Workshop on "Spatio-Temporal Dynamics of Excitons: Bridging the Gap between Quantum Mechanics and Applications" (June 10 – 14, 2024)

June 10, Monday

7:15-8:20 am: Breakfast at the Center (Telluride Intermediate School)

8:20 - 8:30 am: Opening Remarks

Session 1: Spectroscopy and Computational Modeling of Molecular Excitons - Jang

8:30 – 9:10 am (Talk1): Justin Caram, "Exploring the total photon economy of molecules and molecular aggregates"

9:10 – 9: 50 am (Talk 2): Chern Chuang, "Long- and short-range interactions in low-dimensional anisotropic excitonic systems and their spectroscopic and dynamical features"

9:50 – 10:30 am (Talk 3): John Herbert, "The Importance of orbital Invariance in measuring electron-hole separation"

10:30 – 10:50 am: Break

10:50 - 11:30 am (Talk 4): Gabriela Schlau-Cohen, "Sculpting photoproducts with DNA origami"

11:30 am – 12:10 pm (Talk 5): Andres Montoya Castillo, "Symmetry-breaking fluctuations split porphyrin Q-bands"

12:10 - 2:00 pm: Lunch on your own

Session 2: Semiconductor Nanocrystal Excitons - Tretiak

2:00 – 2:40 pm (Talk 6): **Dong Hee Son**, "Hot electrons and coherent photons from stronglyconfined perovskite nanocrystals and their superlattices"

2:40 – 3:20 pm (Talk 7): Eric Bittner, "Dark excitons and dark polaritons in hybrid perovskites"

3:20 – 3:40 pm (Talk 8): **Ari Chakraborty**, "Generation of entangled-photon pair from biexcitonic-to-exciton cascade decay in semiconductor nanoparticles"

3:40 – 4:00 pm: Break

4:00 – 4:40 pm (Talk 9): Carsten Ullrich, "Towards real-time TDDFT for excitons in solids"

4:40 – 5:20 pm (Talk 10): **Aaron Sternbach**, "Interrogation and control of excitons with ultrafast nano optical spectroscopy"

5:20 – 6:00 pm (Talk 11): **Dmitri Kilin**, "First principles dissipative dynamics of excitons: from bound excitons to machine learning"

June 11, Tuesday

7:15-8:20 am: Breakfast at the Center (Telluride Intermediate School)

Session 3: Quantum Effects and Spins - Caram

8:20 - 9:00 am (Talk 12): David Jonas, "Absorption from an extreme Stokes' shift"

9:00 – 9:40 am (Talk 13): Joel Yuen-Zhou, "Organic diradicals as molecular spin qubits"

9:40 – 10:20 am (Talk 14): Li Hao, "Correlated noise enhancement of coherence and fidelity in coupled qubits"

10:20 – 10:40 am: Break

10:40 – 11:20 am (Talk 15): Michael Wasielewski, "Spin dynamics of charge transfer excitons in molecular donor-acceptor co-crystals"

11:20 am – 12:00 pm (Talk 16): **Jeff Cina**, "Interference, coherence, and Berry's phase development in an energy-transfer trimer"

12:00 – 1:30 pm: Lunch at the Center

Session 4: Intersystem Crossing, Defects, and Disorder - Cina

1:30 – 2:10 pm (Talk 17): William Barford, "Singlet triplet-pair production and singlet fission in carotenoid systems"

2:10 – 2:50 pm (Talk 18): **Sean Roberts**, "Imaging energy migration within singlet fission materials"

2:50 – 3:10 pm: Break

3:10 – 3:50 pm (Talk 19): **Svetlana Kilina**, "Unveiling the role of chemical defects in carbon nanotubes: Simulating pathways and understanding defect-related excitons"

3:50 – 4:30 pm (Talk 20): **Joel Eaves**, "Realistic quantum noise: Averaged trajectories without averaging"

6:30 pm: Telluride Town Talk (Telluride Convention Center, Mountain Village)

June 12, Wednesday

7:15-8:20 am: Breakfast at the Center (Telluride Intermediate School)

Session 5: Spatio-temporal evolution of excitons – Montoya Castillo

8:20 – 9:00 am (Talk 21): **Naomi Ginsberg**, "A vision for detecting and discerning the spatiotemporal evolution of multiple forms of energy as they interconvert and explore heterogeneous material structure"

9:00 – 9:40 am (Talk 22): Jianshu Cao, "Unusual quantum diffusivity in disordered materials"

9:40 – 10:20 am (Talk 23): Irene Burghardt, "Quantum dynamical simulations of H, J, and HJ aggregates: Adiabatic and non-adiabatic exciton transport driven by soft modes"

10:20 - 10:40 am: Break

10:40 – 11:20 am (Talk 24): **Art Bragg**, "Exciton dynamics in templated and scaffolded molecular assemblies"

11:20 am – 12:00 pm (Talk 25): **Doran Raccah**, "Size-invariant scaling simulations of exciton dynamics and spectroscopy"

12:00 – 1:30 pm: Lunch at the center

Session 6: Dynamics of Molecular Excitons - Burghardt

1:30 – 2:10 pm (Talk 26): **Cathy Wong**, "In situ transient absorption during molecular aggregation"

2:10 – 2:50 pm (Talk 27): Kuniyuki Miwa, "Quantum dynamics of photoexcited electronic systems coupled to anharmonic oscillator environments"

2:50 – 3:10 pm: Break

3:10 – 3:50 pm (Talk 28): Richard Hildner, "Energy transport in complex supramolecular nanostructures"

3:50 – 4:30 pm (Talk 29): **Sergei Tretiak**, "Non-adiabatic excited state molecular dynamics: Bridging the gap between quantum mechanics and applications to molecules"

5:30 pm: Picnic & Barbecue (Tent behind dchool, Families welcome)

June 13, Thursday

7:15-8:20 am: Breakfast at the Center (Telluride Intermediate School)

Session 7: Probing and Utilizing Excitonic Effects in Dynamics -Yuen-Zhou

8:20 - 9:00 am (Talk 30): Libai Huang, "Exciton interactions and quantum transport"

9:00 – 9:40 am (Talk 31): **Roel Tempelaar**, "Mixed quantum–classical modeling of exciton–phonon scattering in solids"

9:40 – 10:20 am (Talk 32): Chad Cruz, "Making the connection: searching for spectroscopic signatures that inform device behavior"

10:20 – 10:40 am: Break

10:40 – 11:20 am (Talk 33): **Milan Delor**, "Imaging, controlling and extracting ballistic excitons in van der Waals semiconductors"

11:20 am – 12:00 pm (Talk 34): **Seogjoo Jang**, "Fermi's golen rule and Magnus expansion for exciton transfer rates and dynamics"

12:00 - 5:00 pm - Lunch (on your own) & Group hiking

6:00 – 8:00 pm – Group dinner

June 14, Friday

7:15-8:20 am: Breakfast at the Center (Telluride Intermediate School)

Discussion & Informal Meetings