

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 Science & Innovation Center, 300 S Townsend St. Telluride, CO

• **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).

Meet & Greet:

Friday, June 13, **5:00-6:30 pm**, cash-bar at [Alibi](#) – 157 S. Fir Street, Telluride, CO. A staff member will be on hand to welcome you, distribute badges, and answer any questions.

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: on your own at **12:00 – 2:00 pm** on Saturday through Wednesday

TSRC Picnic:

Monday, June 16th from 5:30-7:00 pm

Location: Telluride Science & Innovation Center, 300 S Townsend St. Telluride, CO

Free BBQ, Beer, Wine and Non-Alcoholic Beverages.

Friends and Family are invited free of charge.

Hike: June 17th, **2:00 pm** meeting near Gondola Station, Telluride (see page 8)

Social Gathering: June 14th (6 pm) and June 17th (5:00 pm) at **Smuggler Union***
(225 S Pine St Telluride, CO 81435)

*subject to change, check for announcements from organizers to confirm

Town Talk: June 17th at 6:30 pm, Telluride Conference Center in Mountain Village

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	D. Kilin	E. Hobbie	S. Ivanov	B. Rasulev	Velizhanin, Kilin, Kilina, Fedik
9:05-9:45	S. Ivanov	A. Forde	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	K. Bolotin	R. Sardar	W. Bricker	ML: molecules
12:00-2:00 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	F. Shakib	K. Velizhanin	A. Star	K. Velizhanin	
2:00-2:40	S. Roberts	Y. Wang	W. Sun		
2:40-3:20	K. Velizhanin	A. Star	D. Balcells		
3:20-3:40 pm	break	break	break	hike	
3:40-4:20	A. Mandal	S. Kilina	V. Sharma		
4:20-5:00	J. Jakowski	S. Piletsky			
5:00-5:40	A. Kryjevski	B. Rasulev		social gathering	
5:30 PM			Picnic		
6:00 PM	social gathering				
6:30 PM				Town Talk	

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: Dmitri Kilin

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

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

Afternoon Session II

2:00 pm - 5:40 pm **SESSION: Many-Body Excitation in Nano-Interfaces**

Chair: Farnaz Shakib

2:00-2:40 **Sean Roberts**, *University of Texas, Austin, TX*;
Reshaping Light via Photon Up- and Down-Conversion

2:40-3:20 **Kirill Velizhanin**, *Los Alamos National Lab, Los Alamos, NM*;
Is there "Nano" in Detonation?

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

3:40-4:20 **Arkajit Mandal**, *Texas A&M University, College Station, TX*;
Cavity Modified Exciton Transport

4:20-5:00 **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

5:00-5:40 **Andrei Kryjevski**, *North Dakota State University, Fargo, ND*;
Dynamics of Photoexcited Janus Semiconductor Nanocrystals: DFT-Based Calculation

6:00-10:00 pm **Social gathering** at Smuggler Union
(225 S Pine St Telluride, CO 81435) – location is subject to change

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: Erik Hobbie

9:05-9:45 **Aaron Forde**, *Los Alamos National Lab, Los Alamos, NM*;
Chiroptical Spectroscopy and Nonadiabatic Dynamics of Excitons in
Nanostructured Lead-Halide Perovskite

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 **Kirill Bolotin**, *Freie University of Berlin, Berlin, Germany*;
Turning New Knobs on Hamiltonians of 2D materials

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

Afternoon Session IV

2:00 pm - 5:40 pm **SESSION: Carbon Nanotubes and Their Optical Properties**

Chair: Kirill Velizhanin

2:00-2:40 **YuHuang, Wang**, *University of Maryland, College Park, MD*;
Finding Dark Excitons in Carbon Nanotubes

2:40-3:20 **Alexander Star**, *University of Pittsburgh, Pittsburgh, PA*;
Carbon Nanotube Sensors for Machine Learning-Assisted Opioid Detection

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

3:40-4:20 **Svetlana Kilina**, *North Dakota State University, Fargo, ND*;
Chiral Molecular Adducts for Controlling Circularly Polarized NIR Emission in
Carbon Nanotubes

4:20-5:00 **Stanislav Piletsky**, *Zuckerman Research Center, New York, NY*;
Handle-Free Functionalization of Carbon Nanotubes for Next-Generation
Nanosensor Development

5:00-5:40 **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 - 12:00 pm **SESSION: NOT II-VI QDs: Optical and Electronic Response**

Chair: Sergei Ivanov

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*;
Telecom Spin Qubits in SiC and Oxides: From Bulk to Nanocrystals

11:20-12:00

Rajesh Sardar, *Indiana University–Purdue University, Indianapolis, IN*;
Engineering of Ultralow Work Function Plasmonic Inorganic Nanocrystals

12:00-2:00

Lunch (on your-own)

Afternoon Session VI

2:00 pm - 4:20 pm **SESSION: Molecular Structures: Optical and Catalytic Properties**

Chair: Alexander Star

2:00-2:40

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

2:40-3:20

David Balcells, *University of Oslo, Oslo, Norway*;
Generative AI for the Chemistry of the Transition Metals

3:20-3:40

Coffee Break

3:40-4:20

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

5:30 pm - 7:00 pm **TSRC Picnic/BBQ** at Telluride Science & Innovation Center,
300 S Townsend St. Telluride CO 81435
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 - 12:00 pm **SESSION: ML From Bio to Nano**

Chair: Bakhtiyor Rasulev

9:05-9:45 **Nikita Fedik**, *Los Alamos National Lab, Los Alamos, NM;*
From Bio to Nano using Machine Learning: Success Stories and Cautionary Tales

