

## NANO2002 Workshop IV: Modeling and Simulation for Materials

### Tuesday November 19, 2002

- 8:30–9:30 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:30–10:30 **Efthimios (Tim) Kaxiras** (Harvard University)  
*Simulations of complex systems across multiple length scales*
- 10:30–11:00 *Break*
- 11:00–12:00 **Emily Carter** (UCLA)  
*Revisiting Old Ideas: Cohesive Laws of Fracture and Solving Directly for Electron Densities of Materials*
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:00 **Weitao Yang** (Duke University)  
*Simulation of chemical reactions in enzymes with a DFT QM/MM free energy method*
- 3:00–4:00 **Dieter Wolf** (Argonne National Lab)  
*Multiscale Simulation of Grain Growth in Nanocrystalline Thin Films\**
- 4:00–4:30 *Break*
- 4:30–5:30 **William Goddard** (California Institute of Technology)  
*Multi Scale Materials Design*
- 5:30–7:00 *Wine/Cheese Reception (Hosted by IPAM)*

### Wednesday November 20, 2002

- 9:00–9:30 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:30–10:30 **Russel Caflisch** (UCLA)  
*Simulation for Epitaxial Growth with Strain*
- 10:30–11:00 *Break*

*(Wednesday schedule continued on next page)*



*(Wednesday schedule continued from previous page)*

- 11:00–12:00 **Arthur Voter** (Los Alamos National Laboratory)  
*Accelerated Molecular Dynamics Methods*
- 12:00–1:30 *Lunch (on your own)*
- 1:30–2:30 **Weinan E** (Princeton University)  
*Heterogeneous multiscale modeling*
- 2:30–3:30 **Rob Phillips** (California Institute of Technology)  
*Physics of DNA Packing: From Viruses to Chromosomes*
- 3:30–4:00 *Break*
- 4:00–5:00 **Tamar Schlick** (New York University)  
*Mesoscale modeling of chromosomal DNA*
- 5:00–6:00 **Christopher Wolverton** (Ford Motor Company)  
*The Role of Quantum Mechanics in Virtual Aluminum Castings*
- 6:00–7:15 *Dinner (Hosted by IPAM)*

### Thursday November 21, 2002

- 9:00–9:30 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:30–10:30 **George Gilmer** (Lawrence Livermore National Laboratory)  
*Atomistic modeling of silicon device processing, front and back ends.*
- 10:30–11:30 **David Srolovitz** (Princeton University)  
*Faceted Film Growth*
- 11:30–11:45 *Break*
- 11:45–12:45 **Peter Smereka** (University of Michigan)  
*Hybrid Methods for Computing Epitaxial Growth*
- 12:45–2:00 *Lunch (on your own)*
- 2:00–3:00 **Mark Gyure** (HRL Laboratories)  
*Ab-initio based modeling of III-V semiconductor surface equilibrium and growth*
- 3:00–4:00 **Achi Brandt** (Weizmann Institute of Science)  
*Systematic Upscaling of Molecular Computation*

## Friday November 22, 2002

- 9:00–9:30 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:30–10:30 **Boris Yakobson** (Rice University)  
*Learning nanomechanics of the ~1D-materials: wires, tubes and their siblings*
- 10:30–11:00 *Break*
- 11:00–12:00 **Gerhard Hummer** (National Institute of Health)  
*Water and proton transport through hydrophobic channels: from carbon nanotubes to proteins*
- 12:00–2:00 *Lunch (on your own)*
- 2:00–3:00 **Michael Griebel** (University of Bonn, Germany)  
*Multiscale methods in nano- and biotechnology*
- 3:00–4:00 **Antonio Redondo** (Los Alamos National Laboratory)  
*Current Issues in modeling and simulation of nanomaterials*
- 4:00–4:30 *Break*
- 4:30–5:30 **Mitchell Luskin** (University of Minnesota, Twin Cities)  
*Metastability, Phase Transformation, and Microstructure in Structural Phase Transformations*

