Title: Computational Study of Nanoporous Materials for Energy-Related Applications

Abstract: Nanoporous materials such as zeolites and metal-organic frameworks (MOFs) have drawn consideration attention for their potential in energy-related applications. To facilitate their development, computational studies can play an important role in identifying promising structures and achieving molecular-level understandings. In this presentation, I will first give an overview of our research and briefly introduce computational methods used in my group. A few selected projects for computational discoveries of materials will be then discussed. Specifically, I will first discuss our recent efforts on investigating MOFs for water harvesting, with a particular focus on the methods and details associated with such computational study. For instance, the widely used method to compute adsorption isotherms of porous materials - grand canonical Monte Carlo (GCMC) simulations - can converge very slowly due to its inefficient sampling of the dense water phase adsorbed in porous materials and may therefore yield unreliable results. I will demonstrate a method from a class of flat histogram methods, which can sample the accessible states of the water adsorption system much more efficiently. Through employing this method to study a number of MOFs, our results identify promising candidates as well as shed light on the structure-property relationships. Subsequently, I will talk about our recent studies on nanoporous membranes for alcohol/water separation and water desalination. By employing molecular dynamics calculations, we demonstrate the potential of several classes of materials in these separation applications. Finally, our recent efforts on developing approaches to characterize the surface area of MOFs will be discussed in this talk.