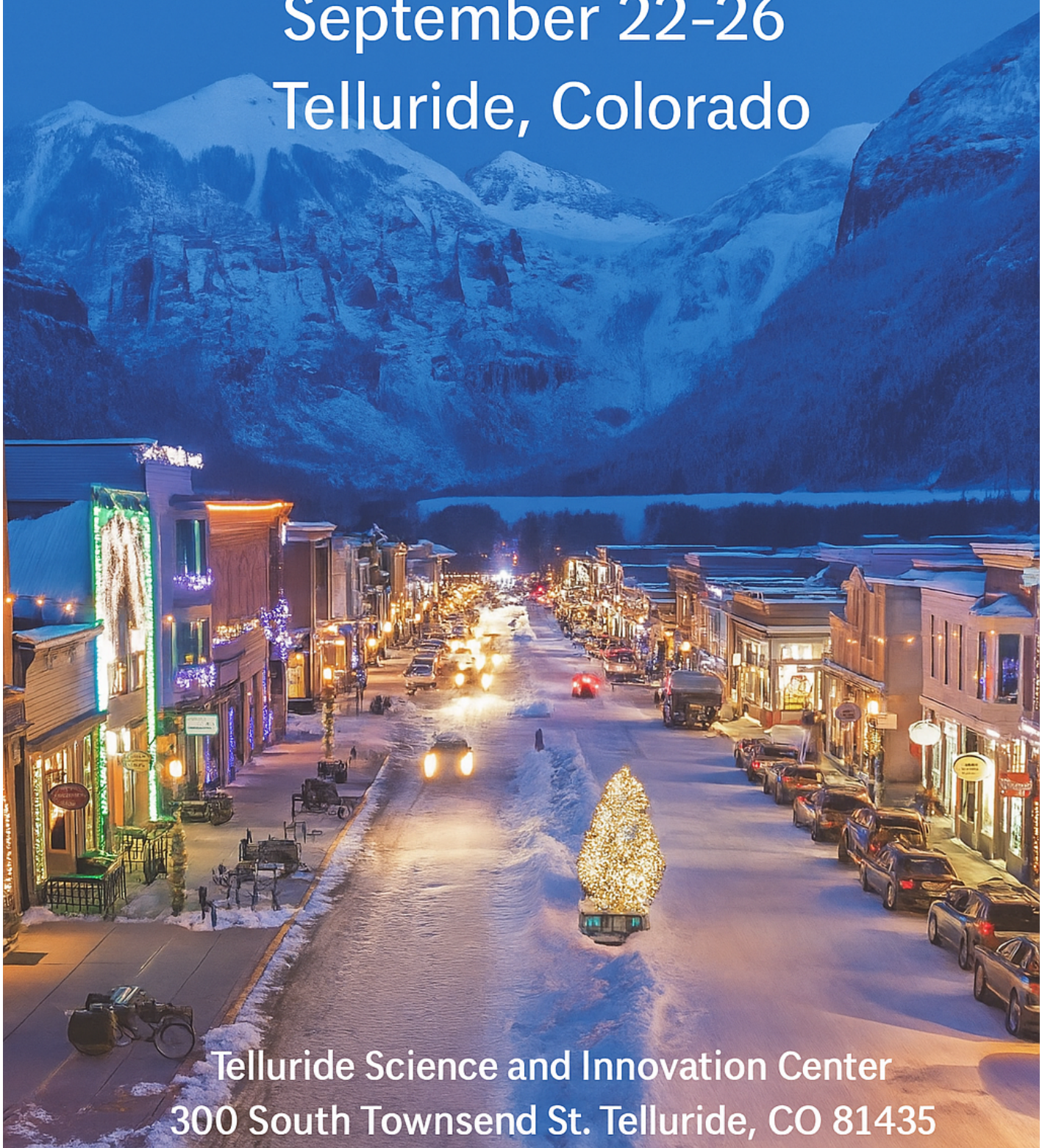
Exciton/Photon

Interactions for Quantum Systems

September 22-26

Telluride, Colorado



Telluride Science and Innovation Center

300 South Townsend St. Telluride, CO 81435

Contents

About

Exciton/Photon Interactions for Quantum Systems: 09/22/2025 - 09/26/2025

Organizers

- Hao Li (Université de Montréal)
- Carlos Silva (Université de Montréal)
- Andrei Piryatinski (LANL)

Meeting Description: This workshop builds upon a history of four highly successful prior TSRC workshops focused upon quantum coherences and collective behavior that evolve due to the strong coupling between matter and a quantized radiation field. Here, we expand the scope of our workshop beyond cavity QED systems and consider a broader range of physical effects stemming from strong light-matter interactions. Topics will include excited-state dynamics, nonlinear spectroscopy, quantum optics, quantum computing, cavity QED effects, polaritons and polariton condensation, and quantum nonlinear optics. The workshop is honoring the 60th birthday of Professor Eric Bittner (Department of Physics, University of Houston) and his seminal contributions to the theories of quantum dynamics and a broad range of fields covered by the workshop.

We wish to ensure an intimate workshop setting, with no more than 20 to 25 participants. If you are interested in attending, but have not received an invitation, please contact the workshop organizer before registering.

Telluride Science is about expanding the frontiers of science, exploring new ideas, and building collaborations. The workshop schedule will allow for substantial unstructured time for participants to talk and think. All participants are expected to stay for the entire duration of the workshop. Scientists are encouraged to consider bringing family or friends. Telluride offers a number of options for children's camps (including Telluride Academy, Aha School for the Arts, and Pinhead Institute). There is more information on childcare, camps, and family activities on Telluride Science's website. Feel free to contact Telluride Science's staff to help with any planning and/or coordinating care.

