Evaluation of Metal-Organic Frameworks as Adsorbent Materials with Applications in Hydrogen Storage and Carbon Dioxide Separations

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The task of designing porous materials for use in specific applications requires a detailed understanding of the adsorption process and how adsorption is affected by material properties. Applications of interest include maximizing gravimetric or volumetric adsorption capacity for hydrogen and carbon dioxide and increasing the selectivity for carbon dioxide in mixtures with other light gasses. Metal-Organic Frameworks (MOFs) are a new class of microporous materials that are synthesized via self-assembly in a “building-block” approach such that the pore size, geometry, and chemical composition can be “tailor made” to produce materials that exhibit specific adsorption and chemical behavior. This study uses a mix of classical simulations, (e.g. simulating adsorption using grand canonical Monte Carlo), as well as quantum calculations, to investigate how best to design these materials for hydrogen storage and carbon dioxide separations. Ultimately, material design guidelines, in terms of surface area, free volume, and heat of adsorption were determined that would enable a material to meet DOE’s hydrogen storage requirements. Short studies were also performed to test ideas for increasing the heat of adsorption in MOFs. Finally, the behavior of carbon dioxide adsorption is investigated, which provides insight into how various materials might perform in adsorption separations.

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