VI.D.7 New Concepts for Optimized Hydrogen Storage in Metal-Organic Frameworks

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Objectives

- Improvement of mass and volumetric H_2 density in metal-organic frameworks (MOFs).
- Examination of polarization effects of the aromatic rings on hydrogen uptake.
- Characterization of hydrogen sorption as a function of temperature and pressure.
- Modeling of hydrogen uptake in MOFs.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- B. Weight and Volume
- C. Efficiency
- M. Hydrogen Capacity and Reversibility

Technical Targets

New concepts for optimized hydrogen storage in MOFs:

This project is concerned with conducting studies on new MOF structures and their hydrogen sorption properties. Insights gained from these studies will be applied toward the design and synthesis of hydrogen storage materials that meet the DOE 2010 hydrogen storage targets, especially for capacity and reversibility.

Approach

MOFs are new materials that have only recently shown promising levels of hydrogen uptake. Thus, their viability in hydrogen storage applications will require continued synthetic developments and new approaches to their design and modification. We will assess gravimetric and volumetric H_2 storage capacities of MOFs that possess interpenetration to explore this topological feature as a strategy for increasing uptake. We will also employ guests to eliminate open space at the centers of the pores. These guests are expected to serve as binding sites for hydrogen, thus increasing gas storage density.

We will implement three major strategies that minimize open space while increasing total surface area for H_2 binding. Initially, we will use linkers with exposed edges, resulting in ultra-high surface area MOFs. A prototypical example is MOF-177 (see Figure 1). We will also take these frameworks and impregnate the large pores with guests designed to adsorb hydrogen. Finally, catenation will be explored as a strategy to decrease open space not participating in gas binding. To explore these approaches, equilibrium H_2 uptake will be determined as a function of structure under DOE 2010 targets. Raman spectroscopy, inelastic neutron scattering, and modeling will be employed to aid in these efforts.

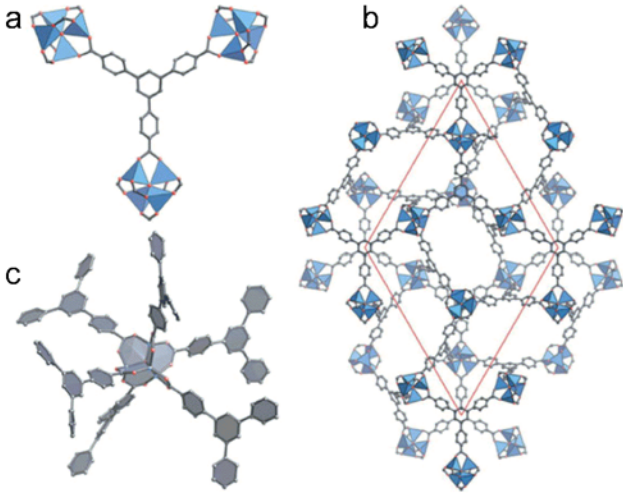

Figure 1. MOF-177 Structure (a) A BTB unit linked to three OZn_4 units (H atoms are omitted). ZnO_4 tetrahedra are shown in blue, and O and C atoms are shown as red and black spheres, respectively. (b) The structure projected down [001]. Colors as for a. For clarity, only about half the *c*-axis repeat unit is shown. (c) A fragment of the structure radiating from a central OZn_4: six-membered rings are shown as grey hexagons and Zn atoms as blue spheres.

Accomplishments

- We chose MOF-177 for initial impregnation studies and commenced scale-up.
- We acquired a high-pressure volumetric sorption analyzer from VTI Corporation that can measure uptake to nearly 100 bar. This system can also study reversibility through desorption isotherms.