Autobiography of Eric Bittner

Professor Eric Bittner received his Ph.D.in 1994 from the University of Chicago and was an NSF Postdoctoral Fellow at the University of Texas at Austin from 1994-1996 and Stanford University. Since 1997, he has been a professor at the Univ. of Houston, where his main research interests concern the quantum dynamics of excitons in materials, quantum optics, many-body theory, quantum trajectory methods, stochastic models of quantum dynamics, and nonlinear spectroscopy. Honours include fellowships in the American Physical Society, the American Association for the Advancement of Science, and the Royal Society of Chemistry. He is a 2007 Guggenheim Fellow and a 2012 Fulbright Fellow. He currently holds the Hugh Roy and Lillian Cranz-Cullen Distinguished Professorship of Chemical Physics at the University of Houston and was the Stanislaw Ulam Distinguished Visiting Scholar at the Los Alamos National Laboratory in 2022-2023. Outside interests include backpacking, sailing, historical fencing, and playing guitar.

List of Participants

Confirmed as of September 17, 2025,

	Name	Institute	Email Address
	Eric Bittner	University of Houston	bittner@central.uh.edu
	Alfonso N Castillo Gonzalez	University of Houston	ancasti4@CougarNet.uh.edu
	Sameer Dambal	University of Houston	sadambal@central.uh.edu
	Kimberley Hall	Dalhousie University	Kimberley.Hall@Dal.Ca
	Suggy Jang	City University of New York (Queens College)	Seogjoo.Jang@qc.cuny.edu
	Ajay Kandada	Wake Forest University	srimatar@wfu.edu
	Hao Li	Université de Montréal	hao.li.3@umontreal.ca
	Jeremy Maddox	Western Kentucky University	jeremy.maddox@wku.edu
	Ognjen Miljanic	University of Houston	miljanic@uh.edu
	Frank Natia	University of Nevada, Reno	nfrank@unr.edu
	Andrei Piryatinski	Los Alamos National Laboratory	apiryat@lanl.gov
	Bill Poirier	University of Vermont	Bill.Poirier@uvm.edu
	Oleg Prezhdo	University of New Mexico	prezhdo@unm.edu
	Doran Raccah	University of Texas at Austin	doran.raccah@utexas.edu
	Raphael Ribeiro	Emory University	raphael.ribeiro@emory.edu
	Jonathan Snow	Louisiana State University	jesnow@lsu.edu
	Alan Steinberg	Independent Consultant	alaneilsteinberg@gmail.com
	Sergei Tretiak	Los Alamos National Laboratory	serg@lanl.gov
	Bhavay Tyagi	University of Houston	btyagi@CougarNet.uh.edu
	Jiri Vanicek	École Ploytechnique Fédérale de Lausanne	jiri.vanicek@epfl.ch
	Yu Zhang	Los Alamos National Laboratory	zhy@lanl.gov

Topical Sessions

- 2D TMD materials & vdW heterostructures
  - correlated excitons
  - magneto-excitons
  - exciton condensations
- Polariton physics and cavity QED
  - Strong coupling between matter/radiation
  - polariton condensation
- organic/solid state quantum emitters
- Plasmonic cavities
- Spectroscopic methods
- Material synthesis & characterization.

Daily Schedule

Day 1: Monday, September 22

7:00–9:00	**Badge Pickup & Breakfast available at site**		
8:45–9:00	**Workshop Opening**		
Session 1	**Stochastic Quantum Mechanics**		
9:00–9:40	IT	**Eric Bittner** University of Houston	Synchronization of Quantum States: Exploring how noise, topology, and dimensionality affect quantum phase coherence
9:40–10:20	IT	**Bhavay Tyagi** University of Houston	On 'Noise-Friendly' Quantum Systems
10:20–10:40	**Coffee Break**		
Session 2	**Quantum Optics and Spectroscopy**		
10:40–11:20	IT	**Kimberley Hall** Dalhousie University, Canada	Laser Driving Schemes for Solid-State Emitters using Engineered Optical Pulses
11:20–12:00	IT	**Ajay Ram Srimath Kandada** Wake Forest University	Quantum Signatures and Spectral Fluctuations: New Windows into Molecular Condensates and Excitonic Complexes
12:00–14:00	**Lunch (on your own) & Discussion**		
Session 3	**Quantum Materials and Computation**		
14:00–14:40	IT	**Natia Frank** University of Nevada, Reno	Optical Gating of Spin-based Quantum States for QISE
14:40–15:20	IT	**Andrei Piryatinski** LANL	TBA
15:20–15:40	**Coffee Break**		
15:40–16:20	IT	**Jeremy Maddox** Western Kentucky University	Numerical methods and benchmark results for interacting quantum trajectories in 1D and 2D model systems
16:20–17:00	IT	**Carlos Silva** Université de Montréal	TBA

Day 2: Tuesday, September 23

7:00–9:00	**Breakfast available at site**		
Session 4	**Quantum Dynamics I**		
9:00–9:40	IT	**Sergei Tretiak** LANL	Four years of adventure in the land of chirality
9:40–10:20	IT	**Doran Raccah** UT Austin	TBA
10:20–10:40	**Coffee Break**		
10:40–11:20	IT	**Oleg Prezhdo** University of New Mexico	Ab Initio Nonadiabatic Molecular Dynamics in Cavities: Anisotropic Exciton-Polariton Relaxation and Phonon Bottleneck in Metal Halide Perovskites
11:20–12:00	IT	**Raphael Ribeiro** Emory University	TBA
12:00–14:00	**Lunch (on your own) & Discussion**		
Session 5	**Quantum Dynamics II**		
14:00–14:40	IT	**Seogjoo Jang** CUNY - Queens College	Molecular Excitons and Quantum Sensing
14:40–15:20	IT	**Jiri Vanicek** EPFL, Switzerland	Vibrationally resolved electronic spectra from Hagedorn wavepacket dynamics
15:20–15:40	**Coffee Break**		
15:40–16:20	IT	**Alan Steinberg** Independent Consultant	A Trek Through Data Fusion
16:20–17:00	**Informal Discussion**		
17:30–	**Eric's Birthday Party (catered dinner on site)**		

