

Grand Challenges in Modeling the Assembly and Properties of Nanomaterials

Wednesday, August 20

- 8:30 AM –8:45 AM **Robert Rosner**, ANL
- 8:45 AM - 9:15 AM **Samuel Bader**, ANL
Overview of the Center for Nanoscale Materials at ANL
- 9:15 AM - 9:55 AM **Stephen Gray**, ANL
Computational Nanoscience at the CNM
- 9:55 AM -10:10 AM *Coffee break*
- 10:10 AM -10:50 AM **Tamar Seideman**, Northwestern University
Current-driven dynamics in molecular electronics: From surface
nanochemistry to molecular machines
- 10:50 AM -11:30 AM **Michel Dupuis**, Pacific Northwest National Lab
Nano-tailored Reactivity: Models, Tools, and Examples
- 11:30 AM -11:50 AM **Tijana Rajh**, ANL
Healing of the Nanoparticle Surface: Opportunity for Charge
Transfer across Nanoparticle Junction
- 12:00 noon – 1:30 PM *Lunch*
- 1:30 PM 2:10 PM **Krishnan Raghavachari**, University of Indiana
Quantum Chemical studies of semiconductor surface chemistry
using cluster models
- 2:10 PM - 2:50 PM **Qiang Cui**, University of Wisconsin-Madison
Exploring mechanochemical coupling in molecular motors with
molecular simulations
- 2:50 PM - 3:10 PM *Coffee Break*
- 3:10 PM - 3:50 PM **Susan Sinnott**, University of Florida
Computational Studies of the Chemical Modification of Carbon
Nanotube-Based Structures
- 3:50 PM - 4:20 PM **Barry Smith**, ANL
PETSc: Linear and Nonlinear Solvers for PDE Simulations
- 4:20 PM - 5:00 PM **Robert Harrison**, Oak Ridge National Lab
TBA

Thursday, August 21

- 9:00 AM – 9:40 AM **Jim Chelikowsky**, University of Minnesota
Optical properties and doping of semiconductor nanocrystals
- 9:40 AM – 10:20 AM **Serdar Ogut**, University of Illinois at Chicago
First Principles Dielectric Screening in Si Quantum Dots
- 10:20 AM – 10:40 AM *Coffee Break*
- 10:40 AM – 11:20 AM **Evelyn Goldfield**, Wayne State University
Molecular hydrogen confined in a nanotube
- 11:20 AM – 12:00 noon **Deepak Srivastava**, NASA Ames Lab
Computational Nanotechnology of Materials and Devices
with Carbon Nanotubes and Fullerenes
- 12:00 noon – 1:30 PM *Lunch*
- 1:30 PM - 2:10 PM **Karl Freed**, University of Chicago
Thermodynamics of competition between polymerization and
phase separation in equilibrium polymerization
- 2:10 PM - 2:50 PM **Woods Halley**, University of Minnesota
Simulation of Electrochemical Interfaces and Nanoparticles
Using Self Consistent Tight Binding Methods.
- 2:50 PM - 3:10 PM **Millicent Firestone**, ANL
Nanostructured Biocomposite Materials for Energy Transduction
- 3:10 PM - 3:30 PM *Coffee Break*
- 3:30 PM - 4:10 PM **Boris Yakobson**, Rice University
Modeling 1D materials: Nanowires, Nanotubes and Their
Assemblies
- 4:10 PM - 4:30 PM **Axel Hoffmann**, ANL
Magnetic Anisotropies in coupled antiferromagnetic/ferromagnetic
systems
- 4:30 PM - 5:10 PM **Mark Ratner**, Northwestern University
Simple Junctions and Beyond

Friday, August 22

- 9:00 AM - 9:40 AM **Pawel Keblinski**, Rensselaer Polytechnic Institute
Heat Flow and Role of Interfaces in Carbon-Nanotube Composites
- 9:40 AM - 10:20 AM **Vincent Meunier**, Oak Ridge National Lab
Theory of electronic transport properties in carbon nanostructures
- 10:20 AM - 10:40 AM *Coffee Break*
- 10:40 AM - 11:00 AM **John Carlisle**, ANL
Nanostructured carbon materials: Experimental issues and the need for theory and simulation.
- 11:00 AM - 11:40 AM **Sergei Rashkeev**, Vanderbilt University
Band Offsets and Charge-Carrier Dynamics in Ultra-Thin Oxides and Nanostructures by Second Harmonic Generation
- 11:40 AM - 12:00 noon **Gary Wiederrecht**, ANL
Near-field microscopy and ultrafast spectroscopy of metal nanoparticles and nanoparticle arrays
- 12:00 noon - 1:30 PM *Lunch*
- 1:30 PM - 2:10 PM **George Schatz**, Northwestern University
Optical properties of silver and gold nanoparticles and nanoarrays
- 2:10 PM - 2:30 PM **Orlando Auciello**, ANL
Ferroelectricity in the nanoscale
- Peter Zapol**, ANL
- 2:30 PM – 2:45 PM Closing Remarks
- 3 PM *Adjourn*