9:45-10:25 **Rose Cersonsky**, *University of Wisconsin-Madison, 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

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

2:00 pm - 7:30 pm **HIKE & BEYOND** (see page 8 for details)

2:00-5:00 Hiking to Bear Creek Falls

5:00-6:30 pm **Social gathering at Smuggler Union**
(225 S Pine St Telluride, CO 81435)

6:30-7:30 **Town Talk** at Telluride Conference Center in Mountain Village
Steve Corcelli, *University of Notre Dame, IN;*
Animating the Invisible: Molecular Movies and the Science They Reveal

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 - 12:00 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 Materials

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

Facilitators: Nikita Fedik and Svetlana Kilina

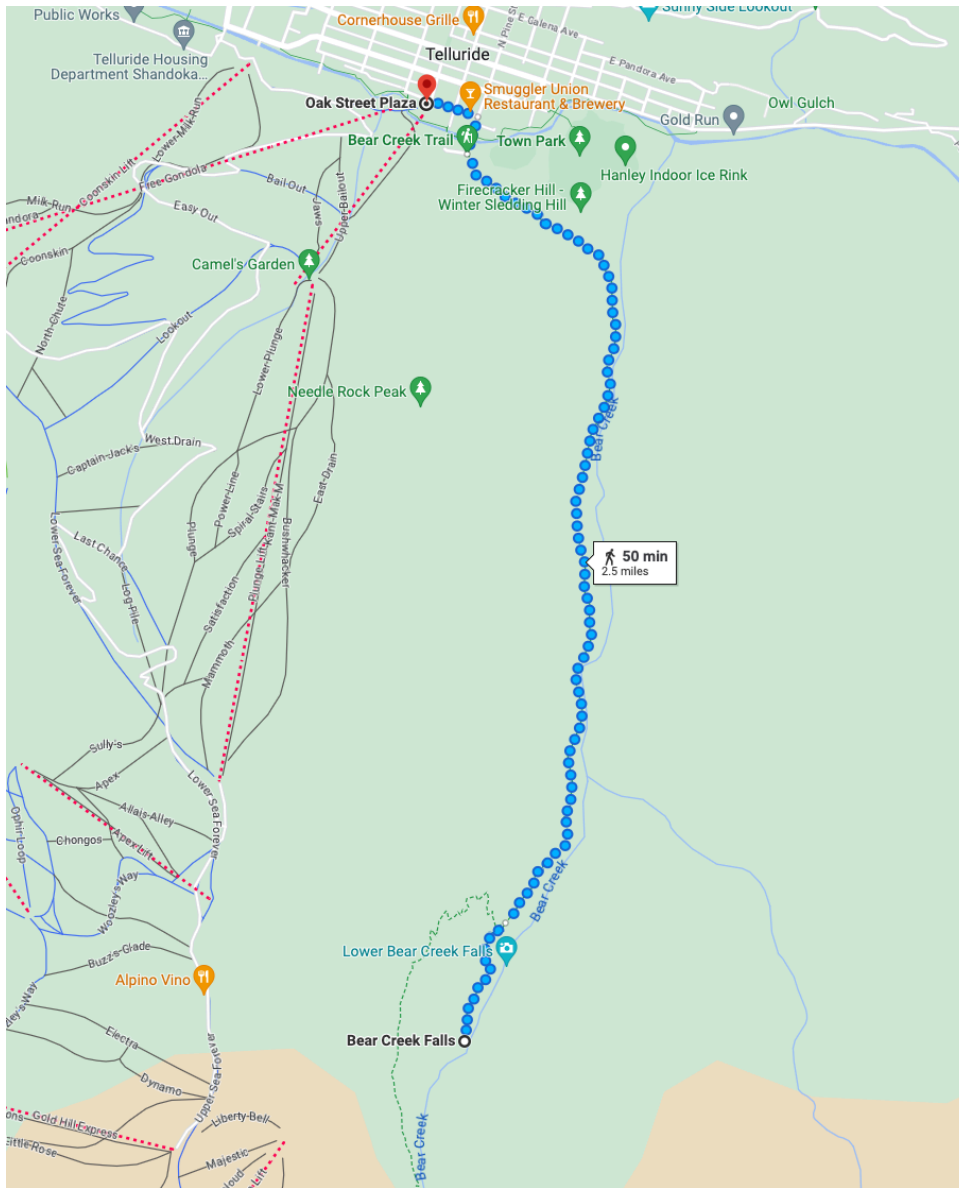
10:40-11:20 ML for Carbon-based Materials: Carbon Nanotubes and Carbon Dots

11:20-12:00 ML for Excited State Processes in Metal-Organic Complexes

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

2:00 pm **Adjourn**

Addendum: Hike & Beyond (June 17th, 2:00pm – 7:30pm)



- **2:00 pm:** Starting at Oak Street Plaza (near Gondola): <https://goo.gl/maps/ztgkHVYRkSRruP2G8> or on your own
- Hiking to Bear Creek Falls: <https://goo.gl/maps/AEMLBCPtqoESDfhT8>
- **5:00 pm:** Well-deserved visit to Smuggler Union Restaurant & Brewery (shown conveniently on the map): <https://goo.gl/maps/sVfARtYbFra4LTow6> ... or some other place? Let's decide!
- **6:30 pm:** Town Talk - "***Animating the Invisible: Molecular Movies and the Science They Reveal***" by **Steve Corcelli**, University of Notre Dame. Location: Telluride Conference Center in Mountain Village (580 Mountain Village Blvd, Mountain Village, CO); <https://maps.app.goo.gl/x8bVWDXL5PQUKeNw9>
<https://telluridescience.org/town-talks/>