Thayalaraj Christopher Jeyakumar

List of Publications by Year
in descending order

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18	172	1040056 9	1125743 13
papers	citations	h-index	g-index

19	19	19	63
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Isolation and biological evaluation 7-hydroxy flavone fromAvicennia officinalisL: insights from extensiveinÂvitro, DFT, molecular docking and molecular dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2848-2860.	3.5	5
2	Water soluble Cu(II) and Zn(II) complexes of bidentate-morpholine based ligand: synthesis, spectral, DFT calculation, biological activities and molecular docking studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1074-1083.	3.5	19
3	Computational studies of adsorption of dinitrogen over the group 8 metal-borazine complexes. Chemical Papers, 2022, 76, 1539-1552.	2.2	0
4	Group 13 monohalides [AX (AÂ=ÂB, Al, Ga and In; XÂ=ÂHalogens)] as alternative ligands for carbonyl in organometallics: Electronic structure and bonding analysis. Computational and Theoretical Chemistry, 2022, 1209, 113587.	2.5	17
5	Experimental and theoretical studies of novel Schiff base based on diammino benzophenone with formyl chromone â€“ BPAMC. Journal of Molecular Structure, 2022, 1265, 133450.	3.6	7
6	Indolyl-4H-chromenes: Multicomponent one-pot green synthesis, in vitro and in silico, anticancer and antioxidant studies. Journal of Molecular Structure, 2022, 1266, 133464.	3.6	15
7	Vanillin based colorimetric and fluorometric chemosensor for detection of Cu(II) ion: DFT calculation, DNA / BSA interaction and molecular docking studies. Inorganic Chemistry Communication, 2022, 143, 109716.	3.9	13
8	Coordination of indium monohalide with group-10 metal carbonyls [TM(CO)3(InX)]: a DFT study. Chemical Papers, 2021, 75, 311-324.	2.2	13
9	Theoretical studies of group 10 metal gallylene complexes [TM(CO)3(GaX)]. Computational and Theoretical Chemistry, 2021, 1197, 113139.	2.5	13
10	Synthesis, characterization, DFT calculation, biological and molecular docking of Cu(II) complex of pyrimidine derived Schiff base ligand. Journal of Saudi Chemical Society, 2021, 25, 101225.	5.2	16
11	Chemistry of group-10 metals monohaloalumylene complexes [TM(CO)3AlX]: a DFT study. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	10
12	Construction of frustrated Lewis pair from nitride and phosphine for the activation and cleavage of molecular hydrogen. Applied Organometallic Chemistry, 2020, 34, e5811.	3.5	0
13	A DFT study on structural and bonding analysis of transition-metal carbonyls with terminal haloborylene ligands [M(CO)3(BX)] (MÂ=ÂNi, Pd, and Pt; XÂ=ÂF, Cl, Br, and I). Computational and Theoretical Chemistry, 2020, 1177, 112750.	2.5	15
14	Dehydrogenation of formic acid catalysed by M-embedded nitrogen-doped graphene (M = Fe, Ru, Os): a DFT study. New Journal of Chemistry, 2019, 43, 1440-1448.	2.8	15
15	Possibility of reducing the coordinated dinitrogen into ammonia and hydrazine using [Ru-L] (L =) Tj ETQq1 1 0.784314 rgBT /Overlock	1.5	10
16	Application of Density Functional Theory in Coordination Chemistry: A Case Study of Group 13 Monohalide as a Ligand. , 0, , .		0
17	Molybdenum bound nitrogenâ€doped graphene catalyst for reduction of N ₂ to NH ₃ and NH ₂ NH ₂ , using FLP as a coâ€catalyst: A DFT study. Applied Organometallic Chemistry, 0, , .	3.5	3
18	â€œMicellar catalysis on the electron transfer reactions of iron(III)-polypyridyl complexes with sulfur-containing amino acidsâ€• Chemical Papers, 0, , 1.	2.2	0