Day 3: Wednesday, September 22

7:00–9:00	**Breakfast available at site**		
Session 6	**Introduction to Local Geology**		
8:30–12:30	IT	**Jon Snow** Louisiana State University	Group Hike/Photoshoot
12:30–14:00	**Lunch (on your own) & Discussion**		
Session 7	**ML & Quantum Computing**		
14:00–14:40	IT	**Bill Poirier** University of Vermont	Full-dimensional Schrödinger wavefunction calculations using tensors and quantum computers: the Cartesian component-separated approach
14:40–15:20	IT	**Yu Zhang** LANL	TBA
15:20–15:40	**Coffee Break**		
15:40–16:20	IT	**Alfonso Castillo** University of Houston	TBA
16:20–17:00	**Informal Discussion**		
17:30–	**TSRC BBQ Picnic**		

Day 4: Thursday, September 25

7:00–9:00	**Breakfast available at site**		
Session 8	**Quantum Spectroscopy**		
9:00–9:40	IT	**Ognjen Š. Miljanić** University of Houston	Guest Binding in Cyclobenzoin Derivatives
9:40–10:20	IT	**Sameer Dambal** University of Houston	Quantum Spectroscopy with Biphotons: Lyapunov-Based Input–Output Dynamics
10:20–10:40	**Coffee Break**		
10:40–11:20	IT	**Hao Li** Université de Montréal	Stochastic Exciton Scattering Theory for Multidimensional Spectroscopy
11:20–12:00	**Informal Discussion**		
12:00–14:00	**Lunch (on your own) & Discussion**		
14:00–17:00	**Informal discussion & Collaboration**		

Day 5: Friday, September 26

7:00–9:00	**Breakfast available at site**
all day	**Informal discussion & Collaboration**

Abstracts for Invited and Contributed Talks

Synchronization of Quantum States: Exploring how noise, topology, and dimensionality affect quantum phase coherence

Eric R. Bittner IT

Department of Physics, University of Houston

When we think of noise in quantum systems, we usually picture it as the great spoiler—washing out delicate superpositions and destroying entanglement. But the story is more interesting. Just as pendulum clocks on the same wall can spontaneously tick in unison, quantum systems can also synchronize, sometimes because of the noise in their environment rather than in spite of it. In this talk, I will explore how the structure of noise, the connectivity of a system, and even its dimensionality and topology, shape the way quantum states maintain—or lose—phase coherence. Drawing on examples that range from pairs of coupled spins to extended lattices and topological chains, I will show how correlations in the environment can protect certain collective modes, leading to unexpected resilience against decoherence. Along the way, we will see how ideas from classical synchronization, network theory, and topological physics converge in the quantum realm. The broader message is that noise and dissipation, usually treated as adversaries, can sometimes be harnessed as resources—pointing toward new strategies for stabilizing coherence in quantum devices and materials.

Quantum Spectroscopy with Biphotons: Lyapunov-Based Input–Output Dynamics

Sameer Dambal[a], ***Ajay Ram Srimath Kandada***[b], ***Eric Bittner***[a]

[a] Department of Physics, University of Houston, Houston, Texas 77204, United States
[b] Department of Physics and Center for Functional Materials, Wake Forest University, 1834 Wake Forest Road, Winsto-Salem, NC 27109, United States

We develop a Lyapunov-based framework to model the evolution of entangled biphotons interacting with cavity and material modes. Using Gaussian-preserving dynamics and Møller operators, we map input joint spectral amplitudes to experimentally measurable joint spectral intensities. Our model reproduces key features of observed spectra and reveals off-diagonal correlations arising from cavity decay, providing a scalable and tractable tool for quantum spectroscopic analysis

References

[1] S. Dambal, A. R. S. Kandada, and E. R. Bittner, arXiv preprint arXiv:2504.14086 (2025).

Optically Bistable Spin Systems for Quantum Science

Natia L. Frank IT

Department of Chemistry, University of Nevada Reno, Reno NV 89557

Quantum sensing utilizes the exquisite sensitivity of quantum states to external field (magnetic, electric, thermal, and electromagnetic) to detect and measure physical quantities of interest with unprecedented sensitivity and accuracy. Here we propose an indirect strategy for quantum sensing in molecular systems based on the response of structurally bistable ligands to external stimuli, which in turn modulate the quantum states of central transition metal ions. We have recently reported the optical gating of spin-charge states in cobalt semiquinones from a $ls{-}Co(III)catSQ.(doubletS$ =1/2$qubitstate)toa$hs-Co(II)(SQ.-)$_2$ (entangled $hs-Co(II)S=3/2$ bis semiquinone $(S=$) qudit) state via photochromic ligands. Magnetization and optical spectra are consistent with photoisomerization induced spin achreg process, in which photoisomerization leads to changes in the driving force for charge coupled spin transititon process, leading to a long lifetime of $10s$ at room temperature. Here we demonstrate optical gating of the g-anisotropy via cw X-band EPR between the two states from a $Co(III)catSQ.$ (doublet $S=1/2$ qubit state) isotropic $g\approx 2.00$ to $hs-Co(II)(SQ.-)_2$ with g-factors or $g\approx 2.48$ and 5.0. Pulsed EPR experiments lowed characterization of the spin dynamics (T1 and Tm) in the $Co(III)$ state via inversion recovery and Hahn echo sequences. The spin lifetime was found to be quite long (Tm $\approx$ ms) consistent with an organic radical, suggesting external manipulations feasibly fall within the long coherence times observed. The strategy is extended to simple isotropic spin systems in which significant changes in coherence times are observed with ligand isomerization. By leveraging bistable systems that respond to the local environment, an indirect strategy for quantum sensing is proposed whereby a subtle shift in environment leads to changes in quantum state populations and energies for quantum information protocols.

