

# Nanomaterials: Computation, Theory, Machine Learning and Experiment

**June 10 – 14, 2023**

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

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

- **Workshop Location:**

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

- **Workshop Starting/Ending :**

Saturday (June 10/2023) at 1:30 pm by Wednesday (June 14)

- **Questions:**

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

**Meet and Greet:**

**Friday, June 9, 5:00 pm to 6:30 pm**

**Location:** The Liberty (121. S Fir Street)

This is a good chance to meet up with fellow participants prior to our meeting.

A staff member will be on hand to welcome you and distribute badges.

**Breakfast:**

From Saturday to Wednesday – It 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:** at **12:00 – 2:00 pm** by your-own.

**TSRC Picnic:**

**Monday, June 12th 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.

**Telluride Science Town Talk**

**Tuesday, June 13, 6:30 pm to 7:30 pm**

**Location:** Telluride Conference Center in Mountain Village

Cash Bar, Doors Open at 6:00pm

**Talk Title:** Polymers- Smart Programmable Sponges

**Featured Speaker:** Omar Farha, Northwestern University

## SCHEDULE

**All Talks** are scheduled for 40 minutes, with 30-35 minutes for the presentation and 5-10 minutes for questions and discussions.

	Saturday June 10	Sunday June 11	Monday June 12	Tuesday June 13	Wednesday June 14
<b>Breakfast</b>	8:30-9:00	8:30-9:00	8:30-9:00		
<b>Session: 9:00-12:00</b>	<b>Welcome &amp; Introduction</b>	<b>QD &amp; Interfaces</b> Chair: Ivanov	<b>Spin Dynamics</b> Chair: Beard	<b>Excited org/inorg systems</b> Chair: Kilina	Nanocarbon Chair: Velizhanin
9:00-9:40 9:40-10:20	Taking badges	Sean Roberts	Han Htoon	Xiwen Gong	Alex Star
		Masaru Kuno	Louis Bouchard	Timo Thonhauser	Dinesh Thapa
<b>Coffee Break</b>	Introductory words from organizers <b>1:30-2:00 pm</b>	<b>10:20-10:40</b>	<b>10:20-10:40</b>	<b>10:20-10:40</b>	<b>10:20-10:40</b>
10:40-11:20 11:20-12:00		C. Mora Perez	Ryan Beck	Wenfang Sun	Evert Jan Meijer
		Dmitri Kilin	Jinsoo Park	Aaron Forde	Nikita Fedik
<b>Lunch Break</b>	<b>12:00-1:30</b>	<b>12:00-2:00</b>	<b>12:00-2:00</b>	<b>12:00-1:00</b>	<b>12:00-2:00</b>
<b>Session: 2:00-5:00</b>	<b>QD &amp; Interfaces</b> Chair: Kilin	<b>Excitons &amp; ML</b> Chair: Lindsey	<b>Bond Breaking</b> Chair: Meijer	<b>Hike</b>	Closing remarks
2:00-2:40 2:40-3:20	Matt Beard Igor Fedin	Andrei Kryjevski Eric Bittner	Kirill Velizhanin R. Lindsey	<b>Meet at 2:00 pm at Gondola Station</b>	Adjourn
<b>Coffee Break</b>	<b>3:20-3:40</b>	<b>3:20-3:40</b>	<b>3:20-3:40</b>		
3:40-4:20 4:20-5:00	Sergei Ivanov Svetlana Kilina	Adela Habib Bakhtiyor Rasulev	Chris Mauney	<b>Continue at Smugglers at 5:00 pm</b>	
<b>TSRC events</b>			<b>Picnic/BBQ</b> 5:30-7:30 pm (the tent near the school)	<b>Town Talk</b> 6:30-7:30 pm (cash bar starts at 6:00 pm)	

