

**Computational Materials Theory  
Program Overview  
NSF Division of Materials Research**

**June 19**

7:30-8:30am.	Continental Breakfast
8:30-8:45am	Logistics. Duane Johnson, UIUC
8:45-9:15am	Objectives of Overview and ITR. Bruce Taggart & Daryl Hess NSF
9:15-9:45am	Materials Computation Center. Duane Johnson, UIUC
9:45-10:00am	Break
10:00-10:30am	KDI: Multiscale Simulation in Materials Behavior. Sam Trickey, Florida
10:30-11:00am	KDI: Simulation and Modeling of Non-Crystalline Semiconductors. Paulette Clancy, Cornell
11:00-11:30am	Theoretical Solid State Physics. Marvin Cohen, UC-Berkeley
11:30-11:45am	High performance Algorithms for Electronic Materials. Jim Chelikowsky, Minnesota
12:00-1:00pm	Lunch
1:00-1:15pm	Electronic Structure of Condensed Matter. Richard Martin, UIUC
1:15-1:30pm	ITR: Large Scale Quantum Mechanical MD Simulations. Chakram Jayanthi, Louisville
1:30-1:45pm	ITR: Simulations of Carbon Nanotubes. Mark Jarrell, Cincinnati
1:45-2:00pm	ITR: Scalability of PDE Simulations. Georgy Korniss, RPI
2:00-2:15pm	Break
2:15-2:45pm	ITR: Novel Scalable Simulation Techniques. Roberto Car, Princeton
2:45-3:15pm	NIRT: Coherence and Correlation in Electronic Nanostructures. Harold Baranger, Duke
3:15-3:30pm	ITR: Modeling and Simulation of Quantum Phenomena in Semiconductor Structures of Reduced Dimensions. M.-Y. Chou, Georgia Tech
3:30-7:00pm	Poster Session

**June 20**

8:30-8:45am	ITR: Computational Tools for Multicomponent Materials Design. Ling-Qing Chen, Penn State
8:45-9:00am	ITR: Large-Scale Dislocation Dynamics Simulations. Lizhi Sun, Iowa
9:00-9:30am	Screening in Strongly Correlated Electron Systems. Bernd Schuttler, Georgia
9:30-10:00am	FRG: Multiscale Simulation of Atomistic Processes in Nanostructured Materials. Rajiv Kalia, LSU
10:00-10:15am	Break

10:15-10:30am	ITR: Billion Atom Multiscale Simulations on a Grid. Priya Vashishta, LSU
10:30-11:00am	ITR: Multiscale Models of Microstructure Simulation and Process Design. Bob Haber, UIUC
11:00-11:30am	NIRT: Multiscale Simulation of POSS Materials. Peter Cummings, Tennessee
11:30-12:00pm	KDI: Multiscale Modeling of Defects in Solids. Jim Sethna, Cornell
12:00-1:00pm	Lunch
1:00-1:30pm	Computational Studies of Dynamical Phenomena in Nanoscale Ferromagnets. Mark Novotny, Mississippi State
1:30-2:00pm	NIRT: Evolution and Self-Assembly of Quantum Dots. Peter Voorhees, NWU
2:00-2:30pm	ITR: Multiscale Biomolecular Simulations. Celeste Sagui, NCSU
2:30-2:45pm	Break
2:45-3:00pm	ITR: Explorations and Control of Condensed Matter Qubits. Whaley, UCB
3:00-3:30pm	ITR: Center for Modeling of Quantum Dynamics, Relaxation and Decoherence in Solid State Physics. Vladimir Privman, Clarkson
3:30-4:00pm	ITR: Foundations of Solid State Quantum Information Processing. Paul Kwiat, UIUC