

Mohammad Jane Alam

List of Publications by Year in descending order

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66
papers

1,143
citations

361045

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454577

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docs citations

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times ranked

1166
citing authors

#	ARTICLE	IF	CITATIONS
1	Photon harvesting and light trapping in pentacene and PTCDI-C13H27 for organic solar cell application. <i>Optik</i> , 2022, 258, 168931.	1.4	1
2	Tunable luminescence in Ce ³⁺ / Mn ²⁺ co-doped ZrO ₂ nanophosphor integrated with theoretical studies on possible (ZrO ₂) _n clusters using DFT method. <i>Journal of Alloys and Compounds</i> , 2021, 853, 157378.	2.8	4
3	Fabrication of a new 2D Co(II)-organic framework tuned by semi-flexible dicarboxylate and 1,4-bis(4-pyridinylmethyl)piperazine ligands: Topology, DFT/UB3LYP calculations, Hirshfeld surface analysis and magnetic studies. <i>Journal of Molecular Structure</i> , 2021, 1229, 129616.	1.8	4
4	Potential Third-Order Nonlinear Optical Response Facilitated by Intramolecular Charge Transfer in a Simple Schiff Base Molecule: Experimental and Theoretical Exploration. <i>ACS Omega</i> , 2021, 6, 6185-6194.	1.6	31
5	FTIR and FT-Raman spectra of 6-(dimethylamino)purine and its theoretical studies of anharmonic vibrational analysis using quantum chemical calculations. <i>Vibrational Spectroscopy</i> , 2021, 113, 103224.	1.2	5
6	Experimental and computational investigation of novel dihydrated organic single crystal of 2,4,6-triaminopyrimidine and 3,5-dinitrobenzoic acid: Linear and nonlinear optical response with limiting performance. <i>Journal of Solid State Chemistry</i> , 2021, 300, 122255.	1.4	22
7	Electron scattering from molecules relevant to Titan's atmosphere. <i>International Journal of Mass Spectrometry</i> , 2021, 470, 116708.	0.7	5
8	A Proton Transfer Complex Containing 5-Hydroxyisophthalic Acid with 3,3'-bis(4-dimethylpiperazine) Tetraethylammonium Bromide. <i>Journal of ChemistrySelect</i> , 2021, 6, 10201-10207.	0.7	10
9	Z-scan screening of proton-shifted monohydrated organic salt: the linear, nonlinear, and optical limiting characteristics for photonic applications. <i>Journal of Materials Science: Materials in Electronics</i> , 2021, 32, 28750-28764.	1.1	16
10	Impact of annealing on the structural and optical properties of ZnO nanoparticles and tracing the formation of clusters via DFT calculation. <i>Arabian Journal of Chemistry</i> , 2020, 13, 2207-2218.	2.3	48
11	Biosynthesis of silver nanoparticles and its application against phytopathogenic bacterium and fungus. <i>International Journal of Environmental Analytical Chemistry</i> , 2020, 100, 1390-1401.	1.8	17
12	Experimental thermophysical properties and DFT calculations of imidazolium ionic liquids and 2-butanol mixtures. <i>Fluid Phase Equilibria</i> , 2020, 508, 112447.	1.4	9
13	Curcumin induced photodynamic therapy mediated suppression of quorum sensing pathway of <i>Pseudomonas aeruginosa</i> : An approach to inhibit biofilm in vitro. <i>Photodiagnosis and Photodynamic Therapy</i> , 2020, 30, 101645.	1.3	50
14	3 ² -Acetoxy cholest-5-ene crystals: Catalytic synthesis, structural elucidation, contribution of intermolecular interactions and density functional theory calculations. <i>Journal of Molecular Structure</i> , 2020, 1221, 128833.	1.8	0
15	Synthesis, characterization and DFT studies of water stable Cd(II) metal-organic clusters with better adsorption property towards the organic pollutant in waste water. <i>Inorganica Chimica Acta</i> , 2020, 512, 119872.	1.2	23
16	Exploring charge transfer dynamics and photocatalytic behavior of designed donor-acceptor complex: Characterization, spectrophotometric and theoretical studies (DFT/TD-DFT). <i>Journal of Molecular Liquids</i> , 2020, 310, 113213.	2.3	34
17	Crystal structure investigation and natural charge analysis of monohydrated salt of 2,3-pyrazinedicarboxylic acid and 2-amino-5-bromo-6-methyl-4-pyrimidinol. <i>AIP Conference Proceedings</i> , 2020, . .	0.3	0
18	Cocrystallization of 2,3-dimethylquinoxaline with 3,5-dinitrobenzoic acid: Crystal structure, Hirshfeld surface, spectroscopic features and DFT studies. <i>Journal of Molecular Structure</i> , 2019, 1198, 126894.	1.8	16

