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Elucidation of the electronic structure of metal-oxo reactive species in porous media for the oxidation of methane and ethane

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High-valent metal-oxo species attract considerable interest due to their catalytic role in oxygenation reactions as active intermediates. A synthetic route that has successfully applied in functional materials is the introduction of reactive species inside porous materials that mimic the nuclearity and reactivity of active sites of enzymatic analogues, such as the methane mono-oxygenase and non-heme enzymes. Metal-organic frameworks (MOFs) and zeolites are porous materials that can offer advantageous coordination environments for the formation of such highly reactive species. Two such examples will be discussed. The first is the iron-containing MOF, Fe0.1Mg1.9(dobdc) (dobdc4- = 2,5-dioxido-1,4-benzene-dicarboxylate), which was reported to catalyze the oxidation of ethane to ethanol in the presence of nitrous oxide. The catalytic activity of the iron-containing MOF was attributed to an uncommon high-spin iron (IV)-oxo intermediate. The second part of this talk is related to the unique $[Cu_3O_3]^{2-}$ ring intermediate deposited on the mordenite zeolite. The tricopper cluster site was reported to catalyze the oxidation of methane to methanol. The multireference character of this single-site active site affects its catalytic behavior and thus, its electronic structure was examined by multi-configurational wave function methods.

Biography

Konstantinos D Vogiatzis completed his BS in Chemistry at the University of Athens, Greece, in 2006 and he obtained his Master's (MSc) in Applied Molecular Spectroscopy from the University of Crete, Greece, in 2008. He received his PhD in 2012 from the Karlsruhe Institute of Technology, Germany, where he developed a highly accurate coupled-cluster scheme in the group of Prof. Wim Klopper. After an eight-month Post-doctoral appointment at the Institute of Nanotechnology at the Karlsruhe Institute of Technology, Germany, he moved to the University of Minnesota (UMN) in 2014 where he performed Post-doctoral Research in the group of Prof. Laura Gagliardi. His research at the UMN focused on the catalytic and sorption properties of metal-organic frameworks (MOFs), and on the development and application of strongly correlated methods. In 2016, he joined the University of Tennessee as an Assistant Professor of Theoretical and Computational Chemistry.

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