**2013 Telluride Conference**

**Advances In Photoreactions: When Spin-Orbit Coupling, Optical Excitation, and Motion of Nuclei are of Equal Importance?**

**Location**: Telluride Intermediate School at 725 W. Colorado Ave

**Workshop** Organizers: Svetlana Kilina and Dmitri Kilin

**TSRC Hosts**: Nana Naisbitt at 970-708-0004 and Rory Sullivan at 970-708-4542

**Tentative Agenda**

**June 24**

***Monday Evening***

**6:00 – 9:00 pm** Welcome Reception at the New Sheridan Bar at 231 W. Colorado, cash bar, free pool

**June 25**

***Tuesday Afternoon***

**1:00-1:30 pm Refreshment / Social gathering at TSRC**

**1:30-1:45 pm** Welcome and Opening Remarks

**1:45-5:00 pm Section I**: ***Photoexcited Dynamics in Carbon-Based Materials***

*Chair: Joel Eaves - Toru Shiozaki*

1:45-2:30 Kirill Velizhanin, Los Alamos National Lab, NM

*“Curious Thermodynamics of Functionalized Graphene”*

2:30-3:15 Heather Jaeger, Lehigh University, PA

“*Decoherence in the Nonradiative Relaxation Pathways of Photo-Excited Graphitic Nanostructures”*

**3:15-3:30 Coffee Break**

3:30- 4:15 Jacek Jakowski, Oak Ridge National Lab / University of Tennessee, TN

“*Modeling Materials at the Nanoscale”*

4:15- 5:00 Spiridoula Matsika, Temple University, PA

*“Exciplexes and Conical Intersections in Pi-Stacked Dimers of Nucleobases”*

**6:00-7:15 TSRC Town Talk** at the Historic Sheridan Opera House at 110 N. Oak Street

**June 26**

***Wednesday Morning***

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

**9:00-9:05** Organizational Remarks

**9:05 am -12:20 pm Section II: *Photophysical Properties of Materials Activated***

***by f-Elements***

*Chair: Jeffrey Pietryga-* *Spiridoula Matsika*

9:05-9:50 Mary Berry, University of South Dakota, SD

*“Photodissociation Dynamics of Lanthanide-Based Metal Organic Complexes”*

9:50-10:35 Dmitri Kilin, University of South Dakota, SD

*“Non-adiabatic Processes in Lanthanide Activated Materials”*

**10:35-10:50 Coffee Break**

10:50- 11:35 Stanley May, University of South Dakota, SD

*“Metal-Surface-Enhanced NIR-to-Visible Upconversion in Lanthanide-Doped Nanocrystals”*

11:35- 12:20 Xiaodong Wen, Los Alamos National Lab, NM

*“Performance of Screened Hybrid Functional on Actinide Oxides”*

**12:20-2:00 Lunch** (by your own)

***Wednesday Afternoon***

**2:00 pm -5:00 pm Section III: *Computational Approach to Spin-Polarization in Solids and Molecules***

*Chair: Benjamine Levine*

2:00-2:45 Toru Shiozaki, Northwestern University, IL

*“Fully Relativistic 4-Component Electronic Structure Methods for 100 Atomic Systems”*

2:45-3:30 Vladimir Turkowski, University of Central Florida, FL

*“Time-Dependent Spin-Density Functional Theory for Photo-Excitations in Strongly Correlated Electron Materials”*

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

3:45- 4:30 Shruba Gangopadhyay, IBM, CA

“*Application of DFT+U to Understand Atomic Scale Magnetism”*

4:30- 5:00 Discussion (Moderator: Dmitri Kilin)

**6:00-dark TSRC Picnic** at the Ah Haa Art School at 300 S. Townsend

**June 27**

***Thursday Morning***

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

**9:00-9:05** Organizational Remarks

**9:05 am -12:20 pm Section IV: *Photodynamics in Semiconductor Nanocrystals***

*Chair Stanley May-Elena Jakubikova*

9:05-9:50 Jeffrey Pietryga, Los Alamos National Lab, NM

*“The Surprising Influence of Metal Impurities on the Optical and Magnetic Properties of Semiconductor Nanocrystals”*

9:50-10:35 Benjamine Levine, Michigan State University, MI

*“A Multireference Approach to Modeling Semiconductor Photodynamics”*

**10:35-10:50 am Coffee Break**

10:50- 11:35 Richard Schaller, North Western University / Argon National Lab, IL

*"Probing Energy Migration in Semiconductor Nanocrystals for Sensing and Energy Applications"*

11:35- 12:20 Kenneth Lopata, Louisiana State University, LA

*“Shedding Light on Excited States with Real-Time Time-Dependent Density Functional Theory: Valence, Core, Spin-Orbit, and Auto-Ionizing Excitations.”*

**12:20-2:00 Lunch** (by your own)

***Thursday Afternoon***

**2:00 pm -5:00 pm Section IV: *Photophysics of Chemically Functionalized Nanoparticles***

*Chair: Richard Schaller*

2:00-2:45 Aleksey Kuznetsov, North Carolina State University, NC

*Structural and Electronic Properties of Bare and Capped Cd33Se33 and Cd33Te33 Nanoparticles”*

2:45-3:30 Svetlana Kilina, North Dakota State University, ND

*“Verifying Conditions for Electron Transfer in Quantum Dots Functionalized by Organometallic Complexes”*

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

3:45- 4:30 Sergei Ivanov, Sandia National Lab, NM

“*Uncovering the Origin of Fluorescence in Ligand-Protected Small Gold Clusters”*

4:30- 5:00 Discussion (Moderator: Kirill Velizhanin)

**June 28**

***Friday Morning***

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

**9:00-9:05** Organizational Remarks

**9:05 am -12:20 pm Section IV: *Photophysics of Chromophores for Photovoltaics***

Chair: Mary Berry

9:05-9:50 Elena Jakubikova, North Carolina State University, NC

*“Toward Computational Design of Iron-Based Chromophores for Solar Energy Conversion”*

9:50-10:20 Naveen Dandu, North Dakota State University, ND

*“Computational Insights into Optical Transitions in Pt (II) and Ir(III) Complexes”*

**10:20-10:35 am Coffee Break**

10:35-11:20 Joel Eaves, University of Colorado, Bolder, CO

*“Exciton Dynamics in Carbon Nanotubes: A View From the*

*Luttinger Liquid”*

11:20-12:05 Andriy Zhugayevych, Los Alamos National Lab, NM

*"Ultrafast Exciton Dissociation in Small-Molecule Bulk-Heterojunction Solar Cells"*

12:05-12:30 Discussion (Moderator: Sergei Ivanov)

**12:30-1:30 Lunch** (by your own)

***1:30-6:00 Hiking* (Bear Creek Trail)**

**June 29**

***Saturday Morning***

**9:00-10:00** Breakfast at TSRC for participants

**10:00-12:00** Closing Remarks/ Discussion/ Farewell