

U.S. Department of Energy

Theory Focus Session on Hydrogen Storage Materials

Office of Hydrogen, Fuel Cells and Infrastructure Technologies, Energy Efficiency and Renewable Energy

Office of Basic Energy Sciences, Office of Science

Monday, March 24, 2008 (8:30 am to 5:30 pm), Room Golden Gate C3, San Francisco Marriott Hotel, San Francisco, CA

Co-organizers: Shengbai Zhang (Rensselaer Polytechnic Institute), Chris Wolverton (Northwestern University), Vidvuds Ozolins (UCLA)

DOE Contacts: John Vetrano (BES) and Sunita Satyapal (EERE)

Objectives

- Identify critical areas, key barriers and gaps in current theory/modeling approaches for hydrogen storage materials and technologies
- Provide an overview of the 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
- Follow up on issues and problems identified in the 2006 Theory Focus Session, and identify progress or opportunities in these areas. (Information regarding this previous 2006 session is given at the following website:
http://www1.eere.energy.gov/hydrogenandfuelcells/wkshp_theory_focus.html)

Agenda

8:30-8:40 am Opening Remarks

Session #1: Cutting Edge Methodologies (beyond DFT)

Moderator: Shengbai Zhang (NREL/RPI)

Topics to be addressed: Benchmarking state-of-the-art approaches, accurate energy landscape. Identify problems with the current DFT-LDA and GGA approaches and possible pathways to overcome these problems.

8:40-8:45 am Moderator Introduction

8:45-9:10 am Jonathan DuBois (LLNL), "Quantum Monte Carlo benchmarks for dispersive interactions".

9:10-9:35 am	Martin Head-Gordon (Berkeley), “Recent advances in electronic structure methods with application to hydrogen binding problems”.
9:35-10:05 am	Discussion
10:05 – 10:25 am	Coffee Break

Session #2: Kinetics

Moderator: Vidvuds Ozolins (UCLA)

Topics to be addressed: Catalyst design for accelerated hydrogen uptake and release, multi-length scale physics methods and accelerated molecular dynamics.

10:25 - 10:30 am	Moderator Introduction
10:30 -10:55 am	Damien West (NREL), “Stochastically accelerated molecular dynamics and application to H diffusion on graphene”.
10:55 – 11:20 am	Mei-Yin Chou (Georgia Tech), “Catalytic effect of Ti for hydrogen cycling in NaAlH ₄ ”.
11:20 – 11:45 am	Chris van de Walle (UCSB), “Effects of point defects and impurities on kinetics in NaAlH ₄ ”.
11:45 – 12:20 pm	Discussion
12:20 – 1:50 pm	Lunch

Session #3: Thermodynamics

Moderator: David Sholl (Georgia Tech)

Topics to be addressed: State-of-the-art DFT isotherm calculation and development of DFT-based effective approaches.

1:50 – 1:55 pm	Moderator Introduction
1:55 – 2:20 pm	Gerbrand Ceder (MIT), “Cluster expansion approaches for the determination the imide structures”.
2:20 – 2:45 pm	Eric Majzoub (U. Missouri - St. Louis), “Monte Carlo global optimization method”.
2:45 – 3:15 pm	Discussion
3:15 – 3:35 pm	Coffee Break

Session #4: Prediction of New Materials/Properties

Moderator: Vincent Crespi (Penn State)

Topics to be addressed: Metastable hydride alloys and adsorbents with potential to meet the DOE gravimetric and volumetric targets, nano materials, and the effect of surfaces.

3:35 – 3:40 pm	Moderator Introduction
3:40 – 4:05 pm	Zhenyu Zhang (Oak Ridge), “Kinetic stability of metal coated carbon structures”.
4:05 – 4:30 pm	Boris Yakobson (Rice U.), “Spillover mechanism for hydrogen storage”.
4:30 – 4:55 pm	Don Siegel (Ford), “Thermodynamic guidelines for the prediction of hydrogen storage reactions, and their application to new hydrides and hydride composites”.
4:55 – 5:30 pm	Discussion
5:30 pm	Workshop Adjourns