Prashant Kumar

List of Publications by Year
in descending order

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22	365	840776 11	794594 19
papers	citations	h-index	g-index

33	33	33	420
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Combining Molecular Dynamic Information and an Aspherical-Atom Data Bank in the Evaluation of the Electrostatic Interaction Energy in Multimeric Protein-Ligand Complex: A Case Study for HIV-1 Protease. Molecules, 2021, 26, 3872.	3.8	6
2	TAAM: a reliable and user friendly tool for hydrogen-atom location using routine X-ray diffraction data. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 296-306.	1.1	22
3	Intermolecular Interactions in Ionic Crystals of Nucleobase Chloridesâ€"Combining Topological Analysis of Electron Densities with Energies of Electrostatic Interactions. Crystals, 2019, 9, 668.	2.2	11
4	Extension of the transferable aspherical pseudoatom data bank for the comparison of molecular electrostatic potentials in structureâ€"activity studies. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 398-408.	0.1	25
5	Phytochemicals As Uropathognic Escherichia Coli FimH Antagonist: In Vitro And In Silico Approach. Current Molecular Medicine, 2019, 18, 640-653.	1.3	10
6	A tetranuclear CuII2DyIII2 coordination cluster as a Suzuki (Câ€"C) coupling reaction promoter. Dalton Transactions, 2018, 47, 17202-17205.	3.3	14
7	Universal Method for Electrostatic Interaction Energies Estimation with Charge Penetration and Easily Attainable Point Charges. Journal of Chemical Theory and Computation, 2018, 14, 6336-6345.	5.3	10
8	Catalytic and conductivity studies in two dimensional coordination polymers built with a thiazole based ligand. Polyhedron, 2018, 150, 21-27.	2.2	5
9	Protonated nucleobases are not fully ionized in their chloride salt crystals and form metastable base pairs further stabilized by the surrounding anions. IUCrJ, 2018, 5, 449-469.	2.2	9
10	New models of electron density for electrostatic interaction energy estimation. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e302-e302.	0.1	0
11	3d/4f Coordination Clusters as Cooperative Catalysts for Highly Diastereoselective Michael Addition Reactions. Inorganic Chemistry, 2017, 56, 9563-9573.	4.0	43
12	Interplay of point multipole moments and charge penetration for intermolecular electrostatic interaction energies from the University at Buffalo pseudoatom databank model of electron density. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 598-609.	1.1	9
13	Experimental charge densities of nucleobase chlorides from intermolecular interaction perspective. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1439-C1439.	0.1	0
14	Highly Efficient Tetranuclear ZnII2LnIII2 Catalysts for the Friedelâ€"Crafts Alkylation of Indoles and Nitrostyrenes. Catalysts, 2016, 6, 140.	3.5	15
15	Efficient Ni^{II}₂Ln^{III}₂ Electrocyclization Catalysts for the Synthesis of trans-4,5-Diaminocyclopent-2-enones from 2-Furaldehyde and Primary or Secondary Amines. Inorganic Chemistry, 2016, 55, 6988-6994.	4.0	55
16	Phosphine-free chiral iridium catalysts for asymmetric catalytic hydrogenation of simple ketones. RSC Advances, 2016, 6, 39335-39342.	3.6	4
17	Structural and Dynamical Aspects of Electrostatic Interactions by Applying Aspherical Atom Model in HIV-1 Protease. Biophysical Journal, 2016, 110, 380a.	0.5	6
18	Tetranuclear Zn/4f coordination clusters as highly efficient catalysts for Friedelâ€"Crafts alkylation. Chemical Communications, 2016, 52, 7866-7869.	4.1	59

#	Article	IF	Citations
19	Tetranuclear Zn₂Ln₂ coordination clusters as catalysts in the Petasis borono-Mannich multicomponent reaction. RSC Advances, 2016, 6, 79180-79184.	3.6	21
20	A Universal and Straightforward Approach to Include Penetration Effects in Electrostatic Interaction Energy Estimation. ChemPhysChem, 2016, 17, 2455-2460.	2.1	15
21	A Comparative Study of Transferable Aspherical Pseudoatom Databank and Classical Force Fields for Predicting Electrostatic Interactions in Molecular Dimers. Journal of Chemical Theory and Computation, 2014, 10, 1652-1664.	5.3	25
22	A comparative study of transferable theoretical aspherical pseudoatom data bank and classical force field in predicting the electrostatic interaction in molecular dimers. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, s547-s548.	0.3	0