

Agenda

U.S. Department of Energy Theory Focus Session on Hydrogen Storage Materials

DOE Hydrogen Program
Basic Energy Sciences (Office of Science) and
Office of Hydrogen, Fuel Cells and Infrastructure Technologies (Energy Efficiency and
Renewable Energy)
Thursday, May 18, 2006 (1 pm to 6 pm)
Crystal Gateway Marriott, Crystal City, VA
(In conjunction with the DOE Hydrogen Program Annual Merit Review, May 16-19)

Salon IV First Floor

Co-organizers: Chris Wolverton (Ford), Karl Johnson (U. of Pittsburgh), Maciek Gutowski (Pacific Northwest National Laboratory)

Objectives:

- Identify critical areas, key barriers and gaps in current theory/modeling approaches for hydrogen storage materials and technologies
- Provide an overview of current state of the art and most recent technical progress in theory and modeling of hydrogen storage from experts in the field
- Promote potential theory/modeling research collaborations, identify and reduce duplication and create and strengthen partnerships

1:00-1:05pm – Introductory Remarks

1:05-2:15pm - Session #1: Prediction of Novel Reactions and Materials

Chair: Karl Johnson

Topics to be addressed:

Prediction of Novel Crystal Structures
Prediction of Stable Mixtures of Known Compounds
Predicting Stable Decomposition Products

Speakers:

1:05-1:30pm - Predictions of New Hydrogen Storage Compounds and Mixtures -
Vidvuds Ozoliņš (UCLA)

1:30-1:55pm - Prediction of Novel Hydrogen Storage Reactions – **Kazutoshi Miwa (Toyota)**

1:55-2:15pm – Discussion

2:15-4:05pm - Session #2: Thermodynamics of Storage Materials

Chair: Chris Wolverton

Topics to be addressed:

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Accuracy of DFT (and other) Methods: ΔH , ZPE, Thermodynamics/Entropies
Potential to Use DFT as a “Screen” for Discovery of New Compounds

Speakers:

2:15-2:40pm Solid-state (metal and complex) hydrides – **Susanne Opalka (UTRC)**

2:40-3:05pm Chemical hydrides - **Dave Dixon (Alabama)**

3:05-3:20pm – Coffee Break

3:20-3:45pm Weakly-bound/Physisorbed Materials – **Andrew Williamson (LLNL)**

3:45-4:05pm Discussion – Thermodynamics of Storage Materials

4:05-5:15pm - Session #3: Kinetics of Storage Materials

Chair: Maciek Gutowski

Topics to be addressed:

Reaction Barriers: TST, NEB vs. other transition-state finders

Methods for modeling "infrequent events" (e.g., rate-limiting, high kinetic barrier events)

“Catalytic” Effects: Making “thermodynamically reversible” systems, also “kinetically reversible”

Speakers:

4:05-4:30pm - Simulation of Kinetic Events at the Atomic Scale - **Graeme Henkelman (Texas)**

4:30-4:55pm - Accelerated Dynamics Methods for Infrequent Events - **Art Voter (LANL)**

4:55-5:15pm – Discussion

5:15-6:00 - Session #4: Mesoscale Modeling

Chair: Art Voter

Topics to be addressed:

Beyond the Atomic Scale: Longer length-/time-scale Modeling

Microstructural Evolution of Hydride Systems

Phase-separation/decomposition mechanisms (e.g., mass transport of Al in NaAlH_4)

5:15-5:40pm – Chemical Kinetics, Mechanics, and Microstructure Evolution in Solid Hydrogen Storage Media – **Anter El-Azab (Florida State)**

5:40-6:00pm - Discussion
