

Workshop on Coarse-Grained Modeling of Polymers and Soft Materials for the Materials Genome Initiative

August 6-7, 2014

National Institute of Standards and Technology (NIST)
Gaithersburg, MD

Sponsored by

- Material Measurement Laboratory (MML), NIST
- Center for Hierarchical Materials Design (CHiMaD)

Organizing Committee

- Juan de Pablo, University Chicago/CHiMaD
- Jack F. Douglas, NIST
- Frederick R. Phelan Jr., NIST
- Rob Riggelman, University of Pennsylvania

Program Schedule – Day 1

Wednesday August 6, 2014

Green Auditorium

9:00 AM	Welcome and Introductions	Fred Phelan, NIST James Warren, NIST Juan de Pablo, CHiMaD
	Session I: Developments in Quantitative Coarse-Graining and Bottom-Up Methods	Moderator: Fred Phelan
9:25 AM	Announcements and Session Introduction	
9:30 AM	Challenges for Coarse-Graining the Structure And Thermodynamics of Soft Materials	Will Noid, Penn State
10:00 AM	Structural Coarse-Graining for Polymers Under Different Conditions - Opportunities and Limitations	Roland Faller, UC Davis
10:30 AM	<i>Coffee Break (30 minutes)</i>	
11:00 AM	Driving Innovation for Advanced Materials & Systems Soft Matter Modeling	Pieter in 't Veld, BASF
11:30 AM	Multi-Scale Coarse-Graining of Non-Conservative Interactions in Molecular Systems and its Application to Coarse-Graining of Molecular Explosives	Sergei Izvekov, ARL
12:00 PM	Discussion Session I	
12:30 PM	<i>Lunch (70 minutes)</i>	NIST Cafeteria
	Session II: Mesoscale Modeling, Material Properties and Non-Equilibrium Dynamics	Moderator: Rob Riggelman
1:40 PM	Announcements and Session Introduction	
1:45 PM	A Coarse-Graining Method that Preserves the Free Energy, Structural Correlations, and Thermodynamic State of Polymer Melts From the Atomistic to the Mesoscale	Marina Guenza, Oregon
2:15 PM	Nonlinear Rheology Predictions of Highly Entangled Polymers from Coarse-Graining Atomistic Simulations	Jay Schieber, IIT
2:45 PM	<i>Coffee Break (45 minutes)</i>	
3:30 PM	Mechanical Properties of Glassy Polymers from Coarse-Grained Simulations	Mark Robbins, Johns-Hopkins
4:00 PM	Simulating Morphology Transitions in Block Copolymer Materials	Marcus Müller, Göttingen
4:30 PM	Discussion Session II	
5:00 PM	Day 1 Adjournment – Announcements and Travel Logistics	
6:30 PM	Dinner(Cash)	That's Amore!, Gaithersburg

Program Schedule – Day 2

Thursday, August 7, 2014

Green Auditorium

	Session III: Scale-Bridging, Mesoscale Continuum Models and Applications	Moderator: Jack Douglas
8:55 AM	Announcements and Session Introduction	
9:00 AM	Equilibrium and dynamical coarse-graining of polymer nanoparticle mixtures	Venkat Ganesan, UT Austin
9:30 AM	Polymeric and Composite Electrolyte Membranes: Insights from Multiscale Modeling	James Elliott, Cambridge
10:00 AM	<i>Coffee Break (30 minutes)</i>	
10:30 AM	Ionic Bilayers Tail Packing and Mesoscale Geometry	Monica Olvera de la Cruz, Northwestern
11:00 AM	Phase-Field Modeling of Polycrystalline Solidification: From Needle Crystals to Spherulites	Laszlo Granasy, Wigner Research Centre for Physics
11:30 AM	Discussion Session III	
12:00 PM	<i>Lunch (1 hour)</i>	NIST Cafeteria
1:00 PM	Session IV: Plotting the Path Forward - Opportunities for Scale Linking - Discussion of CALPHAD for Polymers Approach - High Level Data Containers and Data Mining	Moderator: Juan de Pablo
2:00 PM	Adjournment	