Mohammad Jane Alam

List of Publications by Year
in descending order

66	1,143	361045	454577
papers	citations	20 h-index	30 g-index

66	66	66	1166
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Anharmonic vibrational studies of l-aspartic acid using HF and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 992-1004.	2.0	54
2	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
3	Curcumin induced photodynamic therapy mediated suppression of quorum sensing pathway of Pseudomonas aeruginosa: An approach to inhibit biofilm in vitro. Photodiagnosis and Photodynamic Therapy, 2020, 30, 101645.	1.3	50
4	FTIR, FT-Raman, UVâ€“Visible spectra and quantum chemical calculations of allantoin molecule and its hydrogen bonded dimers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 961-978.	2.0	49
5	Spectroscopic (FTIR, FT-Raman, 1H NMR and UVâ€“Vis) and DFT/TD-DFT studies on cholesteno [4,6-b,c]-2â€²,5â€²-dihydro-1â€²,5â€²-benzothiazepine. Journal of Molecular Structure, 2019, 1178, 570-582.	1.8	48
6	Impact of annealing on the structural and optical properties of ZnO nanoparticles and tracing the formation of clusters via DFT calculation. Arabian Journal of Chemistry, 2020, 13, 2207-2218.	2.3	48
7	Molecular structure, anharmonic vibrational analysis and electronic spectra of o-, m-, p-iodonitrobenzene using DFT calculations. Journal of Molecular Structure, 2014, 1059, 239-254.	1.8	39
8	Quantum chemical and spectroscopic investigations of 3-methyladenine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 653-664.	2.0	39
9	The novel iminium surfactant p-benzylidene benzyldodecyl 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
10	Synthesis, spectroscopic, computational (DFT/B3LYP), AChE inhibition and antioxidant studies of imidazole derivative. Journal of Molecular Structure, 2018, 1151, 327-342.	1.8	38
11	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
12	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
13	Exploring charge transfer dynamics and photocatalytic behavior of designed donor-acceptor complex: Characterization, spectrophotometric and theoretical studies (DFT/TD-DFT). Journal of Molecular Liquids, 2020, 310, 113213.	2.3	34
14	Potential Third-Order Nonlinear Optical Response Facilitated by Intramolecular Charge Transfer in a Simple Schiff Base Molecule: Experimental and Theoretical Exploration. ACS Omega, 2021, 6, 6185-6194.	1.6	31
15	FT-IR and FT-Raman spectra, MEP and HOMOâ€“LUMO of 2,5-dichlorobenzonitrile: DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 464-472.	2.0	29
16	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
17	Computational studies of vibrational spectra and molecular properties of 6-methyluracil using HF, DFT and MP2 methods. Indian Journal of Physics, 2011, 85, 239-260.	0.9	24
18	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

#	Article	IF	Citations
19	Synthesis, characterization and DFT studies of water stable Cd(II) metalâ€“organic clusters with better adsorption property towards the organic pollutant in waste water. Inorganica Chimica Acta, 2020, 512, 119872.	1.2	23
20	Quantum chemical calculations and analysis of FTIR, FTâ€“Raman and UVâ€“Vis spectra of temozolomide molecule. Journal of Molecular Structure, 2015, 1099, 453-462.	1.8	22
21	Experimental and computational investigation of novel dihydrated organic single crystal of 2,4,6-triaminopyrimidine and 3,5-dintrobenzoic acid: Linear and nonlinear optical response with limiting performance. Journal of Solid State Chemistry, 2021, 300, 122255.	1.4	22
22	Computational and anti-tumor studies of 7a-Aza-B-homostigmast-5-eno [7a, 7-d] tetrazole-3Î²-yl chloride. Journal of Molecular Structure, 2016, 1108, 411-426.	1.8	21
23	DFT/TD-DFT calculations, spectroscopic characterizations (FTIR, NMR, UVâ€“vis), molecular docking and enzyme inhibition study of 7-benzoyloxycoumarin. Computational Biology and Chemistry, 2018, 73, 65-78.	1.1	21
24	DFT, Hirshfeld surfaces, spectral and inÂvivo cytotoxic studies of 7a-Aza-B-homostigmast-5-eno [7a,7-d] tetrazole. Journal of Molecular Structure, 2015, 1099, 588-600.	1.8	20
25	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
26	Synthesis, X-ray crystallography, spectroscopic (FT-IR, 1H &13C NMR and UV), computational (DFT/B3LYP) and enzymes inhibitory studies of 7-hydroximinocholest-5-en-3-ol acetate. Journal of Molecular Structure, 2016, 1116, 317-332.	1.8	17
27	Growth, structure, Hirshfeld surface and spectroscopic properties of 2-amino-4-hydroxy-6-methylpyrimidinium-2,3-pyrazinedicorboxylate single crystal. Journal of Molecular Structure, 2018, 1155, 695-710.	1.8	17
28	Biosynthesis of silver nanoparticles and its application against phytopathogenic bacterium and fungus. International Journal of Environmental Analytical Chemistry, 2020, 100, 1390-1401.	1.8	17
29	Anharmonic vibrational and electronic spectral study of 2-amino-4-hydroxy-6â€“methylpyrimidine: A combined experimental (FTIR, FT-Raman, UVâ€“Vis) and theoretical (DFT, MP2) approach. Journal of Molecular Structure, 2017, 1148, 89-100.	1.8	16
30	Cocrystallization of 2,3-dimethylquinoxaline with 3,5-dinitrobenzoic acid: Crystal structure, Hirshfeld surface, spectroscopic features and DFT studies. Journal of Molecular Structure, 2019, 1198, 126894.	1.8	16
31	Z-scan screening of proton-shifted monohydrated organic salt: the linear, nonlinear, and optical limiting characteristics for photonic applications. Journal of Materials Science: Materials in Electronics, 2021, 32, 28750-28764.	1.1	16
32	FTIR, FT-Raman and UVâ€“Vis spectral studies of d-tyrosine molecule. Journal of Molecular Structure, 2016, 1105, 169-177.	1.8	15
33	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
34	Anharmonic vibrational spectroscopy and investigation of intramolecular mode couplings in adenine. Vibrational Spectroscopy, 2011, 56, 51-59.	1.2	12
35	DFT and TD-DFT computation of charge transfer complex between o-phenylenediamine and 3,5-dinitrosalicylic acid. AIP Conference Proceedings, 2016, , .	0.3	12
36	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

