Computational Design of Nanomaterials for Gas Storage and Separation Applications

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A variety of novel nanomaterials have been used/tested for next-generation gas storage and separation applications. However, in many cases little is known about their properties and performance, although such fundamental understanding is essential for further advances in gas storage and separation technologies. Experiments may yield many clues to the behavior of those materials, but the interpretations are often controversial due largely to the difficulty of direct characterization. Under such circumstances, first principles-based computational modeling has emerged as one of the most powerful tools for design and development of new nanomaterials for specifically targeted applications. This talk will focus on introducing our ongoing efforts in first principles modeling of nanomaterials for gas separation and storage. In the first part of my talk, I will discuss the properties and performance of amorphous silica-based membranes for hydrogen separation and purification, particularly the doping of transition metals and its impacts on the microstructure, hydrothermal stability, and permeation properties of thin amorphous silica films.