Agenda for the 2010 NIST Workshop on Atomistic Simulations for Industrial Needs
NIST Gaithersburg, Building 101, Lecture Room D

Tuesday, July 27, 2010

08:30 AM	Clear security and the front gate	
09:00 AM	Introduction and Welcome	
09:30 AM	Robust Quantum-Based Interatomic Potentials for Transition Metals	John Moriarty, LLNL
10:00 AM	Limitations of Atomic Modeling for Nanomaterial Applications	Sadasivan Shankar, Intel
10:30 AM	Discussion / break	
11:00 AM	Development and applications of ReaxFF reactive force fields for combustion, catalysis and material failure	Adri Van Duin, Penn. State U.
11:30 AM	Applications of ReaxFF reactive force fields in hydrogen storage	Julius Ojwang, CIW
12:00 PM	lunch (NIST cafeteria)	
01:30 PM	Interatomic potentials for complex systems: recent development	Yuri Mishin, George Mason U.
02:00 PM	Ideas from Multi-state MEAM Applied to the Pu-Ga System	Mike Baskes, LANL
02:30 PM	Molecular dynamics simulations of multicomponent oxide glasses	Jincheng Du, U. North Texas
03:00 PM	Discussion / break	
03:30 PM	Integrating atomic potentials across the interfaces	Yue Qi, GM
04:00 PM	MEAM Interatomic Potential Generation: Coupling MATLAB with Atomistic Codes	Mark Tschopp, MS State U.
04:30 PM	Discussion and daily wrap-up	

07:00 PM Dinner at The Fontina Grille
801 Pleasant Drive, Rockville, MD 20850
301-947-5400

Wednesday, July 28, 2010

09:00 AM	Forcefield parameter determination in and from atomistic scale for non-covalent interactions	Jian-jie Liang, Accelrys
09:30 AM	A comprehensive environment for property prediction and forcefield development	Hannes Schweiger, Materials Design
10:00 AM	Open Knowledgebase of Interatomic Models (OpenKIM.org): an online platform for testing and archiving empirical potentials.	Ellad Tadmor, U. Minnesota
10:30 AM	Towards an API standard for the Knowledgebase of Interatomic Models (KIM)	Valeriu Smiricinschi, U. Minnesota
11:00 AM	Discussion	
12:00 PM	lunch (NIST cafeteria)	
01:00 PM	Role of precipitates in commercial Al and Mg alloys	Bita Ghaffari, Ford
01:30 PM	Development of Interatomic Potentials Appropriate for Simulation of Solid-Liquid Interface Properties in Al-Mg Alloys	Mikhail Mendelev, Ames Nat. Lab.
02:00 PM	Role of Sr in the Atomic Structure of Liquid Al-Si Hypoeutectic Alloys Using High Energy X-Ray Diffraction	Matthew Kramer, Ames Nat. Lab
02:30 PM	Finding long-range orientational order in a metallic glass	Howard Sheng, George Mason U.
03:00 PM	Discussion and workshop wrap-up	