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	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
2	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
3	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
4	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
5	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
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	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
8	Theoretical studies of group 10 metal gallylene complexes [TM(CO)3(GaX)]. Computational and Theoretical Chemistry, 2021, 1197, 113139.	2.5	13
9	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
10	Possibility of reducing the coordinated dinitrogen into ammonia and hydrazine using [Ru-L] (L =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 3	1.5	10
11	Chemistry of group-10 metals monohaloalumylene complexes [TM(CO)3AlX]: a DFT study. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	10
12	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
13	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
14	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
15	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
16	Application of Density Functional Theory in Coordination Chemistry: A Case Study of Group 13 Monohalide as a Ligand. , 0, , .		0
17	Computational studies of adsorption of dinitrogen over the group 8 metal-borazine complexes. Chemical Papers, 2022, 76, 1539-1552.	2.2	0
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