

Nanomaterials: Computation, Theory, and Experiment

July 11 – 15, 2017

- NEW Location: Telluride Intermediate School (NOT Telluride Elementary School as was in 2015 and 2016) located at 725 W Colorado Ave, Telluride, CO 81435
- Invited talks will be 30 minutes plus 10 minutes for questions and discussion
- Contributing talks will be 15 minutes plus 5 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 Erik Hobbie (erik.hobbie@ndsu.edu)
- Any questions about logistics should be directed to TSRC hosts: Mark Kozak (mark@telluridescience.org); phone: (970)-708-4426

Meet and Greet: Monday, July 10, 6:00-9:00 pm at The Phoenix bean is located, 221 W. Colorado Ave Main Street, Telluride, CO. A representative from TSRC will be there 6-8 pm to hand out badges, welcome folks to town, and answer your questions. You will need your badge for the drink specials (cash bar). Guests and family members are welcome.

Badge Pick-Up: Tuesday, July 11, 7:30 am – 11:00 am at the Telluride Intermediate School (available afterwards in the office)

TSRC Town Talk: Tuesday, July 11, 6-7:15 pm, Conference Center in Mountain Village

TSRC Picnic/BBQ: Wednesday, July 12, 6:00-9:00 pm, under the tent at the Telluride Intermediate School (family and guests welcome free of charge)

Breakfast: Wednesday-Saturday is included in the registration cost and will be provided at TSRC from 8:00 – 9:00 am

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

	Tuesday July 11	Wednesday July 12	Thursday July 13	Friday July 14	Saturday July 15
Breakfast	8:00-9:00	8:00-9:00	8:00-9:00	8:00-9:00	8:00-9:00
Session: 9:00-10:20	<i>Badge Pick-Up</i>	Defects in Carbon Nanotubes	Novel Methods for Nanosystems	Surface Effects in Quantum Dots	Organic-Inorganic Interactions
		A. Star	T. Mueller	T. Krauss	S. Tretiak
		Y-H. Wang	B. Rasulev	Y. Dahnovsky	D. Kilin
Coffee Break		10:20-10:40	10:20-10:40	10:20-10:40	10:20-10:40
Session: 10:40-12:20		S. Doorn	A. Chakraborty	R. Sardar	E. Jakubikova
		B. Gifford	E. DePrince	A. Munro	A. Abakumov
		K. Velizhanin	M. Davari	L. Lystrom	S. Brown
Lunch Break		12:30-2:00	12:30-2:00	12:30-2:00	12:30-2:00
1:45-2:00	<i>Open Remarks</i>	Carbon Nanotubes for Energy Conversion	Photo-Processes in QD Solids	Hiking & Free time	The End
Session 2:00-3:20	Quantum Dots: Property Control via Core/Shell				
	M. Beard				
	J. Hollingsworth	B. Flavel	R. Schaller		
Coffee Break	3:20-3:40	3:20-3:40	3:20-3:40		
Session 3:40-5:20	N. Makarov	A. Kryjevski	G. Zimanyi	7:00-10:00 Social gathering at Smugglers Brewpub	
	S. Kilina	G. Tschumper	E. Hobbie		
			J. Vogel		
TSRC events	Town Talk 6:00-7:15 pm	Picnic/BBQ 6:00-9:00 pm			

Full Agenda

July 10: Monday

6:00-9:00 Meet and Greet at The Phoenix bean

located at 221 W. Colorado Ave Main Street, Telluride, CO

July 11: Tuesday (Afternoon Session)

1:00 pm - 1:40 pm Refreshment

1:40 pm - 2:00 pm Open Remarks

2:00 pm - 5:00 pm **SESSION I: Quantum Dots: Property Control via Core/Shell Structures**

Chair: Erik Hobbie

2:00-2:40 Matt Beard, NREL, Golden, CO

Controlling the Properties of Colloidal Quantum Dots for Energy Conversion Applications

2:40-3:20 Jennifer Hollingsworth, LANL, Los Alamos, NM

Non-blinking Nanomaterials: Experimental Success Invites Theoretical Inquiry

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

3:40- 4:20 Nikolay S. Makarov, LANL, Los Alamos, NM

CuInSeS/ZnS Quantum Dots With Near-Unity Quantum Yield: Development, Challenges, and Applications

4:20- 5:00 Svetlana Kilina, North Dakota State University, Fargo, ND

Controlling Phonon-Mediated Photoexcited Processes via Shell Composition in IR-Emitting Quantum Dots

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

July 12: Wednesday (Morning Session)

- 8:00-9:00** Breakfast at TSRC (for participants)
- 9:00 am -12:20 pm** **SESSION II: Defects in Carbon Nanotubes and Their Applications in Sensing and Lightning Technology**
Chair: Andrei Kryjevski
- 9:00-9:40 Alexander Star, University of Pittsburgh, Pittsburgh, PA
Chemical sensing with carbon nanostructures
- 9:40-10:20 YuHuang Wang, University of Maryland, College Park, MD
Tubes²
- 10:20-10:40** **Coffee Break**
- 10:40-11:20 Steve Doorn, Los Alamos National Lab, Los Alamos, NM
Spectroscopy and Dynamics of Carbon Nanotube Defect States
- 11:20-11:40 Brendan Gifford, Oregon State University, Corvallis, OR
Influence of Sidewall and Cap Chemical Functionalization on the Electronic and Optical Properties of Carbon Nanotubes
- 11:40-12:20 Kirill Velizhanin, Los Alamos National Lab, Los Alamos, NM
Exciton relaxation processes in functionalized carbon nanotubes
- 12:30-2:00** **Lunch (on your-own)**

July 12: Wednesday (Afternoon Session)

