

Nanomaterials: Computation, Theory, and Experiment

July 16 – 20, 2019

Organizers: Svetlana Kilina, Dmitri Kilin, and Bakhtiyor Rasulev

TSRC host: Mark Kozak, 970-708-4426

- **Location:** Telluride Intermediate School, 725 W Colorado Ave, Telluride, CO 81435
- Any questions about the schedule should be directed to workshop organizers: Svetlana Kilina (Svetlana.Kilina@nds.u.edu), Dmitri Kilin (Dmitri.Kilin@usd.edu), and Bakhtiyor Rasulev (bakhtiyor.rasulev@nds.u.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 15, 5:00-6:30 pm at Oak located at the base of the gondola at 250 W San Juan Avenue (Gus's Way). Oak offers walk-up counter service for food and drink and is a great place to get together prior to our workshop. Guests and family members are welcome.

Breakfast: Wednesday-Saturday is included in the registration cost and will be provided at TSRC meeting site at **8:30 – 9:00 am** (30-minutes before morning session starts).

Lunch: at **12:40 – 2:00 pm** by your-own.

TSRC Picnic/BBQ: Wednesday, July 17, 6:00-8:00 pm, under the tent outside of the Telluride Intermediate School, 725 W Colorado Ave, Telluride. Family and guests welcome free of charge!

- **Invited Talks** are scheduled for 40 minutes, with 30 minutes for the presentation and 10 minutes for questions and discussion
- **Student Talks** are scheduled for 30 minutes, with 25 minutes for the presentation and 5 minutes for questions and discussion

	Tuesday July 16	Wednesday July 17	Thursday July 18	Friday July 19	Saturday July 20
Breakfast	NA	8:30-9:00	8:30-9:00	8:30-9:00	8:30-9:00
Session: 9:00-10:20	<i>Photoexcited Processes</i> Badge Pick-Up <i>Open Remarks</i>	<i>Plasmonic Effects & Emission</i>	<i>Modeling of MOFs & Perovskites</i>	<i>Advances in Light- Driven Dynamics</i>	<i>Closing Remarks & Future Directions</i>
		R. Sardar	T. Thonhauser	D. Kilin	D. Kilin
		D. Masiello	J. Vogel	D. Trivedi	S. Kilina
Coffee Break	10:30 am	10:20-10:40	10:20-10:40	10:20-10:40	10:20-10:40
Session: 10:40-12:40	S. Roberts	J. Hollingsworth	S. Tretiak	S. Kilina	The End
	A. Kryjevski	A. Piryatinski	H. Liu	E. J. Meijer	
	Y. Dahnovsky	C. Huang	A. Forde	L. Lystrom	
Lunch Break	12:40-2:00	12:40-2:00	12:30-2:00	12:30-2:00	
Session: 2:00-3:20	<i>Carbon Nanotubes as Emitters</i>	<i>Quantum Dots as Emitters</i>	<i>Machine Learning for Photophysics</i>	2:30-7:00 Hiking & Free time	
	A. Star	T. Krauss	B. Rasulev		
	Y-H. Wang	V. Klimov	N. Dandu		
Coffee Break	3:20-3:40	3:20-3:40	3:20-3:40	7:00-10:00 Social gathering at Smugglers Brewpub	
Session: 3:40-5:00	B. Gifford	M. Beard	D. Tandabany		
5:00-5:30	K. Velizhanin	A. Chakraborty	D. Priyakumar		
TSRC events		Picnic/BBQ 6:00-8:00 pm			

Full Agenda

July 16: Tuesday

Late Morning Session

10:30 am - 12:40 pm **SESSION I: Photoexcited Processes in Nanostructures**

Chair: Svetlana Kilina

10:30 - 10:40 **Open Remarks**

10:40-11:20

Sean Roberts, *University of Texas, Austin*

Designing Materials for Photon Up- and Down-conversion

11:20-12:00

Andrei Kryjevski, *North Dakota State University, Fargo, ND*

DFT-Based Study of Charge Separation in Doped Semiconductor Nanoparticles

12:00-12:40

Yuri Dahnovsky, *University of Wyoming, Laramie, WY*

Electronic and magnetic properties of 2D porphyrin type conjugated porous polymers

12:40-2:00

Lunch (on your-own)

Afternoon Session

2:00 pm - 5:00 pm **SESSION II: Carbon Nanotubes as Emitters and Sensors**

Chair: Andrei Kryjevski

2:00-2:40

Alexander Star, *University of Pittsburgh, Pittsburgh, PA*

Advances in Carbon Nanostructure Sensors and Drug Delivery

2:40-3:20

YuHuang Wang, *University of Maryland, College Park, MD*

Dynamic Gating of Infrared Radiation through a Fabric

3:20-3:40

Coffee Break

3:40- 4:20

Brendan Gifford, *Los Alamos National Lab, Los Alamos, NM*

Controlling the Diverse Emission Features in Functionalized Carbon Nanotubes

4:20- 5:00

Kirill Velizhanin, *Los Alamos National Lab, Los Alamos, NM*

Exciton Relaxation in Carbon Nanotubes via Electronic-to-Vibrational Energy Transfer

July 17: Wednesday

Morning Session

8:30-9:00 am Breakfast at TSRC (for participants)

9:00 am -12:40 pm **SESSION III: Plasmonic Effects and Emission in Nanostructures**

Chair: Dhara Trivedi

9:00-9:40 **Rajesh Sardar**, *Indiana University-Purdue University, Indianapolis, IN*
Work Function Pinning of Plasmonic Nanostructures by Conjugated Aromatic Ligands

9:40-10:20 **David Masiello**, *University of Washington, Seattle, WA*
A Reductionist's Approach to Single-Particle Imaging

