Hydrogen Storage Workshop

Advanced Concepts Working Group

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Advanced Storage Techniques/ Approaches in Priority Order

1. Crystalline Nanoporous Materials (15)
2. Polymer Microspheres (12)
   Self-Assembled Nanocomposites (12)
3. Advanced Hydrides (11)
   Metals – Organic (11)
4. BN Nanotubes (5)
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5. Mesoporous materials (4)
   Bulk Amorphous Materials (BAMs) (4)
6. Iron Hydrolysis (3)
7. Nanosize powders (2)
8. Metallic Hydrogen (1)
   Hydride Alcoholysis (1)

Overarching R&D Questions for All Advanced Materials

- Maximum storage capacity – theoretical model
- Energy balance / life cycle analysis
- Hydrogen absorption / desorption kinetics
- Preliminary cost analysis – potential for low cost, high volume
- Safety

Crystalline Nanoporous Materials – Description / Current Status

- Advanced zeolites
- Advantages
  - Cheaply available
  - Chemically and thermally robust
  - Good structural reproducibility
  - Modifiable
  - Environmentally friendly
  - Safe
- Maximum H_2 capacity measured to date: 2.5 wt% (5 kg/m3)

Crystalline Nanoporous Materials – R&D Needs

1. Maximum wt% of H_2 that can be absorbed by physisorption
2. Chemical modifications of zeolite surfaces
3. Best structures for max absorption – small vs. large pore
4. Characterization of internal surface structures
5. Advanced material characterization
6. Zeolite chemistry (e.g., Si/Al)

Polymer Microspheres – Description / Current Status

- Hollow spheres from glassy polymers
  - Segmented polymers hold H_2 at room temperature
  - Goal: Hold liquid H_2 at room temp.
- Advantages: flowable/consistent with GM design, portable, safe storage, microencapsulation, light weight, inexpensive, rechargable/recyclable
- Operate >300 atm
- PTMSP has very high gas permeability
- Issues/Challenges: Room temp leak rate, Manufacture, Identifying correct polymer, turning it on and off

Polymer Microspheres – R&D Needs

- Pressure inside the sphere
- How to get H2 in and out and in/out rate
- Identifying correct polymer
- Turning it on and off
- Room temperature leak rate

Self-Assembled Nanocomposites – Description / Current Status

- Aerogels are the scaffold; template with organic functional groups; physisorption, acid-base reaction
- Advantages
  - Extremely lightweight (0.003-0.5 g/cc)
  - Self assembly in one step (commercial) process
  - Flexibility to control properties – surface groups chemistry, pore structure, incorporation of dispersed metallic clusters
  - Stable materials
  - Molecular “switch” for sorption control
  - Environmentally benign
  - Inexpensive

Self-Assembled Nanocomposites – R&D Needs

1. Studying silica aerogels
2. Modifying aerogels
3. Theoretical Modeling - various chemical structures / materials
4. Functionalization strategies

Advanced Hydride Materials – Description / Current Status

- Advantages:
  - High wt% hydrogen potential
  - Lightweight
  - Reversibility potential (to be explored)

Advanced Hydride Materials – R&D Needs

1. Hydrogen generation from $LiBH_4$
2. How to get H2 in and out
3. Incorporation of LiBH4 into nanoporous materials to see effects on the chemical reaction (for lowering reaction temperature)

Metal Organics – Description / Current Status

- Zeolitic materials using carbon as backbone, polymeric synthesis, using carbon and metals; cross between carbon and zeolitic materials; organic microporous
- Advantages:
  - Flexibility in material composition / structure
  - Larger pore structures with tailored properties
  - Potential to put on advantageous functional groups
  - Capillary effect

Metal Organics – R&D Needs

1. Initial studies of wt% hydrogen absorption
2. Chemical modifications – functional groups

Boron Nitride Nanotubes – Description / Current Status

- Nanotubes based on boron nitride instead of carbon
- Roughly equivalent to carbon nanotubes in terms of advantages, but less pyrophoric

Boron Nitride Nanotubes – R&D Needs

1. Verify wt%
2. Understanding adsorption mechanisms
3. Estimating costs
4. Desorption behavior

Bulk Amorphous Materials (BAMs) – Description / Current Status

- A new approach
  - New class of metallic materials based on multi-component alloy systems
  - Loosely packed with porous defects (interstitial holes for H2 storage) in super cooled liquid phase

- Ti-Al-Fe based BAMs - light weight / low cost
  Can meet 6% target if H/M = 3

- Thermal treatment may be used to control size and distribution of porous defects

Bulk Amorphous Materials (BAMs) – Advantages

- Fast adsoption/desorption kinetics
- Resistance to embrittlement and disintegration
- Multiple types of interstitial sites for H2 absorption
- Chemisorption
- Low cost / volume production

Bulk Amorphous Materials (BAMs) – R&D Needs

1. Verify wt% for Ti-Al-Fe material
2. Low density / low cost materials
3. Demonstrate H2 release
4. Calculate / optimize environment and bonding strengths
5. Detailed experimental information on bond lengths and ordering

Hydrogenated Amorphous Carbon – Description / Current Status

- Carbon skeleton made up in part of stressed graphitic “cages” nanotube sponge)
  - Plasma-assisted chemical deposition process
- Advantages:
  - 6-7 wt% hydrogen
  - stable up to T=300 degrees C
  - potential for high hydrogen content
- Tests indicate rapid H2 release between 200-300 degrees C

Hydrogenated Amorphous Carbon – R&D Needs

1. Reversibility
2. Kinetics – in/out rates
3. Structure / Modeling
   – to determine whether paths are stable, diffuse back and forth, interconnected
4. Fabrication of powders