Dipak Panthi

List of Publications by Year
in descending order

12 papers	79 citations	1651377 6 h-index	1637695 9 g-index
13 all docs	13 docs citations	13 times ranked	99 citing authors

#	Article	IF	Citations
1	Time-Dependent Density Functional Theory Study of Copper(II) Oxo Active Sites for Methane-to-Methanol Conversion in Zeolites. Inorganic Chemistry, 2021, 60, 1149-1159.	1.9	10
2	Copper-Oxo Active Sites in the 8MR of Zeolite Mordenite: DFT Investigation of the Impact of Acid Sites on Methanol Yield and Selectivity. Journal of Physical Chemistry C, 2021, 125, 6684-6693.	1.5	5
3	Methane Câ€“H Activation by [Cu₂O]²⁺ and [Cu₃O₃]²⁺ in Copper-Exchanged Zeolites: Computational Analysis of Redox Chemistry and X-ray Absorption Spectroscopy. Inorganic Chemistry, 2021, 60, 6218-6227.	1.9	5
4	Methane Overâ€Oxidation by Extraâ€Framework Copperâ€Oxo Active Sites of Copperâ€Exchanged Zeolites: Crucial Role of Traps for the Separated Methyl Group. ChemPhysChem, 2021, 22, 1101-1109.	1.0	7
5	Copper-Oxo Active Sites for Methane Câ€“H Activation in Zeolites: Molecular Understanding of Impact of Methane Hydroxylation on UVâ€“Vis Spectra. Inorganic Chemistry, 2021, 60, 8489-8499.	1.9	11
6	DFT Analysis of Methane Câ^'H Activation and Overâ€Oxidation by [Cu₂O]²⁺ and [Cu₂O₂]²⁺ Sites in Zeolite Mordenite: Intraâ€versus Interâ€site Overâ€Oxidation. ChemPhysChem, 2021, 22, 2517-2525.	1.0	2
7	Heterometallic [Cuâ€“Oâ€“M]²⁺active sites for methane Câ€“H activation in zeolites: stability, reactivity, formation mechanism and relationship to other active sites. Catalysis Science and Technology, 2021, 11, 5671-5683.	2.1	3
8	2D-IR studies of cyanamides (NCN) as spectroscopic reporters of dynamics in biomolecules: Uncovering the origin of mysterious peaks. Journal of Chemical Physics, 2020, 152, 074201.	1.2	7
9	Activating Water and Hydrogen by Ligand-Modified Uranium and Neptunium Complexes: A Density Functional Theory Study. Inorganic Chemistry, 2020, 59, 3102-3109.	1.9	2
10	Ground-state actinide chemistry with scalar-relativistic multiconfiguration pair-density functional theory. Journal of Chemical Physics, 2019, 151, 134102.	1.2	12
11	Nitrogen Reduction by Multimetallic trans-Uranium Actinide Complexes: A Theoretical Comparison of Np and Pu to U. Inorganic Chemistry, 2019, 58, 6731-6741.	1.9	7
12	Performance of density functional theory for describing heteroâ€metallic activeâ€site motifs for methaneâ€toâ€methanol conversion in metalâ€exchanged zeolites. Journal of Computational Chemistry, 2018, 39, 2667-2678.	1.5	8