Nanomaterials:
Computation, Theory, Machine Learning and Experiment

June 14 – 18, 2025

Organizers: *Kirill Velizhanin, Svetlana Kilina, Dmitri Kilin, and Nikita Fedik*

TSRC Host: *Mark Kozak, 970-708-4426*

- **Workshop Location:**

  Telluride Intermediate School, 725 W Colorado Ave, Telluride, CO 81435

- **Workshop Starting/Ending :**

  Workshop starts on **Saturday, June 14th** and runs through **Wednesday, June 18th**

- **Questions:**
  - Any questions about the schedule should be directed to workshop organizers: Svetlana Kilina (svetlana.kilina@ndsu.edu); Dmitri Kilin (Dmitri.Kilin@usd.edu); Kirill Velizhanin (kirill@lanl.gov); Nikita Fedik (nfedik@lanl.gov);
  - Any questions about logistics should be directed to TSRC hosts: Mark Kozak (mark@telluridescience.org); phone: (970)-708-4426
  - Any questions about registration fees can be addressed to Cindy Fusting (cindy@telluridescience.org) and Sara Friedberg (sara@telluridescience.org).

Breakfast:

Saturday-Wednesday - is included in the registration cost and will be provided at TSRC meeting site at ***7:30 – 9:00 am*** (come at least 30-minutes before morning session starts).

Lunch: by your-own at ***12:00 – 2:10 pm*** *on Saturday and Sunday*
and **12:40-2:10 pm** *on Monday, Tuesday, and Wednesday*

TSRC Picnic:

Monday, June 16th from 5:30-7:30

Location: The tent behind outside of the Telluride Intermediate School, 725 W Colorado Ave, Telluride.

Free BBQ, Beer, Wine and Non-Alcoholic Beverages.
Friends and Family are invited free of charge.

Hike: **June 17th, 3:00 pm** meeting near Gondola Station, Telluride

Social Gathering: **June 14 th** and **June 17th, 6:00 pm at Smugglers Brewpub**
(*225 S Pine St Telluride, CO 81435)*
Check the announcements to confirm

SCHEDULE

All Talks are scheduled for 40 minutes, with 30-35 minutes for the presentation and 5-10 minutes for questions and discussions. We strongly encourage you to allocate time for discussions!

	Saturday	Sunday	Monday	Tuesday	Wednesday
	June 14	**June 15**	**June 16**	**June 17**	**June 18**
8:00-9:00 am	breakfast	breakfast	breakfast	breakfast	breakfast
9:00-9:05	intro: organizes	announcements	announcements	announcements	announcements
Session:	**II-VI QDs**	**2D Materials**	**NOT II-VI QDs**	**ML: From Bio to Nano**	**Future Direction**
chair					**K. Velizhanin**
9:05-9:45	S. Ivanov	S. Chabi	E. Hobbie	N. Fedik	ML: QDs
9:45-10:25	S. Goupalov	D. Qiu	D. Kilin	R. Cersonsky	ML: 2D materials
10:25-10:40 am	break	break	break	break	break
10:40-11:20	I. Fedin	F. Shakib	J. Zhang (?)	J. Jansen	ML: CNTs
11:20-12:00	A. Chakraborty	Kirill Bolotin	R. Sardar	W. Bricker	ML: molecules
12:00-12:40 pm	lunch on your own	lunch on your own	A. Forde	M. Zwolak	**Closing Remarks**
12:40-2:10 pm	lunch on your own	lunch on your own	lunch on your own	lunch on your own	lunch on your own
Session:	**Many-Body Excitations**	**Carbon Nanotubes (CNT)**	**Molecular Structures**	**hike**	**The End**
chair				**K. Velizhanin**	
2:10-2:50	S. Roberts	Y. Wang	W. Sun		
2:50-3:30	A. Kryjevski	A. Star	D. Badia		
3:30-4:10	A. Mandal	Svetlana Kilina	H. Kulik		
4:10-4:25 pm	break	break	break	**hike**	
4:25-5:05	J. Jakowski	S. Piletsky	V. Sharma		
5:05-5:45	K. Velizhanin	B. Rasulev			
5:30 PM			Picnic		
6:00 PM	social gathering			social gathering	

Agenda

June 14: Saturday

Morning Session I

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

9:00 am - 9:05 am **Open Remarks from Organizers**

9:05 am - 12:00 am **SESSION: II-VI Quantum Dots (QDs) and Their Optical Properties**

Chair: TBA

9:05-9:45 **Sergei Ivanov**, *Los Alamos National Lab, Los Alamos, NM;*
Precision Engineering of II-VI Semiconductor Nanoclusters

9:45-10:25 **Serguei Goupalov**, *Jackson State University, Jackson, MS;*
Is the Exciton Ground State in Nanocrystals Always Dark?