Laser Driving Schemes for Solid-State Emitters using Engineered Optical Pulses

Kimberley C. Hall IT

Department of Physics and Atmospheric Science, Dalhousie University, Canada

Sources of single and entangled photons represent an enabling technology for many areas of quantum photonics, including quantum computation [1], quantum cryptography [2] and quantum sensing [3]. Among candidate physical systems under consideration, solid-state emitters offer enhanced potential for long-term scalability and integration with classical communication hardware [3,4]. Over the past decade, our research group has been developing laser triggering schemes for solid-state quantum emitters that exploit the ability to engineer the light-matter interaction by shaping the laser pulse [5-9]. Arbitrary pulse engineering using both amplitude and phase control enables triggering protocols that are robust to variations in laser pulse parameters such as pulse area and detuning [5,7], facilitating commercial implementation. In addition, shaping eases the technical complexity associated with multiplexing in quantum optical systems [9] and enables several performance metrics of quantum emitters (brightness, indistinguishability, purity) to be optimized simultaneously [8].

We recently proposed a new laser triggering scheme called Notch-filtered Adiabatic Rapid Passage (NARP) that enables resonant pumping in conjunction with spectral rejection of scattered laser light [8]. When combined with optimized photonic structures for enhanced collection efficiency and commercial filters, we estimate that NARP would provide less than 10^{-8} scattered photons per emitted photon with a 4% detection loss, far superior to the minimum 50% loss associated with polarization-based filtering. In this presentation, I will highlight our recent experiments implementing NARP in single semiconductor quantum dots, including InGaAs quantum dots in planar heterostructures, and InAsP quantum dots in nanowire waveguides.

References

[1] J.C. Loredo, M.A. Broome, P. Hilaire, O. Gazzano, I. Sagnes, A. Lemaitre, M.P. Almeida, P. Senellart, and A.G. White, Boson Sampling with Single-Photon Fock States from a Bright Solid-State Source, Phys. Rev. Lett., vol. 118, pp. 130503, 2017.
[2] F. B. Basset, M. Valeri, E. Roccia, V. Muredda, D. Poderini, J. Neuwirth, N. Spagnolo, M. B. Rota, G. Carvacho, F. Sciarrino, and R. Trotta, Quantum key distribution with entangled photons generated on demand by a quantum dot, Sci. Adv. vol. 7, pp. eabe6379, 2021.
[3] M. Atature, D. Englund, N. Vamivakas, S.-Y. Lee, and J. Wrachtrup, Material platforms for spin-based photonic quantum technologies, Nature Review Materials vol. 3, 38, 2018.
[4] P. Senellart, G. Solomon, A. White. “High-performance semiconductor quantum-dot single-photon sources”, Nature Nanotechnology 12, 1026, 2017.
[5] R. Mathew, E. Dilcher, A. Gamouras, A. Ramachandran, H. Y. S. Yang, S. Freisem, D. Deppe, and K. C. Hall, “Subpicosecond adiabatic rapid passage on a single semiconductor quantum dot: phonon-mediated dephasing in the strong-driving regime”, Phys. Rev. B 90, 035316, 2014.
[6] A. Ramachandran, G. R. Wilbur, S. O’Neal, D. G. Deppe, and K. C. Hall, Suppression of decoherence tied to electron–phonon coupling in telecom-compatible quantum dots: low-threshold reappearance regime for quantum state inversion, Optics Letters, 45, 6498 (2020).

[7] A. Ramachandran, J. Fraser-Leach, S. O'Neal, D. G. Deppe, and K. C. Hall, Experimental quantification of the robustness of adiabatic rapid passage for quantum state inversion in semiconductor quantum dots. Optics Express, 29, 41766 (2021).
[8] G. R. Wilbur, A. Binai-Motlagh, A. Clarke, A. Ramachandran, N. Milson, J. P. Healey, S. O'Neal, D. G. Deppe, K. C. Hall, "Notch-filtered Adiabatic Rapid Passage for optically driven quantum light sources", APL Photonics 7, 111302, 2022.
[9] A. Ramachandran, G. R. Wilbur, R. Mathew, A. Mason, S. O'Neal, D. G. Deppe, and K. C. Hall, "Robust parallel driving of quantum dots for multiplexing of quantum light sources", Sci. Rep. 14:5356, 2024.

Molecular Excitons and Quantum Sensing

Seogjoo J. Jang **IT**

Department of Chemistry and Biochemistry, Queens College, City University of New York PhD Programs in Chemistry and Physics, Graduate Center, City University of New York

This talk presents some of our on-going efforts for reliable computational modeling of the dynamics of molecular excitons and for the development of theories and computational methods to utilize molecular excitons for quantum sensing.

First, for molecular excitons, I will highlight our ongoing efforts to elucidate design principles behind natural light harvesting 2 (LH2) complex of purple bacteria, where Frenkel-type excitons are formed. I will highlight the role of disorder and hydrogen bonding in making LH2 a superb exciton harvester and also offer new computational evidence supporting this view.

Second, for quantum sensing (QS), I will start with a general overview addressing key theoretical issues. In particular, quantum estimation theory will be summarized as a central theory of QS, and implication of a new form of quantum Fisher information we derived will be discussed. This will be followed by a simple proposal of using molecular excitons for quantum sensing and preliminary computational data on modeling the nonradiative decay of azulene, which is viewed as a versatile template for developing molecular QS device.

Numerical methods and benchmark results for interacting quantum trajectories in 1D and 2D model systems

Jeremy Maddox IT

Department of Chemistry and Biochemistry, Western Kentucky University, Bowling Green, KY

I will give a brief outline of Poirier and co-workers' interacting quantum trajectories methodology for representing the motion of a quantum mechanical particle in terms of an ensemble of coupled Bohmian trajectories. I will focus on the nonlinear partial differential equation describing the evolution of the quantum trajectory ensemble and discuss my recent numerical work. Benchmark results will be presented for 1D and 2D model problems that show excellent agreement with analytical theory and numerical exact wavefunction-based methods.

