University of Minnesota
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Department of Chemistry

Seminar

9:45 a.m. Thursday, September 4, 2014 • 331 Smith Hall

Professor

Professor Laura Gagliardi

Department of Chemistry
University of Minnesota

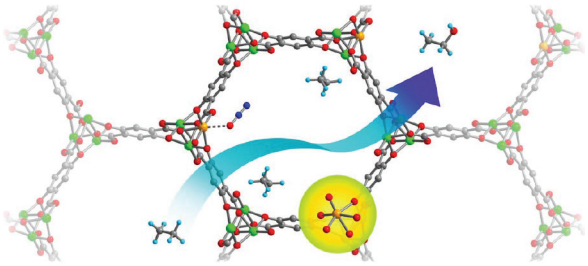
Gas Separation and Catalysis in Metal-Organic Frameworks

Research interests: model chemical systems containing metals and devote special attention to metal-metal multiple bonds and compounds containing lanthanides and actinides. Interested in ground-state and excited-state properties in the gas phase, noble gas matrices, and liquid solution.
Website: http://www.chem.umn.edu/directory/faculty.lasso?serial=2990

Abstract

Metal-organic frameworks (MOFs) are attracting the attention of many scientists because of their high selectivity in gas separations, catalytic activity, and magnetic properties. Many of these properties are linked to the presence of open-site transition metal ions, which may have open shells depending on their d^n configuration and their coordination environments inside the framework. Among this newly popular class of materials, the M_2(dobdc) (M = transition metal, $dobdc^{4-}$ = 2,5-dioxido-1,4-benzenedicarboxylate) systems are particularly noteworthy. They exhibit very high performance for various gas separations and promising catalytic properties.

I will discuss several examples of the interplay between experiment and theory in order to address some of the challenging chemistry that occurs in these materials, including our latest results on the M_2(dobdc) (M= Mg, Fe, Ni, Co) class of materials, obtained using quantum chemical calculations in combination with classical simulations. Our studies[1,2] are aimed at understanding the interaction of various guests, including CO_2, with M_2(dobdc). I will also explain how Fe_2(dobdc) and its magnesium-diluted analogue, $Fe_{0.1}Mg_{1.9}$(dobdc), are able to activate the C–H bonds of ethane and convert it into ethanol and acetaldehyde using nitrous oxide as the terminal oxidant.[3] Electronic structure calculations indicate that the active oxidant is likely to be a high-spin S=2 iron(IV)–oxo species.



1. K. Lee, W. Isley III, A. Dzubak, P. Verma, S. Stoneburner, L.-C. Lin, J. Howe, E. Bloch, D. Reed, M. Hudson, C. Brown, J. Long, J. Neaton, B. Smit, C. Cramer, D. Truhlar, and L. Gagliardi, "Design of a metal-organic framework with enhanced back bonding for the separation of N_2 and CH_4", *J. Am. Chem. Soc.* **136**, 698–704 (2014)
2. N. Planas, A. Dzubak, R. Poloni, L. Lin, A. McManus, T. McDonald, J. Neaton, J. Long, B. Smit, L. Gagliardi, "The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metal - Organic Framework", *J. Am. Chem. Soc.* **135**, 7402-7405 (2013)
3. D. J. Xiao, E. D. Bloch, J. A. Mason, W. L. Queen, M. R. Hudson, N. Planas, J. Borycz, A. L. Dzubak, P. Verma, K. Lee, F. Bonino, V. Crocellà, J. Yano, S. Bordiga, D. G. Truhlar, L. Gagliardi, C. M. Brown, and J. R. Long, Oxidation of ethane to ethanol by N_2O in a metal–organic framework with coordinatively unsaturated iron(II) sites, *Nature Chemistry*, doi:10.1038/nchem.1956 (2014)

Refreshments will be served prior to the seminar.