



**Materials Models and Simulations for Nuclear Fuels**  
MMSNF-4, November 17-18, 2005, Washington DC, U.S.A.  
Omni Shoreham Hotel, Forum Room  
<http://public.lanl.gov/mastan/MMSNF/>



**AGENDA**

**THURSDAY, Nov. 17**

**Session A: Fuel Performance and Characterization.** Chairs: K. Pasamehmetoglu (INL) and M. Stan (LANL).

**1:00 p.m.** K. Pasamehmetoglu (INL), *Review of the Advanced Fuel Cycle Program.*

1: 20 M.S. Veshchunov (IBRAE) and R. Dubourg, *Numerical Simulation of Fission Product Release under Accidental Conditions with the MFPR Code.*

1:40 A. M. Casella (UMC) and S. K. Loyalka, *Simulation of Fission Gas Transport in TRISO Coated Fuels.*

2:00 J.C. Ramirez (LANL), P. Cristea, S. Y. Hu, M. Stan, and M. I. Baskes, *Incorporating Atomistic and Phase Field Calculations into Heat, Oxygen, and Helium Transport Simulations in Nuclear Fuel Rods.*

2:20 Christine Guéneau (CEA), Sylvie Chatain, Jean-Christophe Dumas, Jean-Paul Piron, Jacques Lechelle, Yves Pontillon, Gérard Ducros, Cyril Rado, Françoise Defoort, Karine Froment, Nathalie Dupin, Bo Sundman, Henri Noël, Rudy Konings, *FUELBASE : A Thermodynamic Database for Advanced Nuclear Fuels.*

2:40 *Discussion.*

3:00 COFEE BREAK

3:20 C. R. Stanek (LANL), K.J. McClellan, J.T. Dunwoody, S.L. Voit, S.A. Maloy, T. Hartmann, N. Ashley, and R. W. Grimes, *Nitride Fuel Development for APCI Transmutation: Experiments and Atomistic Simulations.*

3:40 K. Wheeler (Arizona State Univ.), M. Parra, J. Dunwoody, C. Stanek, P. Peralta and K. J. McClellan, *Mechanical Properties and Microstructure of ZrN Pellets as Surrogates for Nitride Fuels: Effect of Sintering Conditions.*

4: 00 Jean-Marc Ricaud (CEA) and Bruno Michel, *A New Approach in Multiscale Behaviour Modelling of Nuclear Fuel. Feasibility Studies in High Temperature Reactor Concept and First Results.*

4:20 M. Stan (LANL), *Towards an Advanced, Theory-Based, Fuel Performance Code.*

4:40 *Discussion.*

**5:00 PM End of session.**



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**FRIDAY, Nov. 18**

**Session B: Models and Simulations of Materials Properties.** Chairs: (J. Tulenko, Univ. of Florida) and S. Srivilliputhur (LANL).

**8:00 a.m.** J. Tulenko (Univ. Florida), *Nuclear Energy Overview.*

8:20 Z. K. Liu (PennState Univ.) *Overview of the NSF Industry/University Cooperative Research Center for Computational Materials Design.*

9:00 M. Bertolus (CEA) and F. Ribeiro, *Mechanisms of Amorphization-induced Swelling in Silicon Carbide: the Molecular Dynamics Answer.*

9:20 J.L. Flèche, Ph. Zeller, A. Chartier, S. Chatain (CEA), and C. Guéneau, *Ab-Initio Calculations Coupled With a Thermodynamic Model to Determine Thermodynamic Properties of Actinide Compounds Versus Temperature.*

9:40 T. B. Besmann (ORNL), N. Kulkarni, K. E. Spear, and John D. Vienna, *Predicting Phase Equilibria and Thermochemistry in Nuclear Waste Glass Systems.*

10:00 COFFEE BREAK

10:20 E. Kotomin (ITU), P. Van Uffelen, and C. Ronchi, *Atomistic Modeling of Radiation and Impurity Defects in UN Nuclear Fuels.*

10:40 Chaitanya Deo (LANL), Blas P. Uberuaga, S. G. Srinivasan, S. A. Maloy, T. Patten, and J. Stubbins, *Multiscale Simulations of Defects in Hyperstoichiometric Uranium Di-Oxide.*

11:00 P. Cristea (LANL) and M. Stan, *Point Defects and Oxygen Diffusion in  $UO_{2+x}$ .*

11:20 S. G. Srivilliputhur (LANL), C. S. Deo, M. Okuniewski, M. I. Baskes, M. R. James, S. A. Maloy, and J. Stubbins, *Multiscale Modeling of Radiation Damage in Reactor Materials.*

11:40 *Discussion.*

**12:00 PM End of workshop.**