Guest Binding in Cyclobenzoin Derivatives

Ognjen Š. Miljanić IT

Department of Chemistry, 3585 Cullen Blvd., University of Houston, Houston, TX 77204-5003, USA

Cyclobenzoins are organic macrocyclic molecules easily prepared by the benzoin condensation of aromatic dialdehydes. Their rigid, shape-persistent cavities are lined with aromatic surfaces, allowing favorable interactions with electric-rich linear guests within the cavity, including environmentally relevant species such as carbon dioxide and C3 hydrocarbons. Their electrochemically addressable nature also means that they are competent organic electrode materials for use in lithium-ion batteries. Very recently, we have discovered that threefold symmetric cyclobenzoins can also complex anions on the outside, using a combination of aromatic and aliphatic C-H bonds to establish convergent anion binding interactions.

Full-dimensional Schrödinger Wavefunction Calculations Using Tensors and Quantum Computers: the Cartesian component-separated approach

Bill Poirier[a], ***Jonathan Jerke***[b]

IT

[a] Department of Chemistry and Biochemistry, and Department of Physics, Texas Tech University, PO Box 41061, Lubbock TX 79409-1061
[b] Quantum Galaxies, LLC

Traditional methods in quantum chemistry rely on Hartree-Fock-based Slater-determinant (SD) representations, whose underlying zeroth-order picture assumes separability by particle. Here, we explore a radically different approach, based on separability by Cartesian component, rather than by particle [1–4]. The approach appears to be very well suited for 3D grid-based methods in quantum chemistry [2–4], and thereby also for so-called "first-quantized" quantum computing [4,5]. We first present an overview of the approach as implemented on classical computers, for which a natural tensor product form is exploited to astronomically reduce the number of stored data elements, by many orders of magnitude. Numerical results are provided that justify performance claims, even when the electrons are strongly correlated (e.g., four-explicit-electron calculations that are equivalent to full-CI matrix diagonalization with nearly 1015 SDs). We then present an implementation for quantum computers for which the number of quantum gates (and to a lesser extent, the number of qubits) can be dramatically reduced, in comparison with other quantum circuitry that has also been envisioned for implementing first-quantized "quantum computational chemistry" (QCC).

References

[1] Jerke, J.; Lee, Y.; Tymczak, C. J.; A Novel Gaussian-Sinc Mixed Basis Set for Electronic Structure Calculations, J. Chem. Phys., 2015, 143, 064108.
[2] Jerke, J.; Poirier, B.; Two-Body Schrödinger Wave Functions in a Plane-Wave Basis Via Separation of Dimensions, J. Chem. Phys. 2018, 148, 104101.
[3] Jerke, J.; Karwowski, J.; Poirier, B; Exact Matrix Elements for General Two-Body Central-Force Interactions, Expressed as Sums of Products, Mol. Phys., 2018, 117, 1264–1275.
[4] Poirier, B; Jerke, J; Full-dimensional Schrödinger wavefunction calculations using tensors and quantum computers: the Cartesian component-separated approach, Phys. Chem. Chem. Phys., 2022, 24, 4437–4454.
[5] Poirier, B; Efficient Evaluation of Exponential and Gaussian Functions on a Quantum Computer, with Application to Quantum Computational Chemistry and Quantum Finance, Phys. Rev. X Quantum (submitted, final stage of review).

Ab Initio Nonadiabatic Molecular Dynamics in Cavities: Anisotropic Exciton-Polariton Relaxation and Phonon Bottleneck in Metal Halide Perovskites

Oleg Prezhdo IT

University of New Mexico

We developed an ab initio quantum dynamics approach to investigate evolution of exciton– polaritons coupled to vibrations, combining non-adiabatic molecular dynamics, real-time timedependent density-functional theory, and the Pauli Fierz cavity model. By applying the approach to a layered lead-halide perovskite, we demonstrated strong dependence of exciton evolution on cavity photon. Hot exciton relaxation is slowed down, because nonadiabatic coupling is decreased by the photon component and the coupling matrix changes structure. In contrast, relaxation to the lowest energy exciton is accelerated, breaking phonon-bottleneck, due to strong, near-resonant interaction with the cavity-photon. Anisotropy of light-matter interaction for photon polarization parallel and perpendicular to the perovskite controls how fast hot excitons access the hybrid exciton-polariton manifold. The developed approach provides means to model quantum dynamics in optical cavities at the ab initio level. The findings demonstrate that anisotropic light–matter coupling can control exciton–polariton dynamics and transport in microcavity-confined lowdimensional materials [1].

References

[1] Jerke, J.; Lee, Y.; Tymczak, C. J.; A Novel Gaussian-Sinc Mixed Basis Set for Electronic Structure Calculations, J. (1) Xu, X.; Han, X.; Stippell, E.; Fang, W.-H.; Prezhdo, O. V.; Long, R., Anisotropic ExcitonPolariton Relaxation and Phonon Bottleneck in Microcavity-Confined Metal Halide Perovskites: Ab Initio Quantum Dynamics. Nano Letters 2025, 25, 13063-13069.

Quantum Signatures and Spectral Fluctuations: New Windows into Molecular Condensates and Excitonic Complexes

Ajay Ram Srimath Kandada IT

Wake Forest University

Recent advances in ultrafast and quantum spectroscopies are reshaping our understanding of collective and correlated phenomena in molecular and hybrid systems. This talk presents three experimental frontiers that illuminate the dynamics, coherence, and fluctuation landscapes of excitonic and polaritonic states. We begin with excitation correlation photoluminescence spectroscopy applied to molecular polariton condensates, revealing the exciton-mediated condensation dynamics [1]. These measurements uncover transient regimes of coherence buildup and decay, offering a dynamic view into polariton formation beyond steady-state photoluminescence. Next, we explore coherent two-quantum spectroscopy as a tool to resolve biexcitonic correlations in lead-halide perovskites [2], where coherent pathways involving double excitations expose hidden couplings and many-body interactions. This approach enables disentanglement of bound and unbound biexciton signatures, with implications for quantum optoelectronics and exciton transport. Finally, we introduce a photon-counting methodology in molecular absorption spectroscopy that tracks rotationally driven spectral fluctuations with unprecedented sensitivity. By quantifying intensity noise and anisotropic modulation in real time, this technique opens a new route to probing molecular environments and dynamic disorder at the single-photon level. Together, these approaches offer a unified perspective on how quantum coherence, many-body interactions, and fluctuation dynamics shape the behavior of complex molecular systems.

