

DRAFT 8/12/2004

Center for Nanophase Materials Sciences

Nanomaterials Theory Institute

2004 Computational Nanoscience Focused User Laboratory

Modeling Molecular and Nano-Electronics

August 16-20, 2004

*Lectures will be held in the Lecture Hall, Bldg. 5100, Room 128.

Sunday, August 15, 2004

7:00 p.m. – 9:00 p.m.	Information Reception – Comfort Inn (Iris Room)	Hempfling
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Monday, August 16, 2004

8:00 a.m.	Bus Departs from ORNL	Hempfling
9:00 a.m. – 10:00 a.m.	Badge pickup at Visitor Center and room assignments in Bldg. 5100	Hempfling
10:00 a.m. – 12:00 p.m.	*Lecture: Quantum Transport Theory	Buttiker
12:00 p.m. – 1:00 p.m.	Lunch: Bldg. 5100, Room 108	Hempfling
1:00 p.m. – 3:00 p.m.	Networking	X. Zhang
3:00 p.m. – 5:00 p.m.	*Lecture: Green's Function Method (Lecture Hall)	Jarrell
5:30 p.m.	Adjourn (Bus to Comfort Inn)	Hempfling

Tuesday, August 17, 2004

8:00 a.m.	Bus Departs from ORNL	Hempfling
9:00 a.m. – 10:00 a.m.	Networking	X. Zhang
10:00 a.m. – 12:00 p.m.	*Lecture: Quantum Transport Theory	Buttiker
12:00 p.m. – 1:00 p.m.	Lunch: Bldg. 5100, Room 108	Hempfling
1:00 p.m. – 3:00 p.m.	Networking	X. Zhang
3:00 p.m. – 5:00 p.m.	*Lecture: Green's Function Method	Jarrell
5:30 p.m.	Adjourn (Bus to Comfort Inn)	Hempfling

Wednesday, August 18, 2004

8:00 a.m.	Depart for ORNL – BUS WILL BE PROVIDED	Hempfling
9:00 a.m. – 10:00 a.m.	Networking	X. Zhang
10:00 a.m. – 12:00 p.m.	Lecture: First-principles Non-equilibrium Transport Modeling (Room 108)	Xue
12:00 p.m. – 1:00 p.m.	Lunch: Bldg. 5100, Room 108	Hempfling
1:00 p.m. – 3:00 p.m.	Networking	X. Zhang
3:00 p.m. – 5:00 p.m.	*Lecture: Tight Binding Approach to Molecular Electronics	Krstic

5:30 p.m.	Adjourn (Bus to Comfort Inn)	Hempfling
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Thursday, August 19, 2004

8:00 a.m.	Bus Departs for ORNL	Hempfling
9:00 a.m. – 10:00 a.m.	Networking	X. Zhang
10:00 a.m. – 12:00 p.m.	Lecture: First-principles Non-equilibrium Transport Modeling (Room 108)	Xue
12:00 p.m. – 1:00 p.m.	Lunch: Bldg. 5100, Room 108	Hempfling
1:00 p.m. – 3:00 p.m.	Networking	X. Zhang
3:00 p.m. – 5:00 p.m.	*Lecture: Methods of Molecular Modeling	Cheng and Chun
5:30 p.m.	Adjourn (Bus to Comfort Inn)	Hempfling
6:30 p.m.	Banquet in Oak Ridge at the American Museum of Science and Energy	Hempfling

Friday, August 20, 2004

8:00 a.m.	Bus Departs for ORNL	Hempfling
9:00 a.m. – 10:00 a.m.	Networking	X. Zhang
10:00 a.m. – 12:00 p.m.	Lecture: Methods of Molecular Modeling (Room 108)	Chun
12:00 p.m. – 1:00 p.m.	Lunch: Bldg. 5100, Room 108 ?see if it ends early	Hempfling
5:30 p.m.	Adjourn (Bus to Comfort Inn)	Hempfling