As global energy demand increases, breakthroughs in clean energy technologies will be needed to meet these demands in a sustainable manner. Metal-organic frameworks (MOFs) are crystalline, nanoporous materials with extreme promise for addressing these challenges. Formed by the assembly of inorganic metal ions and organic ligands, the exceptionally high internal surface areas and chemically tunable structures of MOFs make them ideal candidates for a wide range of clean energy applications such as hydrogen and methane storage, catalysis, and carbon dioxide capture. Over 20,000 distinct MOFs have already been discovered in the past decade and, given the wide range of metal nodes and organic ligands available as chemical building blocks, the potential for identifying further MOFs with promising properties is immense. Chemical instability in the presence of water is one of the last remaining challenges to the widespread use of these materials.

This presentation will discuss the complimentary experimental and molecular modeling techniques that can be used to understand the important structure-property relationships governing chemical stability and adsorption properties in MOFs. I will also highlight instances where molecular modeling can provide information that is not only consistent with experiment, but also allows critical insight into phenomena occurring over length and time scales that are inaccessible to direct experimental observation. To illustrate the power of this highly integrated experimental-computational approach, studies exploring the important role ligand identity plays in dictating the stability and adsorption properties of isostructural MOFs will be presented. Overall, this research lays critical groundwork for addressing the longstanding water stability challenge in MOFs, thus enabling the use of these materials in clean energy applications that could revolutionize the field of adsorption.

Tuesday, January 26, 2016

5326 Stevenson Center
3:10pm – 4:00pm
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Reception at 2:45pm