10:25-10:40 **Coffee Break**

10:40-11:20 **Igor Fedin**, *University of Alabama, Tuscaloosa, AL;*
Synthesis of Cadmium Phosphide Quantum Dots Emitting in the Short-Wave Infrared

11:20-12:00 **Arindam Chakraborty**, *Syracuse University, New York, NY;*
Generation and Decay of High-Energy Excitons in CdTe Quantum Dots Under X-Ray Excitation: Mapping Excitation-Emission Matrix and NIR Emission Pathways

12:00-2:10 **Lunch (on your-own)**

Afternoon Session II

2:10 pm - 5:45 pm **SESSION: Many-Body Excitation in Nano-Interfaces**

Chair: TBA

2:10-2:50 **Sean Roberts**, *University of Texas, Austin, TX;*
Reshaping Light via Photon Up- and Down-Conversion

2:50-3:30 **Andrei Kryjevski**, *North Dakota State University, Fargo, ND*;
Dynamics of Photoexcited Janus Semiconductor Nanocrystals: DFT-Based Calculation

3:30-4:10 **Arkajit Mandal**, *Texas A&M University, College Station, TX*;
Cavity Modified Exciton Transport

4:10-4:25 **Coffee Break**

4:25-5:05 **Jacek Jakowski**, *Oak Ridge National Laboratory, Oak Ridge, TN;*
Real-Time TDDFT for Nonequilibrium Dynamics: Optical Excitations, Beam-Induced Chemistry, and Large-Scale Electronic Response

5:05-5:45 **Kirill Velizhanin**, *Los Alamos National Lab, Los Alamos, NM;*
Is there "Nano" in Detonation?

6:00-10:00 pm **Social gathering at Smugglers Brewpub**
(*225 S Pine St Telluride, CO 81435)*

June 15: Sunday

Morning Session III

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

9:00 am - 9:05 am **Announcements from Organizers**

9:05 am - 12:00 am **SESSION: 2D Materials: Challenges and Opportunities**

Chair: TBA

9:05-9:45 **Sakineh Chabi**, *University of New Mexico, Albuquerque, NM;*
Two-Dimensional Silicon Carbide: Bridging Theory and Experiment.

9:45-10:25 **Diana Qiu**, *Yale University, New Haven, CT;*
Exciton Dynamics and Nonlinear Optics in 2D Materials: From Many-Body to Machine Learning

10:25-10:40 **Coffee Break**

10:40-11:20 **Farnaz Shakib**, *New Jersey Institute of Technology, Newark, NJ;*
Two-Dimensional Electrically Conductive Metal-Organic Frameworks: Challenges and Opportunities

11:20-12:00 **Klrill Bolotin**, *Freie University of Berlin, Berlin, Germany;*
Turning New Knobs on Hamiltonians of 2D materials

12:00-2:10 **Lunch (on your-own)**

Afternoon Session IV

2:10 pm - 5:45 pm **SESSION: Carbon Nanotubes and Their Optical Properties**

Chair: TBA

2:10-2:50 **YuHuang, Wang**, *University of Maryland, College Park, MD;*
Finding Dark Excitons in Carbon Nanotubes

2:50-3:30 **Alexander Star**, *University of Pittsburgh, Pittsburgh, PA*;
Carbon Nanotube Sensors for Machine Learning-Assisted Opioid Detection

3:30-4:10 **Svetlana Kilina**, *North Dakota State University, Fargo, ND;*
Chiral Molecular Adducts for Controlling Circularly Polarized NIR Emission in Carbon Nanotubes

4:10-4:25 **Coffee Break**

4:25-5:05 **Stanislav Piletsky**, *Zuckerman Research Center, New York, NY;*
Handle-Free Functionalization of Carbon Nanotubes for Next-Generation Nanosensor Development

5:05-5:45 **Bakhtiyor Rasulev**, *North Dakota State University, Fargo, ND;*
Machine Learning in Materials: Case Studies of CNTs and C60 Nanomaterials