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19	Structure, vibrational and electronic spectral studies of the SA ²⁻ .AHMP ⁺ crystal: A combined PXRD, FT-Raman, UV-Vis and DFT calculations. AIP Conference Proceedings, 2019, , .	0.3	1
20	Structural investigation of cocrystal, salt and monohydrated salt of chloranilic acid with different donors: A theoretical study. AIP Conference Proceedings, 2019, , .	0.3	1
21	Spectrophotometric and photocatalytic studies of H-bonded charge transfer complex of oxalic acid with imidazole: single crystal XRD, experimental and DFT/TD-DFT studies. New Journal of Chemistry, 2019, 43, 9039-9051.	1.4	36
22	Spectroscopic (FTIR, FT-Raman, ¹ H NMR and UV-Vis) and DFT/TD-DFT studies on cholesteno [4,6-b,c]-2,5-dihydro-1,5-benzothiazepine. Journal of Molecular Structure, 2019, 1178, 570-582.	1.8	48
23	Synthesis, structural investigations and pharmacological properties of a new zinc complex with a N4-donor Schiff base incorporating 2-pyridyl ring. Inorganica Chimica Acta, 2019, 487, 97-106.	1.2	12
24	Structural, vibrational and electronic absorption characteristics of the monohydrate organic salt of 2-amino-5-bromo-6-methyl-4-pyrimidinol and 2,3-pyrazinedicarboxylic acid: A combined experimental and computational study. Journal of Molecular Structure, 2019, 1177, 229-241.	1.8	25
25	Synthesis and characterization of Y ₂ O ₃ nano-material: An experimental and theoretical study. AIP Conference Proceedings, 2018, , .	0.3	3
26	DFT/TD-DFT calculations, spectroscopic characterizations (FTIR, NMR, UV-vis), molecular docking and enzyme inhibition study of 7-benzoyloxycoumarin. Computational Biology and Chemistry, 2018, 73, 65-78.	1.1	21
27	Electron-induced scattering dynamics of Boron, Aluminium and Gallium trihalides in the intermediate energy domain. Molecular Physics, 2018, 116, 1208-1217.	0.8	2
28	Anharmonic vibrational spectra and mode-mode couplings analysis of 2-aminopyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 188, 26-31.	2.0	9
29	Synthesis, spectroscopic, computational (DFT/B3LYP), AChE inhibition and antioxidant studies of imidazole derivative. Journal of Molecular Structure, 2018, 1151, 327-342.	1.8	38
30	Growth, structure, Hirshfeld surface and spectroscopic properties of 2-amino-4-hydroxy-6-methylpyrimidinium-2,3-pyrazinedicarboxylate single crystal. Journal of Molecular Structure, 2018, 1155, 695-710.	1.8	17
31	Synthesis, spectroscopic characterization, X-ray structure, DFT calculations, and antimicrobial studies of diorganotin (IV) complexes of monotopic oxygen nitrogen donor Schiff base. Chemical Papers, 2018, 72, 903-919.	1.0	11
32	Theoretical studies of charge transfer and proton transfer complex formation between 3,5-dinitrobenzoic acid and 1,2-dimethylimidazole. AIP Conference Proceedings, 2018, , .	0.3	3
33	Anharmonic vibrational spectroscopy, NBO charges and global chemical reactivity studies on the charge transfer PDCA ²⁻ .AHMP ⁺ single crystal using DFT calculations. AIP Conference Proceedings, 2018, , .	0.3	2
34	Nature and potency interactions of the hydrogen bond through the NBO analysis for charge transfer complex between 2-amino-4-hydroxy-6-methylpyrimidine and 2,3-pyrazinedicarboxylic acid. AIP Conference Proceedings, 2018, , .	0.3	2
35	Theoretical insights of proton transfer and hydrogen bonded charge transfer complex of 1,2-dimethylimidazolium-3,5-dinitrobenzoate crystal. AIP Conference Proceedings, 2018, , .	0.3	2
36	Experimental vibrational spectroscopy (FTIR and FT-Raman) of D-tryptophan and its anharmonic theoretical studies using density functional theory. Journal of Molecular Structure, 2018, 1171, 315-322.	1.8	14

