

Nanomaterials: Computation, Theory, and Experiment

June 29 – July 4, 2015

- NEW Location: Telluride Elementary School (NOT Intermediate School, as was last years), 447 West Columbia Ave, Telluride CO 81435
- Invited talks will be 30 minutes plus 10 minutes for questions and discussion
- Contributing talks will be 20 minutes plus 10 minutes for questions and discussion
- Any questions about the schedule should be directed to workshop organizers: Svetlana Kilina (Svetlana.Kilina@ndsu.edu); Dmitri Kilin (Dmitri.Kilin@usd.edu) and George Nazin(gnazin@uoregon.edu)
- Any questions about logistics should be directed to TSRC hosts: Mark Kozak (mark@telluridescience.org); phone: (970)-708-4426

Badge Pick-Up: Monday, June 29, 7:30 am – 11:00 am at the Elementary School (available afterwards in the office)

TSRC Town Talk on Tuesday, June 30, 6-7:15 pm, Conference Center in Mountain Village

TSRC Picnic/BBQ: Wednesday, July 1, 6:00-9:00 pm, under the tent at the Elementary School (family and guests welcome free of charge)

Breakfast: Monday-Friday is included in the registration cost and will be provided at TSRC from 8:30 – 9:30 am

Lunch: from 12:30 – 2:00 pm by your-own.

	Monday June 29	Tuesday June 30	Wednesday July 1	Thursday July 2	Friday July 3
Breakfast:	8:30-9:15	8:30-9:30	8:30-9:30	8:30-9:30	8:30-9:30
Intro Remarks:	9:15-9:30 am				
Session: 9:30-10:50	Nanocrystals for En. Conv. V. Klimov T. Krauss	Surface Effects J. Pietryga S. Kilina	Carbon Nanotubes S. Doorn I. Vasiliev	Organic- Inorganic D. Kilin H. Jaeger	Calculations in Nanoscience F. Gygi J. Lewis
Coffee Break	10:50-11:10	10:50-11:10	10:50-11:10	10:50-11:10	10:50-11:10
Session: 11:10-12:30	A. Chakraborty C. Heyes	M. Law M. Beard	Y-H. Wang E. Minot	P. Darancet	Yuning Wu P. Cui
Lunch Break	12:30-2:00	12:30-2:00	12:30-2:00	12:30-2:00	12:30-2:00
Session 2:00-3:20	Nanocrystals for En. Conv. M. Jones A. Kryjevski	Surface Effects G. Galli G. Nazin	2D materials A. Star D. Solenov	Hiking & Free time	Free time
Coffee Break	3:20-3:40	3:30-3:50	3:30-3:50		
Session 3:40-5:40	Y. Dahnovsky M. Sfeir E. Hobbie	C. Stoldt Hong Wang	T. Rahman K. Velizhanin		
TSRC events		Town Talk 6:00-7:15 pm	Picnic/BBQ 6:00-9:00 pm		

Full Agenda

June 29

Monday

8:30-9:20 **Breakfast at TSRC** (for participants)

9:20-9:30 Organizational Remarks

9:30 -12:30 pm **SECTION I (A): Nanocrystals for Energy Conversion**

Chair: Dmitri Kilin

9:30-10:10 Victor Klimov, Los Alamos National Lab, NM
Engineered Quantum Dots for Light Emitting Diodes and Solar Energy

10:10-10:50 Todd Krauss, University of Rochester, Rochester, NY
Semiconductor Nanocrystals for Robust and Efficient Solar Hydrogen Production

10:50-11:10 **Coffee Break**

11:10-11:50 Arindam Chakraborty, Syracuse University, New York, NY
Hard-Shell versus Soft-Shell: Effect of Surface Functionalization on the Optical Properties of Semiconductor Nanoparticles

11:50-12:30 Colin Heyes, University of Arkansas, Fayetteville, AR
Balancing Lattice Strain and Confinement Potential in Multishell Quantum Dots to Improve Their Photoluminescence Properties

12:30-2:00 **Lunch (on your-own)**

2:00 pm - 5:40 pm **SECTION I (B): Nanocrystals for Energy Conversion**

Chair: Matt Law

2:00-2:40 Marcus Jones, U. North Carolina at Charlotte, Charlotte, NC
Probing the Recombination Dynamics of Trions and Multiexcitons in Colloidal Quantum Dots using Multi-Pulse Time-Resolved Fluorescence

2:40-3:20 Andrei Kryjevski, North Dakota State University, Fargo, ND
Enhanced Multiple Exciton Generation in Amorphous Silicon Nanowires: DFT Computation

3:20-3:40 **Coffee Break**

3:40-4:20 Yuri Dahnovsky, University of Wyoming, Laramie, WY
Transition Metal Doped Semiconductor Quantum Dots

4:20-5:00 Matthew Sfeir, Brookhaven Nat. Lab, Upton, NY
In Situ Transient Optical Studies of Charge Transport In Nanostructured Photocatalytic Materials

5:00-5:40 Erik Hobbie, North Dakota State University, Fargo, ND
Nanoscale Carbon and Silicon at the Hard-Soft Interface

6:30-9:00 **Social gathering at Smugglers Brewpub**

June 30

Tuesday

8:30-9:30 Breakfast at TSRC (for participants)

