Carbon Materials Breakout Group Process

- Day 2, Thursday
  - Review results of Day 1 and modify if needed
  - Identify critical R&D needs
  - Outline R&D plan with key milestones
  - Report results to plenary

Carbon Materials Breakout Group

- **Key Results**
  - **Target: get the science right to engineer carbon materials for hydrogen storage**
    - **Integrate theory, experiment, engineering**
    - **Understand mechanisms, effects, and interactions ranging from physisorption to chemisorption**
  - **Theory**
    - **Provide "directional" guidance for experiments (and vice-versa)**
    - **Provide baseline theory to elucidate parameters affecting the number and type of binding sites and the heat of their interaction with H2 (ΔH) for a broad range of (highly) modified carbon materials**
      - **effect of modifying shape , degree of curvature**
      - **chemical/electronic effects of additives and, defects**

Carbon Materials Breakout Group

- **Key Results**
  - Conduct definitive experiments to show where and how hydrogen is stored in SWNT and for various forms of carbon materials
    - develop 2-3 pure SWNT standards for synthesis, purification, activation, and hydrogen adsorption/desorption
    - conduct round-robin testing
      - » role of SWRI, other labs, universities, industry
    - measure isosteric heat at low T, low P
    - develop adsorption isotherms at high P
    - in-situ Raman and IR spectroscopy
    - neutron diffraction measurements
      - » enhanced program needed to produce larger samples

Carbon Materials Breakout Group

- **Key Results**
  - **Experiment**
    - **Conduct definitive experiments to show where and how hydrogen is stored**
      - **measure IR stretch**
      - **measure rate, path, mechanism of hydrogen diffusion**
      - **vary material properties systematically for tests, particularly diameter of NTs, but also chirality**

Carbon Materials Breakout Group

- **Key Results**
  - **Engineering**
    - **Systems model for comprehensive trade-off analysis of storage capacity vs fundamental material properties**
      - **assume mild T & P, high thermal conductivity**
    - **Establish independent laboratory (SwRI?)**
      - **validate materials (structure, H2 adsorption/desorption, etc.)**
      - **provide baseline capability for reproducibility of measurements**
    - **Address parameters for system engineering development**
  - **Integrate Theory, Experiment, and Engineering**
    - **Create secure website to post information, enhance information exchange**
    - **Establish Carbon Materials Working Group**

R&D Roadmap for Carbon Materials

Technical Challenges	R&D Projects/Milestones
Theory 1. confirm interaction of H2-curved C 2. reliably predict heat and entropy of H2 adsorption to rank order candidate materials 3. optimize capacity by structural design	1. form team to examine existing results by 2003 2. identify tractable candidates, use variety of methods to obtain trends 3. develop potential models for cluster surrogates for adsorption sites by 2006 4.
Experiment 1. reproducible synthesis and process 2. develop universal reproducible measurement techniques 3. measurement on perturbation of H-H And C-C bond with degree of interaction 4. synthesize new compositions, esp highly curved C	1. 2. 3. 4.
Engineering 1. specify key transport and equilibrium sorption parameters for Freedom Car 2. address cyclability and durability 3. address poisoning 4.	1. 2. 3. 4.