References

[1] E. J. Kumar, K. A. Koch, R. Kaurav, R. K. Yadav, V. Quiros-Cordero, J. Brinson, V. Menon, A. R. Srimath Kandada, Nonlinear dynamics in the formation of molecular polariton condensates, ArXiv:2505.08674.
[2] K. A. Koch, E. Rojas-Gatjens, M. Gomez-Dominguez, J. Correa-Baena, C. Silva-Acuna, A. R. Srimath Kandada|, Spectroscopic signatures of biexcitons: a case study in Ruddlesden-Popper lead halides, Journal of Chemical Physics, 163, 034202 (2025).

A Trek Through Data Fusion

Alan Steinberg IT

alaneilsteinberg@gmail.com

We examine the concepts, issues, and techniques of modern data fusion; i.e., the process of combining data (or information) to estimate states of measurements, individuals, relationships, situations, processes, etc. Issues include uncertainty representation, multi-modal modeling, and complexity. Frameworks and architectures applicable to diverse requirements and constraints are discussed, with appropriate use cases. We discuss the use of current and emerging machine learning and predictive analytic methods combined with traditional model-based methods to deal with poorly modeled problems. Automated low-level fusion methods – for feature extraction, individual target detection, tracking, characterization and recognition – have matured enormously over the past few decades; with significant success in tactical military applications, as well as in fields ranging from medical diagnostics and cognitive sensing to autonomous vehicles. We survey significant advances made in non-linear tracking, in track-before-detection, in multi-target tracking, and in automated target recognition. Higher-level fusion methods have blossomed in recent years; for relationship, situation and scenario assessment, often in conjunction with planning in uncertain and dynamic environments. Powerful new cognitive tools are being developed for reasoning about human and group-dominated problems of great complexity, variability, and uncertainty. We discuss the roles and methods for data fusion in autonomous and collaborative mission management, including goal-drive data acquisition and exploitation.

Four years of adventure in the land of chirality

Sergei Tretiak IT

Los Alamos National Laboratory, Los Alamos NM, 87545

E-mail: serg@lanl.gov

Chirality is a fundamental molecular property that plays a crucial role in biophysics and drug design. Our simulations demonstrate that X-ray Circular Dichroism (CD) can exploit the localized and element-specific nature of X-ray electronic transitions. X-ray CD therefore is more sensitive to local structures and the chirality probed with it can be referred to as local which in contrast to a conventional Optical CD probing the global molecular chirality. By considering several molecular cases, we find that XCD is capable of distinguishing dichroic contributions combing from a local chirality center and global molecular conformations, along with their complex interplay. We demonstrate that sterically-induced global distortions can be a dominant source of chirality, in the X-ray range, in some cases even destructively interfering with the dichroic response from the chiral center. We further we formulate the concept of chiral populations connecting distribute the dichroic response to the atomic orbital picture. Inducing chiroptical activity into semiconductors is challenging due to difficulties of creating asymmetric crystal structures. We further explore chirality transfer in hybrid perovskite quantum dots capped with chiral ligands. Our atomistic modeling suggests the observed chirality transfer is best rationalized by a dipole – dipole coupling. To maximize the bulk effect, both strategic functionalization and limited conformationally degrees of freedom of the ligands are important for obtaining high-intensity nanomaterial chiroptical signatures through chirality transfer. These computational insights provide synthetic mechanistic guidelines towards improving chiroptical functionality in semiconductor nanomaterials.

Vibrationally resolved electronic spectra from Hagedorn wavepacket dynamics

Jiri Vanicek **IT**

Institute of Chemical Sciences and Engineering, Ecole polytechnique fédérale de Lausanne, Lausanne, Switzerland

Hagedorn functions are carefully constructed generalizations of Hermite functions to the setting of many-dimensional squeezed and coupled harmonic systems [1]. I will describe recent developments that allowed application of Hagedorn wavepackets to vibronic spectroscopy of even anharmonic systems. To evaluate time correlation functions needed for computing spectra, we first derived efficient recursive expressions for the overlaps between Hagedorn bases associated with different Gaussians [2]. To succinctly highlight advantages of Hagedorn wavepackets, I will focus on applications to single vibronic level (SVL) fluorescence experiments, in which the electronically excited initial state is also excited in one or several vibrational modes. In displaced, squeezed, and Duschinsky-rotated globally harmonic systems, Hagedorn functions are exact solutions to the time-dependent Schrödinger equation and can be propagated with the same equations of motion as a simple Gaussian wavepacket; emission spectra from arbitrary vibronic levels can be evaluated using a single trajectory. After validating the method by comparing it with exact quantum calculations [3], we applied it to compute SVL spectra of anthracene by performing wavepacket dynamics on a 66-dimensional harmonic potential energy surface constructed from density functional theory calculations [4]. However, real molecules have anharmonic surfaces. To partially describe effects of anharmonicity on spectra, we combined the Hagedorn approach with local harmonic approximation of the potential [5] and with on-the-fly ab initio dynamics, which allowed us to compute SVL fluorescence spectra of difluorocarbene, a floppy molecule with a very anharmonic potential energy surface [6]. Time permitting, I will also briefly mention other improvements and applications to other spectroscopies, such as evaluating Herzberg-Teller and resonance Raman spectra.