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37	Synthesis, structural, hirshfeld surface, spectroscopic studies and quantum chemical calculation of the proton transfer complex between 2-amino-4-hydroxy-6-methylpyrimidine and salicylic acid. Journal of Molecular Structure, 2018, 1171, 438-448.	1.8	36
38	Electron impact total ionization cross section for C4 and C5 isomeric alcohols. International Journal of Mass Spectrometry, 2018, 431, 37-42.	0.7	8
39	Experimental and theoretical characterization of organic salt: 2-((4-bromophenyl)amino) pyrido[1,2-a] quinoxalin-11-ium bromide monohydrate synthesized via oxidative cyclization. Journal of Molecular Structure, 2018, 1156, 457-464.	1.8	20
40	Detailed molecular, structural and spectral studies of bimetallic salt, [Ni(L)][CoCl ₄] where L=3,7-bis(2-aminoethyl)-1,3,5,7-tetraazabicyclo(3.3.1)nonane. Journal of Molecular Structure, 2017, 1138, 90-101.	1.8	6
41	The novel iminium surfactant p-benzylidene benzyl dodecyl iminium chloride as a corrosion inhibitor for plain carbon steel in 1 M HCl: electrochemical and DFT evaluation. RSC Advances, 2017, 7, 23182-23196.	1.7	39
42	DFT/B3LYP calculations, in vitro cytotoxicity and antioxidant activities of steroidal pyrimidines and their interaction with HSA using molecular docking and multispectroscopic techniques. Bioorganic Chemistry, 2017, 73, 83-99.	2.0	50
43	Anharmonic vibrational spectral analysis of L(-)-xylose molecule. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750059.	1.8	1
44	Anharmonic vibrational and electronic spectral study of 2-amino-4-hydroxy-6-methylpyrimidine: A combined experimental (FTIR, FT-Raman, UV-Vis) and theoretical (DFT, MP2) approach. Journal of Molecular Structure, 2017, 1148, 89-100.	1.8	16
45	Study of molecular structure, anharmonic vibrational dynamic and electronic properties of sulindac using spectroscopic techniques integrated with quantum chemical calculations. Journal of Molecular Structure, 2017, 1147, 603-615.	1.8	11
46	Quantum chemical and spectroscopic investigations of 4-Hydroxy-7-methyl-1,8-naphthyridine-3-carboxylic acid. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650042.	1.8	3
47	DFT and TD-DFT computation of charge transfer complex between o-phenylenediamine and 3,5-dinitrosalicylic acid. AIP Conference Proceedings, 2016, , .	0.3	12
48	Electron impact ionisation cross section for organoplatinum compounds. Molecular Physics, 2016, 114, 3104-3111.	0.8	6
49	Vibrational and electronic spectral analysis of 2,3-pyrazinedicarboxylic acid: A combined experimental and theoretical study. Spectroscopy Letters, 2016, 49, 449-457.	0.5	9
50	FTIR, FT-Raman and UV-Vis spectral studies of d-tyrosine molecule. Journal of Molecular Structure, 2016, 1105, 169-177.	1.8	15
51	Synthesis, X-ray crystallography, spectroscopic (FT-IR, ¹ H & ¹³ C NMR and UV), computational (DFT/B3LYP) and enzymes inhibitory studies of 7-hydroximincholest-5-en-3-ol acetate. Journal of Molecular Structure, 2016, 1116, 317-332.	1.8	17
52	Molecular structure and vibrational analysis of 5-nitro-6-methyluracil molecule based on monomer, dimer and trimer calculations. Indian Journal of Physics, 2016, 90, 503-518.	0.9	4
53	Computational and anti-tumor studies of 7a-Aza-B-homostigmast-5-eno [7a, 7-d] tetrazole-3-yl chloride. Journal of Molecular Structure, 2016, 1108, 411-426.	1.8	21
54	Structural elucidation, density functional calculations and contribution of intermolecular interactions in cholest-4-en-3-one crystals: Insights from X-ray and Hirshfeld surface analysis. Journal of Molecular Structure, 2015, 1084, 274-283.	1.8	23

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55	Quantum chemical calculations and analysis of FTIR, FT-Raman and UV-Vis spectra of temozolomide molecule. <i>Journal of Molecular Structure</i> , 2015, 1099, 453-462.	1.8	22
56	DFT, Hirshfeld surfaces, spectral and <i>in vivo</i> cytotoxic studies of 7a-Aza-B-homostigmast-5-eno [7a,7-d] tetrazole. <i>Journal of Molecular Structure</i> , 2015, 1099, 588-600.	1.8	20
57	Thermal analysis and temperature dependent dielectric responses of Co doped anatase TiO ₂ nanoparticles. <i>AIP Conference Proceedings</i> , 2015, , .	0.3	6
58	FT-IR and FT-Raman spectra, MEP and HOMO-LUMO of 2,5-dichlorobenzonitrile: DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 464-472.	2.0	29
59	FTIR, FT-Raman, UV-Visible spectra and quantum chemical calculations of allantoin molecule and its hydrogen bonded dimers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 961-978.	2.0	49
60	Molecular structure, anharmonic vibrational analysis and electronic spectra of o-, m-, p-iodonitrobenzene using DFT calculations. <i>Journal of Molecular Structure</i> , 2014, 1059, 239-254.	1.8	39
61	Quantum chemical and spectroscopic investigations of 3-methyladenine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 653-664.	2.0	39
62	Anharmonic vibrational studies of l-aspartic acid using HF and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 992-1004.	2.0	54
63	Computational studies of vibrational spectra and molecular properties of 6-methyluracil using HF, DFT and MP2 methods. <i>Indian Journal of Physics</i> , 2011, 85, 239-260.	0.9	24
64	Anharmonic vibrational spectroscopy and investigation of intramolecular mode couplings in adenine. <i>Vibrational Spectroscopy</i> , 2011, 56, 51-59.	1.2	12
65	Anharmonic vibrational analysis of uracil by ab initio Hartree-Fock and density functional theory calculations. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 18-20.	1.5	9
66	Computational and Vibrational Spectroscopy Study of 5-Nitro-6-Methyluracil by Density Functional Theory. , 2008, , .		1