

Agenda

Agenda for the 2009 NIST Workshop on Atomistic Simulations for Industrial Needs Building 223 Room B307 (MSEL Conference Room)

Apr 27, 2009

08:30 AM Clear Security and the front gate
09:00 AM Introduction and Welcome
09:30 AM Siegel Combining computations and experiments to probe interfacial chemistry at the nanoscale
10:00 AM Heinz Simulation of FCC Metals and Metal-Biological Interfaces for Nanoelectronic and Sensor Applications

10:30 AM Break/Discussion

11:00 AM Shankar The Computational Nanomaterial Applications and Needs
11:30 AM Liang Automation in refining nonbond parameters in forcefield development

12:00 PM Lunch (NIST Cafeteria)

01:30 PM Schweiger Materials Modeling using the MedeA software platform: an update
02:00 PM Goddard Advances in force fields for catalysis, pharma, polymers, and complex systems and industrial applications
02:30 PM Kramer Experimental Validation of Atomistic Simulations: Case Studies from Amorphous and Liquid Metals

03:15 PM Break

03:45 PM Sheng Atomistic Modeling of the Structure of Ternary Metallic Glasses
04:15 PM Chaka The Prediction Challenge
04:45 PM Becker The NIST Interatomic Potentials Repository
05:00 PM Discussion
05:30 PM Daily Wrap-up

06:30 PM Dinner at The Flaming Pit
18701 N. Frederick Road
Gaithersburg, MD 20879
(301) 977-0700

Apr 28, 2009

08:30 AM Mishin Atomistic Simulations of the Martensitic Transformation in B2-NiAl
09:00 AM Baskes A Modified Embedded Atom Method Potential for Fe
09:30 AM Ackland Metallic/Covalent/Ionic Interatomic potentials for Ferritic Steels.

10:00 AM Break/Discussion

10:15 AM Kattner Calphad modeling of homogeneity ranges
10:30 AM Foiles Connecting MD info to higher length scale models of grain growth
11:00 AM Qi Modeling, Measuring and Scale Bridging of the Mechanical Properties at Al/Si Interface

11:30 AM Discussion/Closing
12:00 PM Lunch (NIST Cafeteria)

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Participants

<u>Last</u>	<u>First</u>	<u>Affiliation</u>
Ackland	Graeme	University of Edinburgh, UK
Apostol	Florin	George Mason University
Baskes	Mike	Los Alamos National Laboratory
Becker	Chandler	NIST Metallurgy Division
Cahn	John	NIST Metallurgy Division, University of Washington
Chaka	Anne	NIST Physics Laboratory
Cockayne	Eric	NIST Ceramics Division
Cundari	Tom	Univ of North Texas
Elliott	Ryan	University of Minnesota
Foiles	Stephen	Sandia National Laboratory
Frolov	Timofey	George Mason University
Goddard III	William A.	California Institute of Technology
Heinz	Hendrik	University of Akron
Kattner	Ursula	NIST Metallurgy Division
Kramer	Matthew J.	Ames National Laboratory
Lee	Tongsik	Brown University
Levine	Lyle	NIST Metallurgy Division
Liang	Jian-Jie	Accelrys
Mishin	Yuri	George Mason University
Mountain	Ray	NIST Chemical Science and Technology Laboratory
Ojwang	Julius	Carnegie Institute of Washington
Pun	Ganga	George Mason University
Qi	Yue	General Motors
Schweiger	Hannes	Materials Design
Shankar	Sadasivan	Intel Corporation
Sheng	Howard	George Mason University
Siegel	Don	Ford Motor Company
Srivilliputhur	Srinivasan	University of North Texas
Tavazza	Francesca	NIST Metallurgy Division
Wagner	Richard	NIST Metallurgy Division
Wilson	Angela	University of North Texas