Computational Design and Discovery of Nanoporous Materials for Energy- and Environment-related Applications

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Nanoporous materials such as zeolites and metal-organic frameworks (MOFs) have drawn considerable attention for their potential in energy- and environment-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. Selected projects for computational discoveries of materials will be then discussed. Specifically, our recent efforts on investigating MOFs for water adsorption applications will be highlighted. 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 thousands of MOFs, our results identify potential candidates as well as shed light on the structure-property relationships. Besides, with the large-scale computational results at our disposal, the limitations of several geometric and energetic features, which have been traditionally used and are inexpensive to compute, to probe water adsorption behaviors of porous materials will also be discussed. I will subsequently discuss 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 and establish structure-property relationships for future rational design of membranes with an improved performance. We anticipate the outcomes of these studies will facilitate future computational and experimental efforts on the development of nanoporous materials as adsorbents and/or membranes.