IV.H.1 Microporous Metal Organic Materials for Hydrogen Storage

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Contract Number: DE-FC26-05NT42446

Start Date: May 2005
Projected End Date: May 2007

Objectives

- Design and synthesize microporous metal organic materials (MMOMs) with high hydrogen uptake and light-weight metals (for example, lithium and magnesium) incorporated into the MMOMs so as to maintain a low bulk density and promote the formation of small pores, large pore volumes and high surface areas so as to provide a large number of active sites for the adsorption of hydrogen.
- Employ molecular modeling as a tool for understanding the basic physics of adsorption of hydrogen in the synthesized materials and as a method for guiding further experimental synthetic efforts.
- Employ quantum mechanical modeling methods to compute the interaction energies of hydrogen with different MMOMs.
- Employ statistical mechanical modeling to compute adsorption isotherms and probe the effects of changing the structure and composition of the framework on adsorption.
- Employ modeling to help in identifying MMOMs that will be capable of storing much higher weight fractions of hydrogen than current materials. A state-of-the-art computer-controlled pressure-composition isotherm measurement instrument will be used to examine the materials over a wide range of temperature and pressure.

Introduction and Approach

The scope of this work is to design and synthesize MMOMs with high hydrogen uptake. Light-weight metals (for example, lithium and magnesium) will be incorporated into the MMOMs so as to maintain a low bulk density and promote the formation of small pores, large pore volumes and high surface areas so as to provide a large number of active sites for the adsorption of hydrogen. Molecular modeling will be used as a tool for understanding the basic physics of adsorption of hydrogen in the synthesized materials and as a method for guiding further experimental synthetic efforts. Quantum mechanical modeling methods will be used to compute the interaction energies of hydrogen with different MMOMs. Statistical mechanical modeling will be used to compute adsorption isotherms and probe the effects of changing the structure and composition of the framework on adsorption. The ultimate goal of the modeling is to help in identifying MMOMs that will be capable of storing much higher weight fractions of hydrogen than current materials. A state-of-the-art computer-controlled pressure-composition isotherm measurement instrument will be used to examine the materials over a wide range of temperature and pressure.

Accomplishments

Developed a molecular model that demonstrates the basic physics of adsorption of hydrogen into synthesized materials, including the incorporation of light-weight metals (lithium and magnesium) into MMOMs to maintain low bulk density and promote the formation of small pores, large pore volumes, and high surface areas to provide a large number of active sites for the adsorption of hydrogen.

Future Directions

- Develop quantum mechanical models to compute the interaction energies of hydrogen with different MMOMs.
- Develop statistical mechanical models to compute adsorption isotherms and probe the effects of changing the structure and composition of MMOMs on adsorption.
- Identify MMOMs that will be capable of storing much higher weight fractions of hydrogen than current materials.
- Characterize identified MMOMs using a state-of-the-art computer-controlled pressure-composition isotherm measurement instrument over a wide range of temperatures and pressures.