

# SYMPOSIUM PROGRAM

**Sunday, November 11**

5:00 - 8:00 PM      Registration, Submission of Manuscripts  
6:00 - 8:00 PM      Reception

**Monday, November 12**

## INAUGURAL SESSION

9:00 - 9:10 AM      Introductory Remarks  
**Puru Jena**, Symposium Chair, Virginia Commonwealth University, USA

9:10 - 9:20 AM      Welcome Address  
**John B. Fenn**, Nobel Laureate, Virginia Commonwealth University, USA

## SESSION A: Key Note

**Chairman: Constantina Filiou, European Commission, Netherlands**

9:20 - 10:05 AM      “Progress and Challenges of a Hydrogen Economy”  
**Mildred S. Dresselhaus**, Massachusetts Institute of Technology, USA

10:05-10:35 AM      **COFFEE BREAK**

10:35 - 11:35 AM      “DOE Hydrogen Program: Production, Delivery and Fuel Cells:  
Technologies, Challenges, Infrastructure Costs, and Material Needs”  
**Mark D. Paster**, Department of Energy, USA

**11:35 - 1:30 PM      LUNCH**

## SESSION B: Production I

**Chairman: U. (Balu) Balachandran, Argonne National Lab., USA**

1:30 - 2:00 PM      “Materials Issues for Photoelectrochemical Water Splitting: Chalcopyrite  
Thin-Films and III-V Nitrides”  
**John A. Turner**, National Renewable Energy Laboratory, USA

2:00 - 2:30 PM      “Hydrogen Production via Water Splitting in Solar Reactors: The  
Hydrosol Process”  
**Athanasios G. Konstandopoulos**, Aerosol & Particle Technology  
Laboratory, Greece

2:30 - 3:00 PM      “Development of Photocatalysts for Solar Hydrogen Production”  
**Akihiko Kudo**, Tokyo University of Science, Japan

3:00 - 3:15 PM “A Cu/Pt Near-Surface Alloy for Water-Gas Shift Catalysis Studied by STM, XPS, TPD, and DFT”  
**Ronnie T. Vang**, Jan Knudsen, Joachim Schnadt, and Flemming Besenbacher. *Interdisciplinary Nanoscience Center (iNANO and Department of Physics and Astronomy), University of Aarhus, Denmark.*

**3:15 - 3:45 PM COFFEE BREAK**

### **Session C: Storage I (Molecular)**

**Chairman: George Thomas, Department of Energy, USA**

3:45 - 4:15 PM “7.5 wt % Hydrogen Storage in Metal Organic Frameworks”  
**Omar M. Yaghi**, University of California, USA

4:15 - 4:45 PM “Henry’s Law and Isoteric Heats in Physisorbents”  
**Channing Ahn**, California Institute of Technology, USA

4:45 – 5:15 PM “Novel Organometallic Fullerene Complexes for Vehicular Hydrogen Storage”  
**Anne C. Dillon**, National Renewable Energy Laboratory, USA

5:15 - 5:45 PM “Engineered Nano-Materials for High Capacity Hydrogen Storage”  
**Taner Yildirim**, NIST, USA

5:45 - 6:00 PM “Design of materials for storing hydrogen in quasi-molecular form”  
**Qiang Sun**<sup>1,2</sup>, Qian Wang<sup>1</sup>, and Puru Jena<sup>1</sup>, *Physics Department, Virginia Commonwealth University, and Department of Advanced Materials and Nanotechnology, Peking University, China*

**6:00 - 8:00 PM DINNER**

**8:00 - 10:00 PM Poster Session I**

**Tuesday, November 13**

### **Session D: Fuel Cells I**

**Chairman: Gary Sandrock, Department of Energy, USA**

8:30 - 9:00 AM “Materials Challenges in Proton Exchange Membrane Fuel Cells”  
**Biswajit Choudhury**, E. I. du Pont Nemours & Company, USA

9:00 - 9:30 AM “New PEM Fuel Cell Membranes for Higher Temperature, Drier Operating Conditions Based on the Heteropolyacids”  
**Andrew M. Herring**, Colorado School of Mines, USA

- 9:30 - 10:00 AM “Simulation of Reaction and Transport Processes in Fuel Cell Catalysts and Membranes”  
**William A. Goddard, III**, California Institute of Technology, USA
- 10:00 - 10:15 AM “Alternative Materials to Pd Membranes for Hydrogen Purification”  
**Paul S. Korinko** and Thad Adams, Savannah River National Laboratory, USA
- 10:15 - 10:45 AM COFFEE BREAK**

