

Dipak Panthi

List of Publications by Year in descending order

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Version: 2024-02-01

12
papers

79
citations

1478280

6
h-index

1474057

9
g-index

13
all docs

13
docs citations

13
times ranked

90
citing authors

#	ARTICLE	IF	CITATIONS
1	Ground-state actinide chemistry with scalar-relativistic multiconfiguration pair-density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 134102.	1.2	12
2	Copper-Oxo Active Sites for Methane C-H Activation in Zeolites: Molecular Understanding of Impact of Methane Hydroxylation on UV-Vis Spectra. <i>Inorganic Chemistry</i> , 2021, 60, 8489-8499.	1.9	11
3	Time-Dependent Density Functional Theory Study of Copper(II) Oxo Active Sites for Methane-to-Methanol Conversion in Zeolites. <i>Inorganic Chemistry</i> , 2021, 60, 1149-1159.	1.9	10
4	Performance of density functional theory for describing heterometallic active site motifs for methane-to-methanol conversion in metal-exchanged zeolites. <i>Journal of Computational Chemistry</i> , 2018, 39, 2667-2678.	1.5	8
5	Nitrogen Reduction by Multimetallic <i>trans</i> -Uranium Actinide Complexes: A Theoretical Comparison of Np and Pu to U. <i>Inorganic Chemistry</i> , 2019, 58, 6731-6741.	1.9	7
6	2D-IR studies of cyanamides (NCN) as spectroscopic reporters of dynamics in biomolecules: Uncovering the origin of mysterious peaks. <i>Journal of Chemical Physics</i> , 2020, 152, 074201.	1.2	7
7	Methane Over-Oxidation by Extra-Framework Copper-Oxo Active Sites of Copper-Exchanged Zeolites: Crucial Role of Traps for the Separated Methyl Group. <i>ChemPhysChem</i> , 2021, 22, 1101-1109.	1.0	7
8	Copper-Oxo Active Sites in the 8MR of Zeolite Mordenite: DFT Investigation of the Impact of Acid Sites on Methanol Yield and Selectivity. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6684-6693.	1.5	5
9	Methane C-H Activation by [Cu ₂ O] ²⁺ and [Cu ₃ O ₃] ²⁺ in Copper-Exchanged Zeolites: Computational Analysis of Redox Chemistry and X-ray Absorption Spectroscopy. <i>Inorganic Chemistry</i> , 2021, 60, 6218-6227.	1.9	5
10	Heterometallic [Cu-O-M] ²⁺ active sites for methane C-H activation in zeolites: stability, reactivity, formation mechanism and relationship to other active sites. <i>Catalysis Science and Technology</i> , 2021, 11, 5671-5683.	2.1	3
11	Activating Water and Hydrogen by Ligand-Modified Uranium and Neptunium Complexes: A Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2020, 59, 3102-3109.	1.9	2
12	DFT Analysis of Methane C-H Activation and Over-Oxidation by [Cu ₂ O] ²⁺ and [Cu ₂ O ₂] ²⁺ Sites in Zeolite Mordenite: Intra-versus Inter-site Over-Oxidation. <i>ChemPhysChem</i> , 2021, 22, 2517-2525.	1.0	2