Multi-scale Modeling of Porous Materials

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Porous materials are seen as promising candidates for a wide variety of energy-related applications including carbon capture, methane/hydrogen storage, catalysis, and sensors. Unfortunately, the number of materials that can be synthesized is extremely large given the diversity of chemistry and structural topologies. In order to expedite the search for the optimal materials, we have developed a multi-scale modeling framework for this presentation. Accordingly, we can start with an experimental/hypothetical materials and use both quantum mechanical and classical simulation methods to obtain material properties such as the adsorption isotherms.