

Viterbi School of Engineering Research Innovation Fund Report

USC SYMPOSIUM ON “STRUCTURE AND FUNCTION OF ENERGETIC MATERIALS”

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1. Summary of the Program

This fund has provided support for a Symposium on “Structure and Function of Energetic Materials,” which was held at USC on July 28-29, 2008. The Symposium has promoted the confluence of ideas and expertise from diverse experimental and theoretical approaches and fostered collaborative activities between USC faculty, researchers from other universities with strong programs in the field of energetic materials, and DoD laboratories in order to accelerate research on energetic materials on the nanometer scale.

The invited speakers of the Symposium and the title of their presentations were:

- Prof. Karl O. Christe (University of Southern California)
“Recent Progress in High-Oxygen Carriers of Interest as Green Replacement for AP and Hydrazine”
- Prof. Kenneth K. Kuo (Pennsylvania State University)
“RDX Thermal Decomposition Kinetics and Combustion Modeling”
- Prof. Naresh Thadhani (Georgia Institute of Technology)
“Multiscale Processes and Mechanisms Controlling Mechanical Stability and Energetics of Reactive Metal Mixtures”
- Prof. Richard Yetter (Pennsylvania State University)
“Nanoparticle Combustion and Microthrusters”
- Prof. Michael R. Zachariah (University of Maryland)
“Understanding and Tuning the Reactivity of NanoEnergetic Materials”

In addition Professors Rajiv K. Kalia and Aiichiro Nakano from USC participated in the Symposium.

2. Exploring New Directions and Funding Opportunities

DARPA is about to launch a major program to develop enabling technologies for the integration of electronics and nano-energetic materials. We have formed an interdisciplinary team of experts on micro-pyrotechnics, energetic microsystems, and nano-energetic materials from the U.S. Army Research Laboratory (ARL), Pennsylvania State University (PSU), and the European Union (EU) to pursue the opportunity: Rajiv Kalia, Aiichiro Nakano, Priya Vashishta (USC); Madan Dubey, Wayne Churaman, Luke Currano, Christopher Morris, Eugene Zakar, Paul

Amirtharaj, Brett Piekarski (ARL, Adelphi, MD); Rich Yetter (PSU); Carole Rossi, Alain Esteve (CNRS, Toulouse, France). In particular, Dr. Anne Hemeryck from CNRS-Toulouse is visiting us from September 2009 to March 2010 to conduct joint USC-CNRS research on nano-energetic materials.

3. Outcomes and Impact

Publications, presentations, and an award resulting from the Symposium are listed below.

Publications

1. “Enhanced reactivity of nanoenergetic materials: a first-principles molecular dynamics study based on divide-and-conquer density functional theory,” F. Shimojo, A. Nakano, R. K. Kalia, and P. Vashishta, *Applied Physics Letters* **95**, 043114: 1-3 (2009).
2. “Multi-million atom molecular dynamics study of combustion mechanism of aluminum nanoparticle,” W. Wang, R. Clark, A. Nakano, R. K. Kalia, and P. Vashishta, *Materials Research Society Symposium Proceedings* **1137**, EE-10-29: 1-6 (2009).

Invited Presentations

- “Multimillion to billion atom simulations of nanosystems under extreme conditions,” *Computational Approaches and Applications in Earth Materials Studies*, American Geophysical Union, San Francisco, CA, December 15-19, 2008.
- “Multibillion-atom simulations of nano-mechano-chemistry on petaflops computers,” *First International Symposium on Global Center of Excellence for Mechanical Systems Innovation*, Tokyo, Japan, February 2, 2009.
- “Large spatiotemporal-scale material simulations on petaflops computers (opening keynote),” *Winter School on Multiscale Simulation Methods in Molecular Sciences*, Jülich, Germany, March 2, 2009.
- “High performance computing for billion atom simulations of nanosystems,” *Scientific Discovery through Advanced Computing, ICCES’2009*, Phuket, Thailand, April 7-11, 2009.
- “Multimillion atom simulations of reactive nanosystems,” *Symposium on Nano-scale Energetic Materials: Fabrication, Characterization and Molecular Modeling*, E-MRS, Strasbourg, France, June 8-12, 2009.
- “Metascalable atomistic simulations of nano-mechano-chemistry on petaflops computers,” *European Materials Research Society 2009 Spring Meeting*, Strasbourg, France, June 10, 2009.
- “Large reactive molecular dynamics simulations of nano-mechano-chemistry on petaflops computers,” *Workshop on “Molecular Dynamics with Reactive Potentials”*, Memphis, TN, August 5, 2009.

Award

- Best Poster Award, W. Wang, *Materials Research Society Fall Meeting* (December 2009).