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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)

Co-organizers: Chris Wolverton (Ford), Karl Johnson (U. of Pittsburgh), Maciek Gutowski (Pacific Northwest National Laboratory)
DOE Contacts: Sunita Satyapal and Dale Koelling

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, University of Pittsburgh

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 CRDL)**
1:55-2:15pm – Discussion

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

Chair: Chris Wolverton, Ford Motor Co.

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, Pacific Northwest National Laboratory

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, Los Alamos National Laboratory

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

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