Workshop on Theory and Modeling in Nanoscience
AGENDA

Friday, May 10, 2002

	Speaker	Title/Subject
8:00 a.m.	Walt Stevens, DOE, Basic Energy Sciences, and Walt Polansky, DOE, Advanced Scientific Computing Research	"The DOE Perspective on Theory and Modeling in the Nanoscience Initiative"
8:30	Bill McCurdy, LBNL	Goals and Purpose of this Workshop
	Session Chair: Bill McCurdy	
9:00	Stanley Williams Hewlett-Packard Laboratories	"Big Theory as the Engine of Invention for Nanotechnology: Losing the Born-Oppenheimer Approximation"
9:45	Uzi Landman Georgia Institute of Technology	"Small is Different: Computational Microscopy of Nanosystems"
10:30	**Break**	
	Session Chair: Ellen Stechel	
11:00	Steven Louie UC Berkeley	"Theory and Computation of Electronic, Transport and Optical Properties on the Nanoscale"
11:45	Dion Vlachos University of Delaware	"Bridging Length and Time Scales in Materials Modeling"
12:30 p.m.	**Lunch – Working, Catered in Conference Room**	
	Session Chair: David Keyes	
1:45	Phil Colella LBNL	"Computational Mathematics and Computational Science: Challenges, Successes, and Opportunities"
2:30	Jerzy Bernholc North Carolina State University	"Quantum Mechanics on the Nanoscale: from Electronic Structure to Virtual Materials"
3:15	**Break**	
	Session Chair: Peter Cummings	
3:45	Sharon Glotzer University of Michigan	"Computational Nanoscience and Soft Matter"
4:30	Alex Zunger National Renewable Energy Laboratory	"Progress and Challenges in Theoretical Understanding of Semiconductor Quantum Dots"
5:15	Adjourn	
7:00	Conference Dinner – Dinner Speaker: Bernd Hamann, University of California, Davis	"Massive Scientific Data Sets: Issues and Approaches Concerning Their Representation and Exploration"

Saturday, May 11, 2002

	Panel	Subject
8:30 a.m.	Paul Boggs, SNL/Livermore Jim Glimm, SUNY Stony Brook Malvin Kalos, LLNL George Papanicolaou, Stanford University Amos Ron, U. of Wisconsin-Madison Yousef Saad, U. of Minnesota	The Role of Applied Mathematics and Computer Science in the Nanoscience Initiative Panel Moderator: Paul Messina, ANL
	Breakout Sessions	***Chair***
10:30	⇒ Well Characterized Nano Building Blocks	James Chelikowsky, U. of Minnesota
	⇒ Complex Nanostructures and Interfaces	Sharon Glotzer, U. of Michigan
	⇒ Dynamics, Assembly and Growth of Nanostructures	Peter Cummings, U. of Tennessee
12:00 p.m.	**Lunch – Working, Catered in Conference Room**	
1:00	**Reports from Breakout Sessions**	
	Breakout Sessions	***Chair***
1:30	⇒ Crossing Time and Length Scales	George Papanicolaou, Stanford University
	⇒ Fast Algorithms	Malvin Kalos, LLNL
	⇒ Optimization and Predictability	Paul Boggs, SNL/Livermore
3:00	**Reports from Breakout Sessions**	
3:15	Closing Discussion of Report of the Workshop	
4:30	Workshop Adjourns	