

Olajumoke Adeyiga

List of Publications by Year in descending order

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| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 1 | 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 |
| 2 | 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 |
| 3 | 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 |
| 4 | 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 |
| 5 | 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 |
| 6 | 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 |
| 7 | 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 |
| 8 | 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 |
| 9 | Pyrazole, Imidazole, and Isoindolone Dipyrrinone Analogues: pH-Dependent Fluorophores That Red-Shift Emission Frequencies in a Basic Solution. <i>Journal of Organic Chemistry</i> , 2019, 84, 11856-11862. | 1.7 | 6 |
| 10 | Ground-state actinide chemistry with scalar-relativistic multiconfiguration pair-density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 134102. | 1.2 | 12 |
| 11 | 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 |
| 12 | 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 |