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.

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<td><strong>Session 9:00-10:20</strong></td>
<td>Badge Pick-Up</td>
<td>Defects in Carbon Nanotubes</td>
<td>Novel Methods for Nanosystems</td>
<td>Surface Effects in Quantum Dots</td>
<td>Organic-Inorganic Interactions</td>
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<td>A. Star</td>
<td>T. Mueller</td>
<td>T. Krauss</td>
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<td>Y.-H. Wang</td>
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<td><strong>Session 10:40-12:20</strong></td>
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<td>K. Velizhanin</td>
<td>M. Davari</td>
<td>L. Lystrom</td>
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<td><strong>Lunch Break</strong></td>
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<td><strong>1:45-2:00</strong></td>
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<td><strong>Session 2:00-3:20</strong></td>
<td>Quantum Dots: Property Control via Core/Shell</td>
<td>Carbon Nanotubes for Energy Conversion</td>
<td>Photo-Processes in QD Solids</td>
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<td>Hiking &amp; Free time</td>
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<td>M. Beard</td>
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<td>J. Hollingsworth</td>
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<td><strong>Coffee Break</strong></td>
<td>3:20-3:40</td>
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<td>7:00-10:00</td>
<td>Social gathering at Smugglers Brewpub</td>
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<td>S. Kilina</td>
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<td><strong>TSRC events</strong></td>
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<td>6:00-7:15 pm</td>
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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/Schell 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

*Tubes^2*

10:20-10:40  **Coffee Break**

10:40-11:20  Steve Doorn, Los Alamos National Lab, Los Alamos, NM

*Energy harvesting with semiconducting single-walled carbon nanotubes*

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 Dakota 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, Takoma, 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