References

[1] G. A. Hagedorn, Ann. Phys. 269, 77 (1998).
[2] J. J. L. Vaníček and Zhan Tong Zhang, J. Phys. A: Math. Theor. 58, 085303 (2025).
[3] Z. Tong Zhang and J. J. L. Vaníček, J. Chem. Phys. 161, 111101 (2024).
[4] Z. Tong Zhang and J. J. L. Vaníček, J. Chem. Theory Comput., in press; DOI: 10.1021/acs.jctc.5c01097; arXiv:2403.00702.
[5] Z. Tong Zhang, M. Visegrádi, and J. J. L. Vaníček, arXiv:2408.11991.
[6] Z. Tong Zhang, M. Visegrádi, and J. J. L. Vaníček, Phys. Rev. A 111, L010801 (2025).

Useful Information

Talks will be held at the **Telluride Intermediate School**. See the map on page 20.

Morning Breakfast: While lunch and dinner are on your own, breakfast in the form of bagels, coffee, juice, danishes, yoghurt, and fruit will be available each morning.

Coffee breaks will be offered to all participants in a common room shared by the concurrent workshops. Snacks, water, and coffee/tea will also be available throughout the day.

Wi-Fi will be available during the conference.

The **TSRC Picnic** will be held sometime, someplace.

Town Talk

In 1991, Telluride Science founders Peter Salamon and R. Stephen Berry started the lecture series in the old elementary school on Thursday nights as a way to give back to the Telluride community. The Town Talks have grown in popularity through the years and have moved locations several times–from the elementary school, to the Wilkinson Public Library to the Palm Theatre to the Telluride Conference Center.

Getting there and getting around

Telluride is nestled in box canyon in the San Juan Mountains of southwest Colorado. Whether you are flying into the region or venturing on a road trip, Telluride offers a unique journey marked with unmatched scenery, heritage and charm. We recommend arriving as early as possible the day before your workshop begins. Once you arrive, it is very easy to familiarize yourself with our mountain paradise. In the meantime, these FAQs might be helpful.

- **Air Travel** The Montrose Regional Airport (**MTJ**) is the primary airport for Telluride, and is a scenic 65 miles away. During the winter months, guests can take advantage of nonstop flights from 10 major hubs, and summer offers nonstop service from 5 major U.S. cities. **RECOMMENDED**

  Telluride Science participants are eligible for discounted shuttle service to and from the Montrose airport with Telluride Express; however, the discounted rate is only available when a reservation is made prior to your arrival with the code TSRC. **RECOMMENDED**

- **Rental cars** are also available at the Montrose Airport, but we recommend the ground transportation option because you do not need a car in Telluride (difficult at best!). Some of the

lodging providers also charge for parking (usually $30/day!).

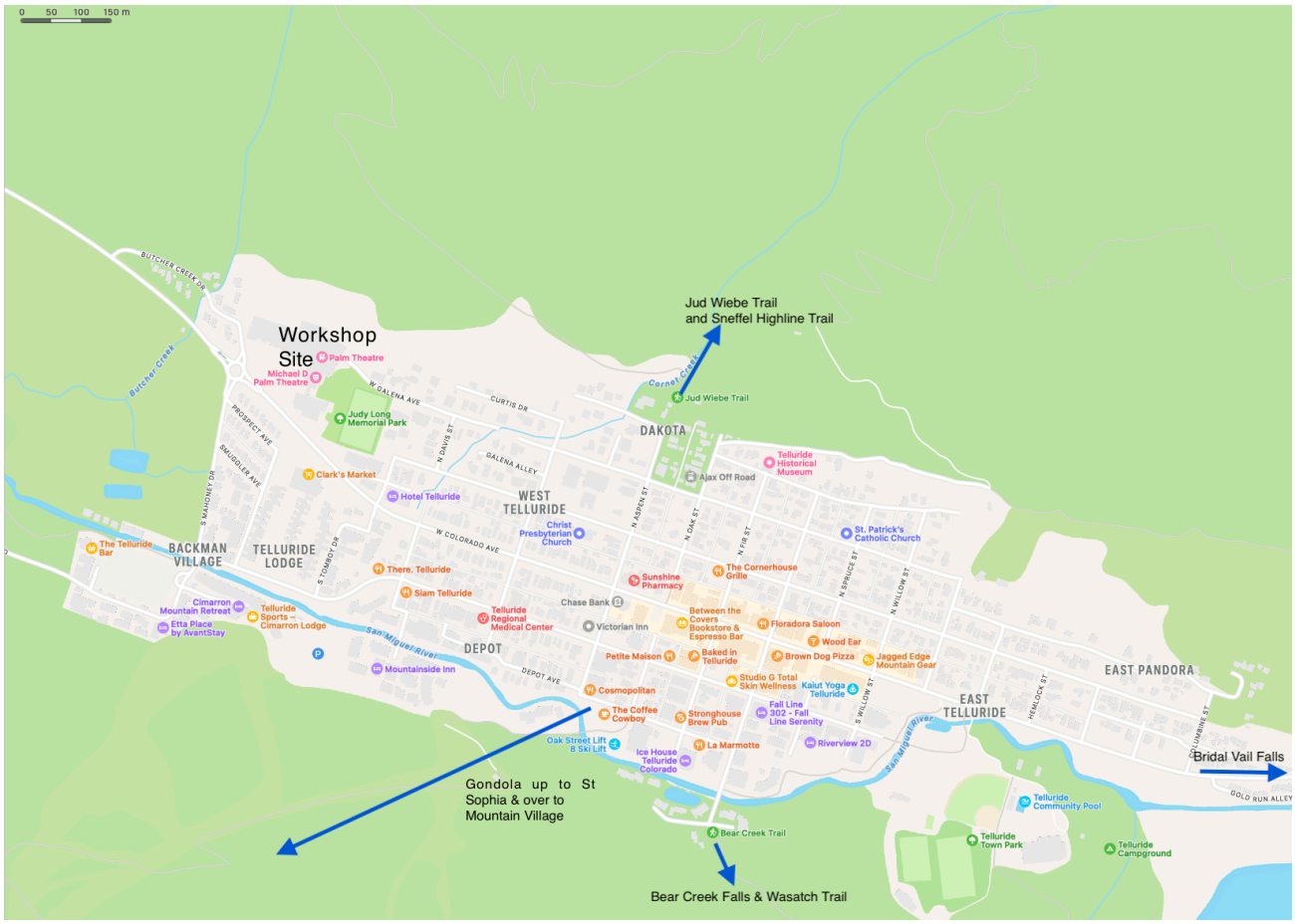
- **The Telluride Airport (TEX)** is located 10 minutes from the town of Telluride. Denver Air Connection offers service from Phoenix and Denver to Telluride and partners with United Airlines, which enables travelers to book and connect through the global United network. **Not-Recommended! These get cancelled on a whim due to the highly unstable summer mountain weather.**

