

Material Modeling and Simulation of Nuclear Fuels Workshop – #8

Sandia National Laboratories
October 19 – 21, 2009



Conference Host

Timothy Bartel
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Material Modeling and Simulation of Nuclear Fuels Workshop – #8
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Agenda

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**



Agenda

Density Functional Theory Session

- 1:00 pm** **Density Functional Theory and F-Electron Systems: Relativity and Exchange-Correlation Functionals**
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
- 3:30pm** **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**



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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**



Agenda

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**



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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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