Physical Chemistry Seminar

Tuesday, January 20, 2015 | **11:00 am** | **Room 1315 Chemistry Building**

Gas Separation and Catalysis in Metal-Organic Frameworks

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Host: Professor Ned Sibert

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 present 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 are aimed at understanding the interaction of various guests, including CO_2, with M_2(dobdc). I will discuss a cooperative insertion mechanism for efficient CO_2 capture in diamine-appended metal-organic frameworks. Spectroscopic, diffraction, and computational studies reveal an unprecedented cooperative process in which, above a metal-dependent threshold pressure, CO_2 molecules insert into metal-amine bonds, inducing a reorganization of the amines into well-ordered chains of ammonium carbamate.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8305F