#	Article	IF	Citations
37	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
38	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
39	A Protonâ€Transfer Complex Containing 5â€Hydroxyâ€isophthalic Acid with 3,3â€²â€(Piperazineâ€1,4â€diylbis) Tj ETQq1 1 0.78431 ChemistrySelect, 2021, 6, 10201-10207.	0.7	10
40	Anharmonic vibrational analysis of uracil by ab initio Hartreeâ€“Fock and density functional theory calculations. Computational and Theoretical Chemistry, 2009, 895, 18-20.	1.5	9
41	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
42	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
43	Experimental thermophysical properties and DFT calculations of imidazolium ionic liquids and 2-butanol mixtures. Fluid Phase Equilibria, 2020, 508, 112447.	1.4	9
44	Electron impact total ionization cross section for C4 and C5 isomeric alcohols. International Journal of Mass Spectrometry, 2018, 431, 37-42.	0.7	8
45	Thermal analysis and temperature dependent dielectric responses of Co doped anatase TiO2 nanoparticles. AIP Conference Proceedings, 2015, , .	0.3	6
46	Electron impact ionisation cross section for organoplatinum compounds. Molecular Physics, 2016, 114, 3104-3111.	0.8	6
47	Detailed molecular, structural and spectral studies of bimetallic salt, [Ni(L)][CoCl 4] where LÂ=Â3,7- bis (2-aminoethyl)-1,3,5,7-tetraazabicyclo(3.3.1)nonane. Journal of Molecular Structure, 2017, 1138, 90-101.	1.8	6
48	FTIR and FT-Raman spectra of 6-(dimethylamino)purine and its theoretical studies of anharmonic vibrational analysis using quantum chemical calculations. Vibrational Spectroscopy, 2021, 113, 103224.	1.2	5
49	Electron scattering from molecules relevant to Titan's atmosphere. International Journal of Mass Spectrometry, 2021, 470, 116708.	0.7	5
50	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
51	Tunable luminescence in Ce3+/ Mn2+ co-doped ZrO2 nanophosphor integrated with theoretical studies on possible (ZrO2)n clusters using DFT method. Journal of Alloys and Compounds, 2021, 853, 157378.	2.8	4
52	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. Journal of Molecular Structure, 2021, 1229, 129616.	1.8	4
53	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
54	Synthesis and characterization of Y2O3 nano-material: An experimental and theoretical study. AIP Conference Proceedings, 2018, , .	0.3	3

#	Article	IF	Citations
55	Theoretical studies of charge transfer and proton transfer complex formation between 3,5-dinitrobenzic acid and 1,2-dimethylimidazole. AIP Conference Proceedings, 2018, , .	0.3	3
56	Electron-induced scattering dynamics of Boron, Aluminium and Gallium trihalides in the intermediate energy domain. Molecular Physics, 2018, 116, 1208-1217.	0.8	2
57	Anharmonic vibrational spectroscopy, NBO charges and global chemical reactivity studies on the charge transfer PDCAâ˜.AHMP+ single crystal using DFT calculations. AIP Conference Proceedings, 2018, , .	0.3	2
58	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
59	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
60	Computational and Vibrational Spectroscopy Study of 5-Nitro-6-Methyluracil by Density Functional Theory. , 2008, , .		1
61	Anharmonic vibrational spectral analysis of L-(-)-xylose molecule. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750059.	1.8	1
62	Structure, vibrational and electronic spectral studies of the SAâ˜.AHMP+ crystal: A combined PXRD, FT-Raman, UV-Vis and DFT calculations. AIP Conference Proceedings, 2019, , .	0.3	1
63	Structural investigation of cocrystal, salt and monohydrated salt of chloranilic acid with different donors: A theoretical study. AIP Conference Proceedings, 2019, , .	0.3	1
64	Photon harvesting and light trapping in pentacene and PTCDI-C13H27 for organic solar cell application. Optik, 2022, 258, 168931.	1.4	1
65	3Î²-Acetoxy cholest-5-ene crystals: Catalytic synthesis, structural elucidation, contribution of intermolecular interactions and density functional theory calculations. Journal of Molecular Structure, 2020, 1221, 128833.	1.8	0
66	Crystal structure investigation and natural charge analysis of monohydrated salt of 2,3-pyrazinedicarboxylic acid and 2-amino-5-bromo-6-methyl-4-pyrimidinol. AIP Conference Proceedings, 2020, , .	0.3	0