

Nanomaterials: Theory and Computation, 07/16/2012 - 07/19/2012

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Meeting Venue: Telluride Intermediate School, 725 West Colorado Telluride CO 81435

Monday Morning July 16

Transport and Dynamics

7:30-8:55 Breakfast at the school, participants only

8:55-9:00 Opening Remarks

9:00-9:45 Oleg Prezhdo, University of Rochester, *Excited state dynamics in nanoscale materials*

9:45-10:30 Dima Mozyrsky, Los Alamos National Lab, *Correlated electron-ion propagation: Novel algorithm for modeling non-adiabatic dynamics*

10:30-10:45 Coffee Break

10:45-11:30 Joongoo Kang, National Renewable Energy Lab, *Nanomaterials for thermal energy storage: first-principles molecular dynamics study*

11:30-12:15 Sergei Tretiak, Los Alamos National Lab, *Vibrational normal modes in non-adiabatic excited state dynamics of conjugated molecules*

12:15-1:30 TSRC Catered Lunch at the meeting site, participants only

Monday Afternoon

Structure and Growth

2:00-2:45 Jerome Delhommelle, University of North Dakota, *How the Relative Stability of Different Polymorphs Influence the Crystallization Process: Insights from Molecular Simulation*

2:45-3:30 Yong Pei, Xiangtan University, China, *Investigating Structural Evolution of Thiolate Protected Gold Clusters from the First-Principles*

3:30-4:15 Benjamin Janesko, Texas Christian University, *Modeling nanostructures using nonlocal density functional theory: New materials, new benchmarks, and new functionals*

Tuesday Morning July 17

Interface between Nanoparticle and Electromagnetic Field

7:30-8:55 Breakfast at the school, participants only

9:00-9:45 George C. Schatz, Northwestern University, *New directions in plasmonics*

9:45-10:30 David J. Masiello, University of Washington, *Molecular-electronic structure in a plasmonic environment: the quantum image effect at finite frequency*

10:30-10:45 Coffee Break

10:45-11:30 Lasse Jensen, Pennsylvania State University, *Understanding the plasmon molecule coupling*

11:30-12:15 Ruth Pachter, Air Force Research Lab, *Aspects of multiscale modeling for optically responsive organic-nanoparticle hybrid material systems*

12:15-1:30 **TSRC Catered Lunch at the meeting site, participants only**

Tuesday Afternoon

Transport and Dynamics

1:30-2:15 Jeff Neaton, Lawrence Berkeley National Lab, *Understanding Charge Transport in Molecular Junctions from First Principles*

2:15-3:00 Michael Galperin, University of California at San Diego, *Thermal transport, heating and cooling in molecular junctions*

3:00-3:15 **Coffee Break**

3:15-4:00 Dan Gezelter, University of Notre Dame, *Simulating mass and heat transport at the interfaces of metallic nanoparticles*

4:00-4:45 Dmitri Kilin, University of South Dakota, *Dynamics of charge transfer at functionalized semiconductor surfaces*

6:00-7:15 **Town Talk**

Wednesday Morning July 18

Hiking (Bear Creek Trail)

12:00 **Group Picture**

12:15-1:30 **TSRC Catered Lunch at the meeting site, participants only**

Wednesday Afternoon

Interface between Nanoparticle and Electromagnetic Field

1:30-2:15 Evan Reed, Stanford University, *Theory of engineered NEMS with 2D materials*

2:15-3:00 Guanhua Chen, Hong Kong University, *QM/EM simulation of emerging electronics: from first-principles to circuit modeling*

3:00-3:15 **Coffee Break**

3:15-4:00 Andrei Piryatinski, Los Alamos National Lab, *Plasmon assisted charge and exciton transport in 1D nanostructures*

4:00-4:30 **Student Award Presentation:** Charles Cherqui, Los Alamos National Lab, *Plasmon assisted polaron effects in carbon nanotubes*

4:30-5:00 **Student Award Presentation:** Emilie Guidez, Kansas State University, *Development of a charge-perturbed particle in a sphere model for electronic structure calculations of ligand-protected gold nanoparticles*

Thursday Morning July 19

Semiconductor Nanomaterials

9:00-9:45 Gustavo M. Dalpian, Universidade Federal do ABC, Brazil, *Surface effects in ZnO nanocrystals*

9:45-10:30 Svetlana Kilina, North Dakota State University, *Modeling of Photoexcitation in Ligated Quantum Dots*

10:30-10:45 Coffee Break

10:45-11:30 Juan Peralta, Central Michigan University, *Magnetic exchange couplings in nanostructures from first-principles*

11:30-12:15 Xiaosong Li, University of Washington, *p-Type Diluted Magnetic Semiconductor*

12:15-1:30 Lunch (Provided by TSRC)

Thursday Afternoon

Interface between Nanoparticle and Ligand

1:30-2:15 Hannu Häkkinen, University of Jyväskylä, Finland, *The gold-sulfur interface at the nanoscale*

2:15-3:00 Zhi-Gang Shuai, Tsinghua University, China, *Modeling organic light-emitting and photovoltaic materials*

3:00-3:15 Coffee Break

3:15-4:00 Sergei Ivanov, Los Alamos National Lab, *Cluster or Not? The Role of Gold in Some Metal-Ligand Systems*

4:00-4:45 Richard Sniatynsky, Texas Christian University, *Density Functional Theory with Screened Hybrid Functionals for Heterogeneous Catalysis*

4:45-5:30 Miguel Jose Yacamán, University of Texas at San Antonio, *"Growth mechanism of nanoparticles: theoretical calculations and experimental results"*

5:30-5:35 Closing Remarks

6:00-dark TSRC Picnic