**Department of Chemical Engineering**

**Seminar Schedule**

**Detailed Understanding of Metal—Organic Frameworks for Energy Applications**

Josh Howe

Postdoctoral Fellow, Georgia Tech

**Abstract**

Metal—Organic Frameworks (MOFs) are a class of hybrid inorganic-organic nanoporous materials that consist of metal-containing nodes coordinated in a highly crystalline network by organic linker components. MOFs have drawn substantial research interest over the past two decades for their potential in various application areas, including adsorption, separations, catalysis, sensing, and gas storage as a result of their tunable chemistries and large internal surface areas. Because there is great freedom in selection of metal node and organic linker, thousands of MOFs have been synthesized and hundreds of thousands more have been predicted. From this immense collection of materials, identifying materials suited to a particular target application is a problem for which computational tools are ideal. Computational models must capture the physics important to the problem of interest to be of any value. I present work aimed at establishing a detailed fundamental understanding of MOFs and the interactions of adsorbates within MOFs, particularly as it pertains to energy applications and especially CO2. These computational studies couple closely with experimental efforts, resulting in new insights into the physics underlying the behavior of MOFs and how MOFs can be useful for a variety of applications.

**Bio**

Joshua D. Howe is a postdoctoral fellow with Prof. David S. Sholl at Georgia Tech in Atlanta, Georgia. Previously, he completed bachelor’s degrees in chemical engineering and physics at Penn State and his Ph.D. in chemical engineering at University of California, Berkeley. His research centers on using computational tools, particularly electronic structure methods, to build fundamental understanding of materials to improve material performance and design.

**Seminar**

**Monday, Feb 26th**

**3:00 pm**

**Livermore 101**