IV.C.7 Room Temperature Hydrogen Storage in Nano-Confined Liquids

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Fiscal Year (FY) 2012 Objectives

- Develop techniques for volumetric measurements of hydrogen solubility in volatile liquid solvents in both bulk form and nano-confined liquid/scaffold composites.
- Demonstrate volumetric measurements of hydrogen solubility in bulk hexane at pressures up to 100 bar.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section (3.3) of the Fuel Cell Technologies Program Multi-Year Research, Development and Demonstration Plan:

(A) System Weight and Volume
(C) Efficiency
(E) Charging/Discharging Rates

Technical Targets

This project is conducting initial studies of enhanced hydrogen solubility in nano-confined liquid solvents. Results from these studies will be applied to developing nano-confined liquid/nano-porous scaffold composite hydrogen storage materials that meet the following DOE targets:

- Specific energy: 6 wt% hydrogen (system)
- Energy density: 50 g/L hydrogen (system)

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Approach

Our approach is to use a composite consisting of a liquid solvent for molecular hydrogen that is nano-confined within a porous scaffold. Nano-confined liquids have been shown to have hydrogen solubilities that are enhanced by up to 50 times compared with bulk solubilities [1]. These enhanced solubilities enable a nano-confined solvent/porous scaffold composite hydrogen storage material with a material basis hydrogen storage density of 6% hydrogen by weight and 50 g/L that operate at room temperature and at pressures <350 bar (Figure 1). These materials could be readily used in current compressed hydrogen tank designs with minimal changes to vehicle engineering and delivery infrastructure, thus facilitating technology transition. The room temperature design also addresses critical shortcomings of current high capacity metal hydride (high temperature) and cryo-adsorbent (coolant and boil off) materials, resulting in significant cost reductions. We will investigate a variety of scaffold material compositions, including those based on carbon (e.g., mesoporous carbon and carbon aerogel) and aluminosilicates (e.g., MCM-41 and zeolites), and hydrogen dissolving liquids to maximize storage capacity. The enthalpy of the stored hydrogen as well as the effect of scaffold pore size will be explored. Storage capacity measurements together with simulations will be used to understand the mechanism of hydrogen storage in nano-confined liquids and optimize performance.

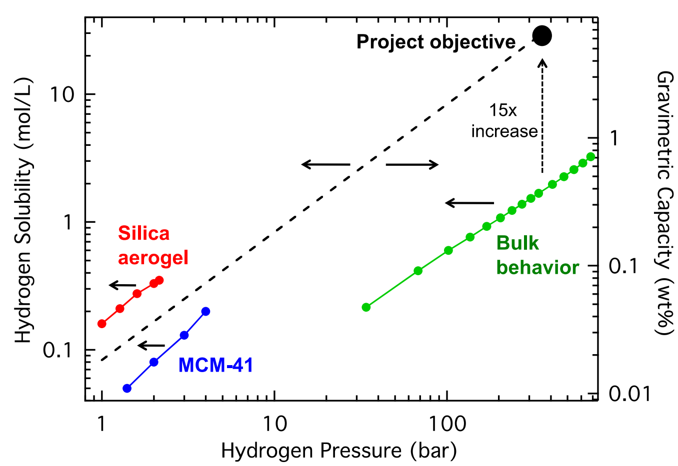

FIGURE 1. Hydrogen storage in nano-confined solvent/porous scaffold composites. Hydrogen solubility (left axis) versus pressure is shown for bulk hexane and nano-confined hexane/silica aerogel and nano-confined hexane/MCM-41 composites. Solubilities for hexane/silica aerogel and hexane/MCM-41 composites indicate ~50x and ~8x enhancements over the bulk, respectively. The project objective and progression (dashed line) are shown in terms of both solubility and hydrogen gravimetric capacity (right axis) based on an ~15x solubility enhancement and a 4 cm^3/g pore volume scaffold.

FY 2012 Accomplishments

- Developed protocols for measuring hydrogen solubility using Sieverts apparatus at pressures between ~10 bar and 50 bar.
- Measured the solubility of hydrogen in n-hexane up to 70 bar using two different Sieverts apparatus and compared with published state-of-the-art measurements.

Future Directions

- We will extend our solubility measurement protocols from bulk liquids to nano-confined solvent/scaffold composites.
- We will develop methods for preparing nano-confined solvent/scaffold composites with specific liquid compositions.
- We will measure the solubility of hydrogen in a nano-confined solvent/scaffold composite, such as hexane/MCM-41.
- We will optimize the confined liquid and the scaffold to maximize hydrogen storage capacities.

FY 2012 Publications/Presentations

1. J.J. Vajo, Room temperature hydrogen storage in nano-confined liquids, Research Performance Progress Report for DOE/EERE, covering March 5, 2012 to June 30, 2012; submitted July 15, 2012.

2. J.J. Vajo, Room temperature hydrogen storage in nano-confined liquids, Poster presentation at the 2012 DOE Fuel Cell Technologies Program Annual Merit Review, May-2012, Crystal City, Virginia.

References

1. V. Rakotovao, R. Ammar, S. Miachon, M. Pera-Titus, "Influence of the mesoconfining solid on gas oversolubility in nanoliquids", *Chem. Phys. Lett.*, **485**, 299-303 (2010).