NIST Workshop on Atomistic Simulations for Industrial Needs
September 11-12, 2012. Building 101, Lecture Room A

Sept. 11, 2012

08:00 AM	Arrive at gate	
ATOMISTICS AND THE MATERIALS GENOME INITIATIVE		
09:00 AM	Welcome and introductions	
09:30 AM	An overview of the MGI	Warren
10:00 AM	Case Study I: 60-GPa Carbon Nanotube Fiber Design Based on Molecular Dynamics Simulations	Cornwell
10:30 AM	*Break*	
11:00 AM	Discussion: What is 'atomistics', and how does it fit into MGI efforts?	
11:30 AM	Discussion: Challenges of using atomistics in the MGI and industry	
12:30 PM	*Lunch (NIST cafeteria)*	
MODELS AND METHODS		
02:00 PM	Development and application of charge optimized many-body (COMB) potentials for modeling surface chemistry and heterogeneous interfacial interactions	Sinnott/Liang
02:30 PM	An interatomic potential for saturated hydrocarbons based on the modified embedded-atom method	Baskes
03:00 PM	A concentration dependent embedded atom method (CD-EAM) potential for light-weight Mg-Li alloys	Karewar
03:30 PM	*Break*	
04:00 PM	Atomistic Simulation of the Structural and Dynamic Inhomogeneity in Supercooled Metallic Liquids	Sheng
04:30 PM	Using molecular simulation to compute interfacial properties	Errington
05:00 PM	Phase boundaries and mixing thermodynamics in model atomic systems	Gelb
05:30 PM	*Adjourn for day*	
07:00 PM	*Dinner: That's Amore, Rockville, MD*	

Sept. 12, 2012

DATA, SOFTWARE AND TOOLS		
08:45 AM	*Announcements*	
09:00 AM	Case Study II: Using Simulations to Guide the Design and Synthesis of a Super Structural Ceramic Composite	Welch/ Devine
09:30 AM	From Atoms to Materials Properties: A Data Perspective	Freiman/Rumble
09:45 AM	A Framework for and Systematic Validation of DFT, Potentials and Forcefields	Saxe
10:00 AM	Strawman for discussion: Property calculation example	Becker
10:15 AM	Discussion: Requirements for models (potentials/forcefields), testing, required metadata, uncertainties, connections between models and software	
10:45 AM	*Break*	
FUNDING AND SUSTAINABILITY		
11:15 AM	MGI at the NSF	Farkas
11:45 AM	Discussion: How do we sustain this? What is a viable business model? Data plans. What are realistic goals? Stretch goals?	
12:30 PM	*Lunch (NIST cafeteria)*	
WHERE DO WE GO FROM HERE?		
01:30 PM	Closing discussions: Where do we go from here? What should be in the white paper?	
03:00 PM	*Adjourn*	