- 2:00 pm - 5:00 pm** **SESSION III: Carbon Nanotubes for Energy Conversion**
Chair: Svetlana Kilina
- 2:00-2:40 Jeff Blackburn, NREL, Golden, CO
Energy harvesting with semiconducting single-walled carbon nanotubes
- 2:40-3:20 Ben Flavel, Karlsruhe Institute of Technology, Germany
Probing the diameter limit of C60:SWCNT solar cells by spectral fitting
- 3:20-3:40** **Coffee Break**
- 3:40- 4:20 Andrei Kryjevski, North Dakota State University, Fargo, ND,
Dynamics of photoexcitations in chiral single-walled carbon nanotubes: DFT-based study
- 4:20- 5:00 Greg Tschumper, University of Mississippi,
Energetics and spectroscopic signatures of halogen bonding interactions in clusters and molecular assemblies
- 6:00 pm - 9:00 pm** **TSRC Picnic/BBQ; under the tent at the Intermediate School**
(family and guests welcome free of charge)

July 13: Thursday (Morning Session)

8:00-9:00 Breakfast at TSRC (for participants)

9:00 am -12:20 pm **SESSION IV: Novel Methods for Nanostructures**

Chair: Dmitri Kilin

- 9:00-9:40 Tim Mueller, Johns Hopkins University, Baltimore, MD
Predicting the structure and properties of nanoscale materials through ab-initio calculations and machine learning
- 9:40-10:20 Bakhtiyor Rasulev, North Dakota State University, Fargo, ND
Adaptation and application of computational and cheminformatics methods in nanomaterials toxicity prediction
- 10:20-10:40** **Coffee Break**
- 10:40-11:20 Arindam Chakraborty, Syracuse University, New York, NY
Development of effective stochastic potential method using random matrix theory for describing electronic excitation in noisy quantum systems
- 11:20-12:00 Eugene DePrince, Florida State University, Tallahassee, FL
Broadband absorption spectra from explicitly time-dependent equation-of-motion coupled-cluster theory
- 11:20-12:20 Mahdi Davari, Stony Brook University, NY
Materials and novel superconductivity discovered through crystal structure prediction
- 12:30-2:00** **Lunch (on your-own)**

July 13: Thursday (Afternoon Session)

2:00 pm - 5:00 pm **SESSION V: Photo-Processes in Quantum Dot Solids, Nanoplates, and Assemblies**

Chair: Kirill Velizhanin

- 2:00-2:40 Victor Klimov, LANL, Los Alamos, NM
Early time photoconductance in quantum-dot solids probed by ultrafast photocurrent spectroscopy
- 2:40-3:20 Rich Schaller, Northwestern/ANL, Chicago, IL
Energy and electron transfer processes in two-dimensional semiconductor nanoplatelets
- 3:20-3:40** **Coffee Break**
- 3:40-4:20 Gergely Zimanyi, UC Davis, CA,
Upconversion, downconversion, transport and the Metal/Insulator Transition in nanoparticle solids
- 4:20-5:00 Erik Hobbie, North Dakots State University, ND
Photoluminescence relaxation in size-purified silicon nanocrystals
- 5:00-5:20 Jon Vogel, University of South Dakota, Vermillion, SD
Photoluminescence in nanostructures

July 14 Friday (Morning Session)

- 8:30-9:00** **Breakfast at TSRC** (for participants)
- 9:00 -12:20 pm** **SESSION VI: Dopant and Surface Effects in Quantum Dots**
Chair: Victor Klimov (?)
- 9:00-9:40 Todd Krauss, University of Rochester, Rochester, NY
Interplay between charge and photoluminescence of individual doped semiconductor nanocrystals
- 9:40-10:20 Yuri Dahnovsky, University of Wyoming, Laramie, WY,
Ferromagnetism in semiconductor nanocrystals
- 10:20-10:40** **Coffee Break**
- 10:40-11:20 Rajesh Sardar, Indiana University-Purdue University, Indianapolis, IN
Efficient hole wave function delocalization in CdSe cluster molecules
- 11:20-12:00 Andrea Munro, Pacific Lutheran University, Tacoma, WA
Examination of the Decomposition of Phenylthiocarbamates during Nanocrystal Ligand Exchange
- 12:00-12:20 Levi Lystrom, North Dakota State University, Fargo, ND
Explaining Improvements in Optical Properties of CdSe Quantum Dots via Hydride Treatment
- 12:30-2:00** **Lunch (on your-own)**
- 2:00 pm - 7:00 pm** **Hiking & Free Time**
- 7:00-10:00** **Social gathering at Smugglers Brewpub**

July 15: Saturday (Morning Session)

- 8:00-9:00** **Breakfast at TSRC** (for participants)
- 9:00 -12:20 pm** **SESSION VII: Organic-Inorganic Interactions and Interfaces**
Chair: Yuri Dahnovsky (?)
- 9:00-9:40 Tretiak Sergei, LANL, Los Alamos, NM
Advances and promises of layered halide hybrid perovskites semiconductors
- 9:40-10:20 Kilin Dmitri, North Dakota State University, Fargo, ND
Photoinduced charge transfer at interfaces of nanomaterials
- 10:20-10:40** **Coffee Break**
- 10:40-11:20 Elena Jakubikova, North Carolina State University, Raleigh, NC
Interfacial electron transfer in dye-semiconductor assemblies: Importance of conformational sampling
- 11:20-12:00 Artem Abakumov, Skol-Tech, Moscow, Russia
Atomic structure and chemistry of nanomaterials with transmission electron microscopy
- 12:00-12:20 Sam Brown, North Dakota State University, Fargo, ND
Silver nanoclusters: computational insight on the photoluminescence
- 12:20-12:30 Closing remarks by organizers