## Agenda

### July 10: Saturday

#### Afternoon Session

**1:30 pm - 2:00 pm** Open Remarks from Organizers

**2:00 pm - 5:00 pm** **SESSION I:**

#### **Photoexcited Properties in Quantum Dots (QDs) and Interfaces**

Chair: Dmitri Kilin

- 2:00-2:40 **Matt Beard**, *NREL, Golden, CO*; Controlling Opto-Electronic Properties of QD and their Assemblies through Beneficial Ligand/QD Interactions
- 2:40-3:20 **Igor Fedin**, *University of Alabama, Tuscaloosa, AL*; Design and Synthesis of Colloidal QDs for Quantum Emitters
- 3:20-3:40** **Coffee Break**
- 3:40-4:20 **Sergei Ivanov**, *Los Alamos National Lab, Los Alamos, NM*; Assessing a Colloidal Route toward Different Magnetic Phases in Cr-Ge-Te Systems
- 4:20-5:00 **Svetlana Kilina**, *North Dakota State University, Fargo, ND*; Charge Transfer in QD-Dye Composites

## June 11: Sunday

### Morning Session

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

**9:00 am -12:00 pm**   **SESSION II:**

#### **Photoexcited Processes in Quantum Dots (QDs) and Interfaces**

*Chair: Sergei Ivanov*

- 9:00-9:40      **Sean Roberts**, *University of Texas, Austin*;  
Designing Hybrid Interfaces for Photon Up- and Down-Conversion
- 9:40-10:20      **Masaru Kuno**, *University of Notre Dame, Notre Dame, IN*;  
Photoluminescence Up-Conversion in CsPbBr<sub>3</sub> Nanocrystals
- 10:20-10:40**      **Coffee Break**
- 10:40-11:20      **Carlos Mora Perez**, *University of Southern California, Los Angeles, CA*;  
Deciphering Perovskite Nanocrystals with Quantum Dynamics  
Simulations: Overcoming Phonon Bottlenecks through Auger Processes
- 11:20-12:00      **Dmitri Kilin**, *North Dakota State University, Fargo, ND*;  
Photo-assisted Nucleation for Fabrication of Nanomaterials:  
Light-to-Matter Interaction Integrated with *Ab initio* Molecular Dynamics

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

### Afternoon Session

**2:00 pm - 5:00 pm**   **SESSION III:**

#### **Excitons and Machine Learning (ML)**

*Chair: Rebecca Lindsey*

- 2:00-2:40      **Andrei Kryjevski**, *North Dakota State University, Fargo, ND*;  
Electronic Structure of Semiconductor Nanoparticles from Stochastic  
Evaluation of Imaginary-Time Path Integral in Kohn-Sham Orbital Basis
- 2:40-3:20      **Eric Bittner**, *University of Houston, Houston, TX*;  
Looking Under the Hood and Unraveling Dark Processes in  
Excitonic Systems
- 3:20-3:40**      **Coffee Break**
- 3:40- 4:20      **Adela Habib**, *Los Alamos National Lab, Los Alamos, NM*;  
Machine Learning Enabled Electron Dynamics in Metal Nanoparticles
- 4:20- 5:00      **Bakhtiyor Rasulev**, *North Dakota State University, Fargo, ND*;  
Machine Learning in Materials Science: Carbon Nanostructures and  
Organometallic Complexes' Case Studies

## June 12: Monday

### Morning Session

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

9:00 am -12:30 pm    **SESSION IV:**

#### **Magnetic Properties and Spin Dynamics in Nanostructures**

*Chair: Matt Beard*

- 9:00-9:40      **Han Htoon**, *Los Alamos National Lab, Los Alamos, NM;*  
Correlated Excitonic Signatures in a Nanoscale van der Waals  
Antiferromagnet
- 9:40-10:20      **Louis Bouchard**, *University of California, Los Angeles, CA;*      The  
Need for Quantum-Grade Materials with Engineered Spin Interactions
- 10:20-10:40      **Coffee Break**
- 10:40-11:20      **Ryan Beck**, *University of Washington, Seattle, WS;*  
Modeling of Electronic Properties in Hybrid Perovskites: From Experimental  
Challenge to Theoretical Understanding
- 11:20-12:00      **Jinsoo Park**, *California Institute of Technology, Pasadena, CA;*  
First-Principles Many-Body Theory of Phonon-Induced Spin Relaxation and  
Decoherence

