

Workshop on Modeling and Simulation of Materials in Soft Matter Science
Iran Thomas Auditorium, Spallation Neutron Source, Building 8600
Oak Ridge National Laboratory, Oak Ridge, TN
November 9-11, 2011

Wednesday, November 9, 2011

1130 Registration opens, Lunch available in SNS cafeteria on your own

1300 Plenary Session

- ORNL Welcome, Kelly Beierschmitt, ORNL
- Workshop welcome – William Heller, ORNL, and Michael Ohl, FZJ
- “Data and Analysis: A Vision for Neutron Sciences”, Robert McGreevy, ORNL
- "Polymer dynamics under confinement: Neutron scattering meets simulation", Dieter Richter, FZJ

1425 – 1500 Questions and break

- “Static and Dynamic Properties of Telechelic Gels”, Walter Kob, Université Montpellier 2
- "Molecular transport and structure of surface modified nanopores: From small ions in nanochannels to nuclear pore complexes", Igal Szleifer, Northwestern University

1610 Summary discussion and session ends.

Dinner on your own

Thursday, November 10, 2011

0800 Registration opens, breakfast available

0900 Complex Materials Session, invited talks

- "Non-equilibrium dynamics of linear and star polymers in solution", Gerhard Gompper, FZJ
- "Simulation Studies of Electrolytes for Batteries and Double Layer Capacitors", Oleg Borodin, Army Research Laboratory

1015 Questions and break

1045 Complex Materials Session resumes, contributed talks

- “Concerted neutron diffraction and MD simulations studies of biomembranes,” J. Alfredo Freites, Univ. California – Irvine
- “Study of water diffusion on single-supported bilayer lipid membranes by quasielastic neutron scattering,” Andrew Miskowiec, University of Missouri

1120 Session summary and lunch with tours of the Spallation Neutron Source

1300 Polymers Session, Invited talks

- "Structure formation of multicomponent polymer materials studied by soft, coarse-grained models", Marcus Mueller, Universität Göttingen
- "Collective dynamics in polymers and glass-forming liquids", Alexei Sokolov, ORNL
- "Computational exploration and design of functional nanostructured materials", Bobby Sumpter, ORNL

1445 – 1530 Discussion and Break

- “Modeling the Miscibility, Self-Assembly and Rheology of Polymer - Nanocomposites”, Sanat Kumar, Columbia Univ.

Contributed talks

- “Structural Characteristics of Polyelectrolyte Dendrimer Solutions Revealed by Neutron Scattering and Atomistic Simulation,” Bin Wu, ORNL

1625 Summary

1730 Poster session begins with heavy hors d’oeuvres

1900 Poster session ends

Friday, November 11, 2011

0830 Biology Session, Invited talks, breakfast available

- Biomolecular Structure and Dynamics from Integration of Simulation and Neutron Scattering, Jeremy Smith, ORNL
- “Structure of biomass components revealed by SANS and simulation”, Loukas Petridis, ORNL
- “Internal Protein dynamics accessed by NSE”, Ralf Biehl, FZJ

1015 – 1045 Summary and break

- "Mechanistic understanding of RNA delivery: simulations of vector-RNA complexation", Sean Smith, ORNL

Contributed talks

- “Statistical inference of structural dynamics of intrinsically disordered proteins using neutron scattering and molecular dynamics simulations,” Arvind Ramanathan, ORNL
- “Redox – Promoting Protein Motions in Rubredoxin” , Jose Borreguero, ORNL

Session summary

1200 Tours of Center for Nanophase Materials Sciences and lunch provided

1300 Workshop Summary session

Workshop report developed

1500 Workshop ends