### **Session E: Storage II (Nano-materials)**

**Chairman: Shengbai Zhang, NREL, USA**

- 10:45 - 11:15 AM “Carbide-Derived Carbons for Hydrogen Storage”  
**Gleb Yushin**, Drexel University, USA
- 11:15 - 11:45 AM “Storage of Molecular Hydrogen in Carbon Based Systems”  
**Sa Li**, Virginia Commonwealth University, USA
- 11:45 - 12:15 PM “Hydride Chemistry in Nanoporous Scaffolds”  
**John J. Vajo**, HRL Laboratories, USA
- 12:15 - 12:30 PM “High Density H<sub>2</sub> Storage on Nanoengineered Scaffolds of Carbon Nanotubes”  
**Carter Kittrell**, A.D. Leonard, S. Chakraborty, H. Fan, W.E. Billups, R.H. Hauge, H.K. Schmidt, M. Pasquali, J.M. Tour, *Department of Chemistry, Rice University, USA*
- 12:30 - 2:00 PM LUNCH**

### **Session F: Production II**

**Chairman: Michelle V. Buchanan, Oak Ridge National Laboratory, USA**

- 2:00 - 2:30 PM “H<sub>2</sub> Binding and Reactivity on Transition Metal Complexes underlying Biomimetic H<sub>2</sub> Production and New Materials for H<sub>2</sub> storage”  
**Gregory J. Kubas**, Los Alamos National Laboratory, USA
- 2:30 - 3:00 PM “Materials Issues in Photobiological Production”  
**Anastasios Melis**, University of California, Berkeley, USA
- 3:00 - 3:30 PM “Hydrogen Production from Hydrocarbons by using Oxygen Permeable Membranes”  
**Hitoshi Takamura**, Tohoku University, Japan
- 3:30 - 3:45 PM “Direct Production of Pressurized Hydrogen from Waste Aluminum without Compressor”  
**T. Hiraki**<sup>a</sup>, N. Okinaka<sup>a</sup>, H. Uesugi<sup>b</sup> and T. Akiyama<sup>a</sup>, <sup>a</sup>*Center for Advanced Research of Energy Conversion Materials, Hokkaido University, Japan*, <sup>b</sup>*Waseda University, Japan*

**3:45 – 5:45 PM**      **FREE TIME/NETWORKING**

**6:00 PM**      **RECEPTION/DINNER:** Jefferson Hotel\*  
**\*Buses leave OMNI at 6:00 PM for Jefferson Hotel**

**SPEAKER:** **Ambassador Reno L. Harnish**, Principal Deputy Assistant Secretary, U.S. Department of State

**Wednesday, November 14**

**Session G: Storage III (Chemical Hydrides)**  
**Chairman: Maciej Gutowski, Heriot-Watt University, UK**

- 8:30 - 9:00 AM      “Indirect, Reversible Hydrogen Storage in Metal Ammine Salts: Recent Progress and Prospects”  
**Claus H. Christensen**, Technical University of Denmark, Denmark
- 9:00 - 9:30 AM      “Alkali Aminoboranes for Hydrogen Storage”  
**Ping Chen**, National University of Singapore, Singapore
- 9:30 - 10:00 AM      “Structure and Dynamics of Ammonia Borane”  
**S. Thomas Autrey**, Pacific Northwest Laboratory, USA
- 10:00 - 10:15 AM      “Molecular Simulation of Structural Changes of Ammonia Borane”  
**Gregory K. Schenter**, Chris Mundy, Shawn M. Kathmann, Vencislav Parvanov, Nancy J. Hess, Wendy J. Shaw, Herman M. Cho and Thomas Autrey, *Pacific Northwest National Laboratory, USA*
- 10:15 - 10:45 AM**      **COFFEE BREAK**

**Session H: Storage IV (Complex Hydrides)**  
**Chairman: Karl Johnson, University of Pittsburgh, USA**

- 10:45 - 11:15 AM      “Characterization of Complex Metal Hydrides by High Resolution Solid State NMR”  
**Robert C. Bowman**, Jet Propulsion Laboratory, NASA, USA
- 11:15 - 11:45 AM      “Hydrogenography: A combinatorial thin film approach to identify the thermodynamic properties of metal hydrides”  
**Bernard Dam**, Vrije University, Netherlands
- 11:45 - 12:15 PM      “First-principles engineering of advanced hydrogen storage materials”  
**Vidvuds Ozolins**, University of California, Los Angeles, USA
- 12:15 - 12:30 PM      “Development of Metal Hydrides for High-Pressure MH Tank”  
**T. Matsunaga\***, T. Shinozawa, K. Washio, D. Mori, M. Ishikiriyama  
*Higashifuji Technical Center, Toyota Motor Corporation, Japan*

**12:30 - 2:00 PM      LUNCH**

### **Session I: Fuel Cells II**

**Chairman: Peter Edwards, Oxford University, UK**

2:00 - 2:30 PM      “Materials Challenges in Solid Oxide Fuel Cells”  
**Subhash C. Singhal**, Pacific Northwest National Laboratory, USA