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

### Afternoon Session

2:00 pm - 4:20 pm    **SESSION V:**

#### **Modeling Reactions and Bond Breaking**

*Chair: Evert Jan Meijer*

- 2:00-2:40      **Kirill Velizhanin**, *Los Alamos National Lab, Los Alamos, NM;*  
Carbon Condensation in Detonations of High Explosives: Theory  
Perspective
- 2:40-3:20      **Rebecca Lindsey**, *University of Michigan, Ann Arbor, MI;*  
Understanding the Chemistry Governing Shockwave-Driven Nanocarbon  
Synthesis
- 3:20-3:40      **Coffee Break**
- 3:40-4:20      **Christofer Mauney**, *Los Alamos National Lab, Los Alamos, NM;*  
Dust Formation in Supernovae Remnants and Evolution in the ISM

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

## June 13 Tuesday

### Morning Session

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

**9:00 am -12:30 pm    SESSION VI:**

#### **Photophysics of Organic/Inorganic Materials**

*Chair: Svetlana Kilina*

- 9:00-9:40      **Xiwen Gong**, *University of Michigan, Ann Arbor, MI;*  
Inorganic Nanomaterials for Wearable Optoelectronics
- 9:40-10:20      **Timo Thonhauser**, *Wake Forest University, Winston-Salem, NC;*  
Combining Modeling and Experiment to Study Molecular Adsorption in  
Metal-Organic Frameworks
- 10:20-10:40      Coffee Break**
- 10:40-11:20      **Wenfang Sun**, *University of Alabama, Tuscaloosa, AL;*  
Impacts of Ligands Benzannulation on the Photophysics and Reverse  
Saturable Absorption of Monocationic Iridium(III) Complexes: A Combined  
Experimental and Theoretical Study
- 11:20-12:00      **Aaron Forde**, *Los Alamos National Lab, Los Alamos, NM;*  
Chirality Induction for Circular Polarization Sensitive Nanomaterials

**12:00-1:00 pm      Lunch (on your-own)**

**2:00 pm - 8:00 pm    Hiking & Telluride/Mountain Village Tour on a Free Gondola**

- 2:00-5:00      Bear Creek Trail**  
Gathering at Gondola Station Telluride (*Oak Street*)
- 5:00-6:30      Social gathering at Smugglers Brewpub**  
(*225 S Pine St Telluride, CO 81435*)
- 6:30-7:30      Telluride Science Town Talk**  
Telluride Conference Center in Mountain Village  
(*Gondola Station St. Sophia*)

## June 14: Wednesday

### Morning Session

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

9:00 am -12:30 pm    **SESSION VI:**

#### **Nanocarbon Materials**

Chair: *Kirill Velizhanin*

- 9:00-9:40      **Alexander Star**, *University of Pittsburgh, Pittsburgh, PA*;  
Advanced Carbon Nanomaterials for Sensing Applications:  
From Functionalized Nanotubes to Holey Graphene
- 9:40-10:20      **Dinesh Thapa**, *North Dakota State University, Fargo, ND*;  
Optical Generation of Trions in Chemically Tweaked Single Walled Carbon  
Nanotubes
- 10:20-10:40      **Coffee Break**
- 10:40-11:20      **Evert Jan Meijer**, *University of Amsterdam, Amsterdam, Netherlands*;  
Novel Insights in the Role of Solvent and Ions in Catalytic Processes
- 11:20-12:00      **Nikita Fedik**, *Los Alamos National Lab, Los Alamos, NM*;  
Bridging the Scales: Chemical Bonding, Machine Learning, and  
Differentiable Physics for Nanomaterials Exploration

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

2:00 pm      **Adjourn**