Material Modeling and Simulation of Nuclear Fuels Workshop – #8

Sandia National Laboratories
October 19 – 21, 2009

Conference Host  Timothy Bartel
Member of Technical Staff
Advanced Nuclear Fuel Cycle Technologies Department
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International Protocol Office  Anisha Quiroz, Protocol Officer
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Monday, October 19, 2009  •  International Programs Building

7:30 am  Depart from Hyatt Place Uptown

7:45 am  Arrive Badge Office

8:15 am  Arrive International Programs Building – Check in

8:25 am  Administrative Announcements
Anisha Quiroz, International Protocol Office

8:30 am  Opening Remarks
Tim Bartel, Sandia National Laboratories
Marius Stan, Los Alamos National Labs

9:00 am  SNL Fuel Disruption Experiments
Steve Wright
Sandia National Laboratories, USA

Multi-Scale Modeling and Simulation Session

9:30 am  Models and Simulations of Nuclear Fuels: Results and Strategy
Marius Stan
Los Alamos National Laboratory, USA

10:00 am  The Results and Perspectives of the Safety of Advanced Nuclear Fuels Project at Institute for Transuranium Elements
Paul Van Uffelen
ITU, Germany

10:30 am  Simulating Xe Redistribution in UO2± x
David Anderson
Los Alamos National Laboratory, USA

11:00 am  Discussion Break

11:30 am  Group Photo

11:45 am  Luncheon in Bistro
Material Modeling and Simulation of Nuclear Fuels Workshop – #8
October 19 – 21, 2009

Agenda

**Density Functional Theory Session**

1:00 pm  
Ann E. Mattson  
Sandia National Laboratories, USA

1:30 pm  
Analysis of Bulk Properties and Defect Energies in –U Y
Benjamin Beeler  
Georgia Institute of Technology

2:00 pm  
DFT+U Modeling of Oxygen Point Defects in Uranium Dioxide: Imposing and Monitoring Occupation Matrices
Boris Dorado  
Commissariat à l'Énergie Atomique -Cadarache, France

2:30 pm  
Break

3:00 pm  
First Principles Study of Noble Gas Impurities and Defects in UO2
Alexander Thompson  
Northwestern University, USA

3:30 pm  
Ab Initio Calculation of Fission Product Gas Dynamics in UO2 as a Function of Lattice Dilation
Torey Semi  
Colorado School of Mines, USA

4:00 pm  
First-Principles Study of Physical Properties of Light Actinide Oxides
Younsuk Yun  
Uppsala University, Sweden

Poster  
Stability and Migration Mechanisms of Volatile Elements in Uranium Carbide
Michel Freyss  
Commissariat à l'Énergie Atomique -Cadarache, France

4:30 pm  
Discussion Break

5:00 pm  
Depart for Hyatt

Sandia National Laboratories  ♦  Albuquerque, New Mexico  USA
Tuesday, October 20, 2009 • International Programs Building

8:00 am  Depart from Hyatt Place Uptown

**Molecular Dynamics Session**

8:30 am  An Atomic Insight of the Primary Irradiation Damages in Nuclear Fuel UO2 with Molecular Dynamics Simulations  
Laurent Van Brutzel  
Commissariat à l’Énergie Atomique - Saclay, France

9:00 am  Grain Boundary Structures and Influence on Segregation Properties in Uranium Dioxide  
Blas Uberuaga  
Los Alamos National Laboratory, USA

9:30 am  The Effect of Electron-Ion Coupling on Radiation Damage Simulations of a Pyrochlore Waste Form  
Paul Crozier  
Sandia National Laboratories, USA

10:00 am  Discussion Break

**Experimental Investigations Session**

10:30 am  Oxygen Diffusion in Relation to P-Type Doping in Uranium Dioxide  
Philippe Garcia  
Commissariat à l’Énergie Atomique - Cadarache, France

11:00 am  XANES and the Electronic State of Americium Oxides  
Chikashi Suzuki  
Japan Atomic Energy Agency, Japan

11:30 am  Core Materials Development for Advanced Fuel Cycle Initiative  
Stuart Maloy  
Los Alamos National Laboratory, USA

12:00 pm  Discussion Break

12:30 pm  Luncheon in Bistro
Mesoscale Modeling Session

1:30 pm  Phase-Field Simulation of Void and Fission-Gas Bubble Evolution in Irradiated Polycrystalline Materials
Paul Millett
Idaho National Laboratory, USA

2:00 pm  Mesoscale Modeling of the Mechanical Response of UO2 Microstructures
Remi Dingreville
Polytechnic Institute of New York University, USA

2:30 pm  Potts Model for Simulating Main Characteristics of High Burnup Structure in UO2 Nuclear Fuels
Jae-Yong Oh
Korea Atomic Energy Research Institute, Korea

3:00 pm  Framework for Mesoscale Simulation of Microstructural Evolution of Nuclear Fuels using Potts Kinetic Monte Carlo Methods
Veena Tikare
Sandia National Laboratories, USA

3:30 pm  Defect Clustering and Xenon Migration in UO2
Ram Devanathan
Pacific Northwest National Laboratory, USA

Poster  Development of a Mesoscale Approach to the Swelling of Nuclear Fuels
Zeke Insepov
Argonne National Laboratory, USA

4:00 pm  Discussion Break

Chemistry and Specie Transport Session

4:30 pm  Thermochemical Modeling of Fluorite-Structure Actinide Oxides
Theodore Besmann
Oak Ridge National Laboratory, USA

5:00 pm  Thermochemical Modeling of Advanced Oxide and Carbide Nuclear Fuels within the FUELBASE Project
Christine Gueneau
Commissariat à l’Énergie Atomique -Saclay, France

5:45 pm  Depart for National Museum of Nuclear Science & History for Hosted Dinner

8:30 pm  Depart for Hyatt
Wednesday, October 21, 2009  ♦  International Programs Building

8:00 am  Depart from Hyatt Place Uptown

**Chemistry and Specie Transport Session-contd.**

8:30 am  Development of a Gibbs Energy Minimizer for Integration into Nuclear Fuel Performance Codes  
Markus Piro  
*Royal Military College of Canada, Canada*

9:00 am  Stoichiometry Drift Behavior of Mixed Oxide Fuel During Air Atmosphere Storage  
Masahiko Osaka  
*Japan Atomic Energy Agency, Japan*

Poster  Advances in Phase-Field Modeling of Laser Flash Experiments  
*Michael Welland*  
*ITU, Germany*

9:30 am  Discussion Break

**Continuum Modeling Session**

10:00 am  Simulations of Dynamic Crack Propagation Using the Material Point Method  
Hongbing Lu  
*University of North Texas, USA*

10:30 am  Fully-coupled Engineering and Mesoscale Simulations of Thermal Conductivity in UO2 Fuel Using an Implicit Multiscale Approach  
Michael Tonks  
*Idaho National Laboratory, USA*

11:00 am  CANDU Fuel Element Behaviour Modeling  
Khaled Shaheen  
*Royal Military College of Canada, Canada*

11:30 am  BISON: An Implicit Solution Framework for Fuel Performance Simulation  
Glen Hansen  
*Idaho National Laboratory, USA*

12:00 pm  Luncheon in Bistro

1:00 pm  Discussion Break

1:30 pm  General Discussion on Direction of MMSNF: Where are we and where are we going?

2:00 pm  Depart to Hyatt or Optional Tour of SNL Experimental Reactor Facility

*Sandia National Laboratories ♦ Albuquerque, New Mexico USA*
Agenda

Participant List

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<th>Wasatch Molecular</th>
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