

Agenda (final) for the 2011 NIST Workshop on Atomistic Simulations for Industrial Needs
NIST Gaithersburg, Building 101, Lecture Room A

Questions: Chandler Becker, 301-975-5344, chandler.becker@nist.gov

Thursday, June 23, 2011

09:00 AM	Clear Security and the front gate	
09:30 AM	Welcome	Frank Gayle, NIST
09:45 AM	Overview and Introductions	Chandler Becker, NIST
10:30 AM	Multi-scale approach to the development of anti-ice coatings	Sonia Tulyani, UTRC
11:00 AM	Computational solutions to industrially-funded simulations	Bill Goddard, CalTech
11:30 AM	<i>Discussion: Experiences and challenges related to industrial use of atomistics and collaborations</i>	
12:15 PM	<i>Lunch</i>	
01:30 PM	Infrastructure for industrial atomistic modeling	Hannes Schweiger, Materials Design
02:00 PM	Ensuring reliability, reproducibility and transferability in atomistic simulations: the Knowledgebase of Interatomic Models (openKIM.org)	Ronald Miller, Carleton Univ.
02:30 PM	The universal interface for testing atomistic potentials	Bohumir Jelinek, Mississippi State Univ.
03:00 PM	Atomic-scale modeling platform for nanoelectronics	Anders Blom, Quantum Wise
03:30 PM	<i>Break</i>	
03:45 PM	<i>Discussion: Linking software, methods, and scales</i>	
05:15 PM	Adjourn	
07:00 PM	Dinner at The Fontina Grille 801 Pleasant Drive, Rockville, MD 20850 301-947-5400	

Friday, June 24, 2011

09:00 AM	New MEAM potentials being developed for the Al, Si, Mg, Cu, and Fe alloy system	Mike Baskes, LANL
09:30 AM	Atomistic modeling of grain boundary motion and grain rotation	Zachary Trautt and Yuri Mishin, George Mason Univ.
10:00 AM	Simulations for primary metals production	Scott Oppenheimer, ATI Allvac
10:30 AM	<i>Break</i>	
11:00 AM	Overview of current ReaxFF applications for metals, alloys, oxides and their surface reactions with hydrocarbons, water and organosulfur compounds	Adri van Duin, Penn. State Univ.
11:30 AM	The use of surface energies at QuesTek	Art Counts, QuesTek Innovations
12:00 PM	<i>Lunch</i>	
01:00 PM	<i>Discussion:</i> <i>* From an academic perspective, what has made industrial collaborations successful?</i> <i>* From an industrial perspective, what are ideas for projects where academics could hope to collaborate?</i> <i>* Is there support for industrial funding of collaborations?</i> <i>* What are outstanding problems that academics might address?</i> <i>* What is the role of national laboratories and government agencies?</i> <i>* What should we do with \$1 million? \$10 million?</i>	
03:00 PM	Adjourn	