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

10:40-11:20 **Jennifer Hollingsworth**, *Los Alamos National Lab, Los Alamos, NM*
A Marriage Made in Heaven: Stable Quantum Emitters and Plasmonic Complex Metal Oxide Nanocrystals Engaging in the Infrared

11:20-12:00 **Andrei Piryatinski**, *Los Alamos National Lab, Los Alamos, NM*
Theory and Simulations of Electron Emission from Semiconductor Nano-tip

12:00-12:40 **Chengkun Huang**, *Los Alamos National Lab, Los Alamos, NM*
Modeling of Electron Emission from the Nano-tip of Diamond Field Emitters

12:40-2:00 **Lunch (on your-own)**

Afternoon Session

2:00 pm - 5:00 pm **SESSION IV: Quantum Dots as Emitters**

Chair: Sean Roberts

2:00-2:40 **Todd Krauss**, *University of Rochester, Rochester, NY*
Explaining the Unusual Photoluminescence of Semiconductor Nanocrystals Doped Via Cation Exchange

2:40-3:20 **Victor Klimov**, *Los Alamos National Lab, Los Alamos, NM*
Hidden Powers of Tiny Particles: From Solar Windows and Lighting Panels to Nanolasers and Ultrastable Sources of Quantum Light

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

3:40- 4:20 **Matt Beard**, *NREL, Golden, CO*
TBA

4:20- 5:00 **Arindam Chakraborty**, *Syracuse University, New York, NY*
Nanoparticles in Noisy Chemical Environments: Insights from a Million Electronic Excitation Calculations

6:00 pm - 8:00 pm **TSRC Picnic/BBQ; under the tent at the Intermediate School**
(family and guests welcome free of charge)

July 18: Thursday

Morning Session

8:30-9:00 am Breakfast at TSRC (for participants)

9:00 am -12:30 pm **SESSION V: Modeling of Hybrid Organic-Inorganic Nanostructures: MOFs and Perovskites**

Chair: Dmitri Kilin

9:00-9:40 **Timo Thonhauser**, *Wake Forest University, Winston-Salem, NC*
Modeling Molecular Adsorption in Nano-Porous Materials

9:40-10:20 **Jon Vogel**, *Sandia National Lab, Albuquerque, NM*
Rare Earth MOFs for Acid Gas Separation and Sensing

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

10:40-11:20 **Sergei Tretiak**, *Los Alamos National Lab, Los Alamos, NM*
Modeling of Electronic Properties in Hybrid Perovskites: From Experimental Challenge to Theoretical Understanding

11:20-12:00 **Hongbin Liu**, *University of Washington, Seattle, WA*
Defect Structure of Cesium-Lead-Halide Perovskites Doped with Trivalent Metal Ions

12:00-12:30 **Aaron Forde**, *North Dakots State University, ND*
Spectral Signatures of Positive and Negative Polarons in Lead-Halide Perovskite Nanocrystals

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

Afternoon Session

2:00 pm - 5:30 pm **SESSION VI: Machine Learning for Predicting Photophysical Properties of Molecules**

Chair: Arindam Chakraborty

2:00-2:40 **Bakhtiyor Rasulev**, *North Dakots State University, ND*
Cheminformatics Methods in Polymers and Nanomaterials: Properties Assessment

2:40-3:20 **Naveen Dandu**, *Argon National Lab, Chicago, IL*
Accurately Predicting Energies of Organic Molecules using Quantum Chemistry Informed Machine Learning

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

3:40-4:20 **Dinadayalane Tandabany**, *Clark Atlanta University, Atlanta, GA*
Computational Study of Noncovalent Interactions between Amino Acids and Graphene

4:20-5:00 **Deva Priyakumar**, *International Institute of Information Technology, India*
Dynamics of Polymer Dispersed Nanoclusters, and *De Novo* Material Design Using Machine Learning

5:00 -5:30 **Jabed Mohammed**, *North Dakota State University, Fargo, ND*
Photophysical and Electrochemical Properties of Small Silver Clusters

July 19 Friday

Morning Session

8:30-9:00 am Breakfast at TSRC (for participants)

9:00 am -12:30 pm **SESSION VII: Advances in Modeling of Light-Driven Dynamics and Charge Transfer in Nanostructures**

Chair: Kirill Velizhanin

9:00-9:40 **Dmitri Kilin**, *North Dakota State University, Fargo, ND*
Spectral Signatures of Excited State Dynamics in Nano-sized Semiconductor Materials

9:40-10:20 **Dhara Trivedi**, *Clarkson University, Potsdam, New York*
Theoretical aspect of Nanoscale Systems: From Carrier Dynamics to Chameleons inspired Nanolaser

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

10:40-11:20 **Svetlana Kilina**, *North Dakota State University, Fargo, ND*
Charge Transfer in QD/Dye Heterostructures

11:20-12:00 **Evert Jan Meijer**, *University of Amsterdam, Amsterdam*
Simulations of Chemical Reactions

12:00-12:30 **Levi Lystrom**, *North Dakota State University, Fargo, ND*
Effect of Surface Passivation by Charged Inorganic and Organic Ligands on the Optical/Electronic Properties and Morphology of Quantum Dots.

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

2:30 pm - 7:00 pm **Hiking & Free Time**

7:00-10:00 **Social gathering at Smugglers Brewpub**
(225 S Pine St Telluride, CO 81435)

July 20: Saturday

Morning Session

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

9:00 am -10:20 am **SESSION VIII: Closing Remarks and Future Directions**

Chair: Bakhtiyor Rasulev

9:00-9:30 **Dmitri Kilin**, *North Dakota State University, Fargo, ND*

9:30-10:00 **Svetlana Kilina**, *North Dakota State University, Fargo, ND*

10:00-10:20 **Coffee Break**

10:20 **Adjourn**