  There are two other regional airports that are two to three hours by car away from Telluride: Grand Junction Regional Airport (GJT) and Durango Regional Airport (DRO). However, the shuttle service from these airports tends to be quite expensive and typically requires a car rental. **Not-Recommended, unless you want to do a fun driving vacation to and from Telluride. It's actually a really nice drive.**

- **Getting around Telluride.** Telluride is 1.5 km long and 0.6 km wide at most, making it a walking friendly town. The scenery is stunning and all hotels are within walking distance to all Telluride Science venues. No points in Telluride are separated by more than a 10-15 min. walk. If you get lost, walk down hill until you get the river or walk uphill until you're clearly heading up a mountain. **Recommend:** Bring a sturdy pair of hiking or walking shoes.

Map of Telluride

Here is a convenient map of Telluride with a few important landmarks highlighted. If you're a first-timer, Colorado Ave is the Main Street through town.



Hiking Trails: The blue arrows indicate the starting point and directions for couple of nice hiking trails heading out of town.

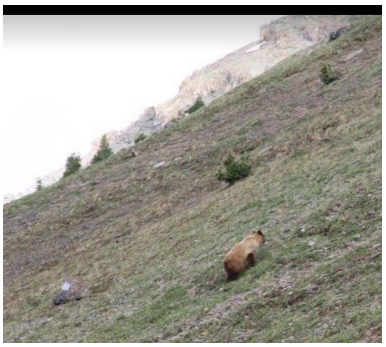


Figure 1: A local black bear (it's a blonde) on the trails around Telluride. It's important to note that you don't need to be able to out run the bear (because you can't), *you just need to outrun your hiking partner*.

Eric's Hiking Guide To Telluride

I've been coming to Telluride for close to 20 yrs and have hiked or climbed most of trails and peaks around Telluride at some point or another. If you go out, take water, a snack, sun screen, rain jacket, your cell phone, a trail map, and ideally a partner.

Importantly, if you go off on one of the longer hikes, let one of the local TSRC staff know where you're going, who you're going with, and what time to expect you to check back in.

- **Bear Creek Trail**: Easy out/back heading up to Bear Creek Falls. About 45 - 60 min up to the falls and 30 min back down. It's a must-do, you can't get lost, and you can enjoy a refreshing swim at the end.


  This is also a great place for a group picture.

- **Jud Wiebe Trail**: Head across the creek at the North end of Aspen St. After a seemingly endless grind up the side of the slope and a few switch-backs, you encounter a fork. Continue to the **right** looping along a trail overlooking the north-side of Telluride. You eventually hit the Liberty Trail. At this point, take a right (DOWNHILL) and eventually come out at about the Telluride Historical Museum. The Cornerhouse Grill is a great place to get a beer after this one, you deserve it. About 1-2.5 hrs depending on your lung capacity for the initial climb. Trail is popular and well

marked.

- **Sneffels Highline Trail**: I consider this to be the best trail in the valley and you have multiple ways to complete it. It's about 14.5 miles as a complete loop if you go the summit and then through Mill Valley. Incidentally, the Tom Waits scene in "Ballad of Buster Scruggs" was filmed just below Dallas Peak. I've done the loop in 5 hrs, I recommend 6-8 hrs. A popular option is to go to the saddle point, enjoy the view and return (4-4.5 hrs round trip). It's also an excellent location for a group photo. Do be forewarned that this goes to almost 13,000' and the last portion is well above the tree line.

- **Bridal Vail Falls.** Super fun! Walk or drive to the trail-head at the end of town and keep walking up. At the top is an old mine that you can partially enter and collect some interesting mineral samples. Also, a great place for a swim and a group photo.


For the more adventurous

Most of the peaks you see from town are climbable without technical gear. The exceptions are Dallas Peak and Pagosa. Ballard Peak requires a good deal of bushwacking and trail finding. An awesome loop is the Wasatch Connection. For this, take the Gondola up to the St. Sophia Station, then walk up the See Forever Trail, connecting to the Wasatch trail on Gold Hill. From here you can head *down* the Bear Creek trail or loop behind Wasatch and Ballard to Blue Lakes, then come down the Bridal Vail Falls trail. This latter option is about 20 miles.

- **Lizard Head**: This is the little thumb you see looking SE from Telluride towards Wilson Peak and on the cover of this book. The formation itself is the core of a long extinct volcano. This 8-9 mile trail takes you to about 13,000' and most of the trail is between 11,000' and 12,000'. Jon Snow and I did this in the summer of 2022. For a day trip, I highly recommend taking 2 cars leaving one at the start and finish to avoid a 2 mile hike back to the trailhead along the highway.

  An alternative hike is to start at the Cross Mountain Trail Head and hike into the cirque below Wilson Peak. This looks like fun!

- **Mt. Sneffels**. This is the beautiful 14,000' mountain you see as you come in from Ridgeway.

You "can" do it as a day hike if you have a 4WD capable of driving into the Yankee Boy Basin from Ouray. Alternatively, you can hike in along the Blue Lakes Trail (different Blue Lakes!) after driving in to the trail-head, camp at about 12,000’ and do either the standard route or a very airy ridge climb. While not a technical climb, you do need a good head for heights! Hao Li and I did this in 2022.