June 16: Monday

Morning Session V

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

9:00 am - 9:05 am **Announcements from Organizers**

9:05 am - 12:40 pm **SESSION: NOT II-VI QDs: Optical and Electronic Response**

Chair: TBA

9:05-9:45 **Erik Hobbie**, *North Dakota State University, Fargo, ND;*
Colloidal Few-Layered 2D SiC Quantum Dots from a Liquid Precursor: Surface Passivation, Photoluminescence, and Self-Assembly

9:45-10:25 Dmitri Kilin, *North Dakota State University, Fargo, ND*
Modeling Synthesis and Excited state Dynamics in Colloidal Nanostructures: SiC and Perovskites

10:25-10:40 **Coffee Break**

10:40-11:20 **Jiefei Zhang**, *Argonne National Lab, Lemont, IL;*
TBA

11:20-12:00 **Rajesh Sardar**, *Indiana University–Purdue University, Indianapolis, IN;*
Engineering of Ultralow Work Function Plasmonic Inorganic Nanocrystals

12:00-12:40 **Aaron Forde**, *Los Alamos National Lab, Los Alamos, NM;*
Chiroptical Spectroscopy and Nonadiabatic Dynamics of Excitons in Nanostructured Lead-Halide Perovskite

12:40-2:10 **Lunch (on your-own)**

Afternoon Session VI

2:10 pm - 5:05 pm **SESSION: Molecular Structures: Optical and Catalytic Properties**

Chair: TBA

2:10-2:50 **Wenfang Sun**, *University of Alabama, Tuscaloosa, AL;*
Transition-Metal Bisterpyridine Complexes Bearing Oligothienyl Substituents: Photophysics and Applications In Phototherapy and Photocatalysis

2:50-3:30 **David Badia**, *University of Oslo, Oslo, Norway*;
Generative AI for the Chemistry of the Transition Metals

3:30-3:45 **Coffee Break**

3:45-4:25 **Heather Kulik**, *Massachusetts Institute of Technology, Cambridge, MA;*
Getting From The Computer to Real World Inorganic Materials Faster With Machine Learning

4:25-5:05 **Vidushi Sharma**, *Princeton Plasma Physics Laboratory, Princeton, NJ;*
Elucidating Photo and Electro-Catalytic Processes Using Multiphysics Modeling Techniques

5:30 pm - 7:30 pm **TSRC Picnic/BBQ;** under the tent at the Intermediate School
Family and guests welcome free of charge

June 17: Tuesday

Morning Session VII

8:00-9:00 am	**Breakfast at TSRC** (for participants)
9:00 am - 9:05 am	**Announcements from Organizers**
9:05 am - 12:40 pm	**SESSION: ML From Bio to Nano**
	Chair: TBA
9:05-9:45	**Nikita Fedik**, *Los Alamos National Lab, Los Alamos, NM;* TBA
9:45-10:25	Rose Cersonsky, *University of Wisconsin-Madisson, Madison, WI;* Representing and Interpreting Chemical Objects in Data Science and Machine Learning: Beyond the Atom and the Black-Box.
10:25-10:40	**Coffee Break**
10:40-11:20	**Jan Jansen**, *Max Planck Institute for Sustainable Materials, Düsseldorf, Germany;* Accelerating Materials Discovery with Machine Learning
11:20-12:00	**William Bricker**, *University of New Mexico, Albuquerque, NM;* Higher-Order Junctions for Multi-Dimensional DNA Nanostructure Design
12:00-12:40	**Michael Zwolak**, *National Institute of Standards and Technology, Gaithersburg, MD;* Biomolecular association, Design, and Assembly
12:40-2:10	**Lunch (on your-own)**
2:30 pm - 6:00 pm	**HIKING & FREE TIME**
6:00-10:00 pm	**Social gathering at Smugglers Brewpub**
	(*225 S Pine St Telluride, CO 81435)*

June 18: Wednesday

Morning Session VIII

8:00-9:00 am	**Breakfast at TSRC** (for participants)
9:00 am - 9:05 am	**Announcements from Organizers**
9:05 am - 12:40 pm	**SESSION: Discussions on Future Directions**
	Facilitators: Kirill Velizhanin and Dmitri Kilin
9:05-9:45	ML for Quantum Dots
9:45-10:25	ML for 2D Martials
10:25-10:40	**Coffee Break**
	Facilitators: Nikita Fedik and Svetlana Kilina
10:40-11:20	ML for Carbon-based Materials: Carbon Nanotubes and Carbon Dots
11:20-12:00	ML for Excited State Processes in Metal-Organic Complexes
12:00-12:40	**Closing Remarks**
12:40-2:10	**Lunch (on your-own)**
2:10 pm	**Adjourn**