	3.6	21
113	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
114	Facile hydrothermal synthesis of highly efficient and visible light-driven Ni-doped V <sub>2</sub> O <sub>5</sub> photocatalyst for degradation of Rhodamine B dye. <i>Journal of Materials Science: Materials in Electronics</i> , 2020, 31, 12913-12925.	2.2	16
115	Zinc-Doped Boron Phosphide Nanocluster as Efficient Sensor for SO <sub>2</sub> . <i>Journal of Chemistry</i> , 2020, 2020, 1-12.	1.9	45
116	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
117	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
118	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
119	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
120	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
121	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
122	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
123	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells. <i>RSC Advances</i> , 2019, 9, 26402-26418.	3.6	115
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