9:30 am -12:30 pm SECTION II (A): Surface Effects in Nanocrystals

Chair: George Nazin

9:30-10:10 Jeff Pietryga, Los Alamos National Lab, Los Alamos, NM
Nanocrystal Surfaces: A Chemist's Perspective

10:10-10:50 Svetlana Kilina, North Dakota State University, Fargo, ND
Contribution of Surface States to Energy Transfer and Energy Dissipation in Quantum Dots: Computational Insights

10:50-11:10 Coffee Break

11:10-11:50 Matt Law, University of California, Irvine, CA
State Filling and Charge Transport in Quantum Dot Films

11:50-12:30 Matt Beard, NREL, WA
Novel Fabrication Strategies for PbS and PbSe QDs via Controllable Cation Exchange Reactions

12:30-2:00 Lunch (on your-own)

2:00 pm - 5:00 pm SECTION II (B): Surface Effects in Nanocrystals

Chair: Matt Beard

2:00-2:40 Giulia Galli, University of Chicago, Chicago, Illinois
TBA

2:40-3:20 George Nazin, University of Oregon, Eugene, OR
Real-Space Spectroscopy of Nanoscale Materials

3:20-3:40 Coffee Break

3:40- 4:20 Conrad Stoldt, University of Colorado, CO
Resonant Light Scattering in Iron Pyrite Colloidal Solutions

4:20- 5:00 Hong Wang, West Virginia University, Morgantown, WV
Gold Nanocatalyst Supported by Facet Anatase (TiO₂) Nanostructures

6:00-7:15 Town Talk at Conference Center in Mountain Village

July 1

Wednesday

8:30-9:30 Breakfast at TSRC (for participants)

9:30 am -12:30 pm SECTION III: Functionalized Carbon Nanotubes

Chair: Kirill Velizhanin

- 9:30-10:10 Steve Doorn, Los Alamos National Lab, Los Alamos, NM
Dopant-Induced Exciton Trapping in Semiconducting Carbon Nanotubes: Spectroscopy and Dynamics
- 10:10-10:50 Igor Vasiliev, New Mexico State University, Las Cruces, NM
Electronic and Transport Properties of Functionalized Carbon Nanostructures
- 10:50-11:10** Coffee Break
- 11:10-11:50 YuHuang Wang, University of Maryland, College Park, MD
Fluorescent Quantum Defects
- 11:50-12:30 Ethan Minot, Oregon State University, Corvallis, OR
Quantum Efficiency of Carbon Nanotube Photodiodes

12:30-2:00 Lunch (on your-own)

2:00 pm - 5:00 pm SECTION IV: 2-D Layered Materials

Chair: Erik Hobbie

- 2:00-2:40 Alexander Star, University of Pittsburgh, Pittsburgh, PA
Sensors and Nano-Carriers Comprising Hybrid Carbon Nanostructures
- 2:40-3:20 Dmitri Solenov, Saint Louis University, Saint Louis, MO
Long-Range Interactions Between Adsorbates via C-Based Mono-Atomic Surfaces
- 3:20-3:40** Coffee Break
- 3:40- 4:20 Talat Rahman, University of Central Florida, Orlando, FL
Absorption Spectrum and Ultrafast Response of Monolayer and Bilayer Transition-Metal Dichalcogenides
- 4:20- 5:00 Kirill Velizhanin, Los Alamos National Lab, Los Alamos, NM
Excitonic Effects in 2D Semiconductors: Path Integral Monte Carlo Approach

6:00 pm - 9:00 pm TSRC Picnic/BBQ; under the tent at the Elementary School
(family and guests welcome free of charge)

July 2

Thursday

8:30-9:30 Breakfast at TSRC (for participants)

9:30 am -12:30 pm SECTION V: Organic-Inorganic Materials and Interfaces

Chair: Svetlana Kilina

9:30-10:10 Dmitri Kilin, University of South Dakota, Vermillion, SD
Simulations of Nonradiative Lifetime in Perovskites and Organic-Inorganic Hybrid Materials

10:10-10:50 Heather Jaeger, Lehigh University, New York, NY
Ab Initio Models of Electronic Processes in Coordination Polymers

10:50-11:10 Coffee Break

11:10-11:50 Pierre Darancet, Argon National Lab, IL
Understanding Non-Equilibrium Charge Transport and Rectification at Nanoscale Interfaces

12:00-1:00 Lunch (on your-own)

1:00 pm - 6:00 pm Hiking & Free Time

6:00-9:00 Social gathering at Smugglers Brewpub

July 3

Friday

8:30-9:30 Breakfast at TSRC (for participants)

9:30 am -12:30 pm SECTION VI: First Principle Calculations for Nanoscience

Chair: Hong Wang / Andrei Kryjevski

9:30-10:10 Francois Gygi, University of California, Davis, CA
First-Principles Molecular Dynamics for Nanoscience Applications

10:10-10:50 James Lewis, West Virginia University, Morgantown, WV
Designing Tunable Au-Based Bimetallic Nanocatalysts

10:50-11:10 Coffee Break

11:10-11:50 Yuning Wu, University of Florida, Gainesville, FL
Giant Molecular Magnetocapacitance

11:50-12:20 Peng Cui, North Dakota State University, Fargo, ND
Conditions for Charge Transfer in CdSe Quantum Dots Functionalized by Metal-Organic Complexes

12:20-12:30 Closing remarks by organizers

12:30-2:00 Lunch (on your-own)