2:30 - 3:00 PM      “The Development of Nano-Composite Electrodes for Natural Gas-Assisted Steam Electrolysis for Hydrogen Production”  
**Raymond J. Gorte**, University of Pennsylvania, USA

3:00 - 3:30 PM      “Near-surface alloys and Core-shell nanocatalysts for reactions involving hydrogen”  
**Manos Mavrikakis**, University of Wisconsin, USA

3:30 - 3:45 PM      “Hybrid Inorganic-Organic Polymer Composites for Polymer-Electrolyte Fuel Cells”  
**Andrea Ambrosini**, Cy H. Fujimoto, Christopher J. Cornelius, *Sandia National Laboratories, Albuquerque, USA*

**3:45 - 4:15 PM      COFFEE BREAK**

### **Session J: Storage V (Complexhydrides)**

**Chairman: Vitalij Pecharsky, Ames Laboratory, USA**

4:15 - 4:45 PM      “Reaction Mechanism and Kinetics of Reactive Hydride Composites”  
**Martin Dornheim**, GKSS Research Centre Geesthacht, Germany

4:45 - 5:15 PM      “Single- and Double-Cations Borohydrides for Hydrogen Storage Applications”  
**Shin-ichi Orimo**, Tohoku University, Japan

5:15 - 5:45 PM      “Tetrahydroboranates: The New Hydrogen Storage Materials”  
**Andreas Borgschulte**, EMPA Materials Science and Technology, Switzerland

5:45 - 6:00 PM      “Storage of Compressed Hydrogen in Multi-capillary Arrays”  
N. K. Zhevago, *Kurchatov Institute, Russia* and **Dan Eliezer**, *Ben Gurion University, Israel*.

**6:00 - 8:00 PM      DINNER**

**8:00 -10:00 PM      Poster Session II**

**Thursday, November 15**

**Session K: Safety & Education**

**Chairman: B. S. Shivaram, University of Virginia, USA**

- 8:30 - 9:00 AM      “Structural-Materials Considerations for Hydrogen Gas Containment”  
**Chris San Marchi**, Sandia National Laboratory, USA
- 9:00 – 9:30 AM      “A National Agenda for Hydrogen Codes and Standards”  
**Chad Blake**, National Renewable Energy Laboratory, USA
- 9:30 -10:00 AM      “Educating Key Audiences about Fuel Cell Technologies”  
**Robert Remick**, National Renewable Energy Laboratory, USA
- 10:00 -10:15 AM      “Hydrogen behavior and coloration of tungsten oxide films prepared by magnetron sputtering and pulsed laser deposition”  
**S. Nagata**<sup>1</sup>, A. Inouye<sup>2</sup>, S. Yamamoto<sup>2</sup>, B. Tsuchiya<sup>1</sup>, T. Shikama<sup>1</sup>,  
*<sup>1</sup>Institute for Materials Reseach, Tohoku University, Japan, <sup>2</sup>Japan Atomic Energy Agency, Takasaki, Japan*
- 10:15 -10:45 AM      COFFEE BREAK**

**Session L: Storage –VI**

**Chairman: Ragaiy Zidan, SRNL, USA**

- 10:45 -11:15 AM      “Hydrogen Storage and Delivery Using Liquid Carriers”  
**Guido Pez**, Air Products and Chemicals Inc, USA
- 11:15 -11:45 AM      “Hydrogen Storage Materials – Playing the Odds”  
**W.I.F. David**, Oxford University, UK
- 11:45 -12:15 PM      “Probing Structure, Bonding, and Dynamics in Hydrogen StorageMaterials by Neutron-Scattering Techniques”  
**Terrence J. Udovic**, NIST Center for Neutron Research, USA
- 12:15 -12:30 PM      “Thermodynamics of Doped Complex Metal Hydrides”  
**J. Karl Johnson**<sup>1,2</sup>, Sudhakar V. Alapati<sup>3</sup>, Bing Dai<sup>1</sup>, David S. Sholl<sup>2,3</sup>  
*<sup>1</sup>Department. of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA 15261, USA; <sup>2</sup>National Energy Technology Laboratory Pittsburgh, PA 15236; <sup>3</sup>Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, USA*
- 12:30 - 2:30 PM      LUNCH**

2:30 - 4:00 PM

**Panel Discussion:**

**Chair: Scott W. Jorgensen**, General Motors, USA  
**Richard Chahine**, Univ. du Quebec a Trois Rivieres, Canada  
**Jeremy P. Meyers**, University of Texas, USA  
**George D. Parks**, Conoco-Phillips, USA  
**Astrid A. Pundt**, University of Goettingen, Germany  
**Yaroslav Filinchuk**, European Synchrotron Radiation Facility