Curriculum Vitae

Professor Lionel William (Bill) Poirier

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Texas Tech University
Department of Chemistry and Biochemistry
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EDUCATION:

University of California Berkeley—Ph.D. in Theoretical Chemical Physics — Fall 1997
Research Advisor: Professor William H. Miller (Chemistry)
Advisor of Record: Professor Robert G. Littlejohn (Physics)
Dissertation Topic: *Optimal Separable Bases and Molecular Collisions*
Dates of Attendance: (except 1991-92 acad. year) — August 1990 to September 1997

University of Maryland College Park—Advanced Special Student in Physics
Research Advisor: Professor Douglas G. Currie (Physics/Astronomy)
Research Project: Chaotic Model of the Solar "Attractor"
Dates of Attendance: (graduate physics classes) — September 1989 to May 1990

Brown University—Sc.B. in Physics with Honors, *magna cum laude* — May 1988
Research Advisor: Professor James C. Baird (Physics/Chemistry)
Thesis Topic: *Fractal Dimension: A New Information-Theoretic Derivation*
A.B. in Mathematics (fulfilled course requirements)
Dates of Attendance: — September 1984 to May 1988

AWARDS AND HONORS:

Phi Kappa Phi
Sigma Xi
Phi Beta Kappa
Outstanding College Students of America
American Association of Physics Teachers

TTU Graduating Senior Named Outstanding Faculty Award—Spring 2022, Spring 2007, Fall 2005.
Apple Polishing Award, TTU Mortar Board—2021.
TTU **Diamond Award** for "Teaching Excellence Under Pressure" during the COVID pandemic—2021.
Texas Tech University **President's Excellence in Teaching Award**—2021.
Invited Professor, Dresden, Germany (Max Planck Institute: Physics of Complex Systems)—2020, 2018, 2015.
TTU Graduate Council Dedicated Service Recognition—2017, 2015.
Celebration of Faculty Excellence Award, TTU Office of Vice President for Research—2017.
Distinguished Guest Scientist Fellow, Hungarian Academy of Sciences, Budapest, Hungary—2017.
Texas Tech University Teaching Academy—2016.
Ferenc Török Memorial Lecture, Budapest, Hungary (Eötvös Loránd University)—2015.
Professeur Invité, Montpellier France (Centre national de la recherche scientifique)—2015, 2011.
Plenary Lecturer, Austrian Academy of Sciences—2013.
Texas Tech System Barnie E. Rushing, Jr. **Faculty Distinguished Research Award**—2013.
Texas Tech System Chancellor's Council **Distinguished Research Award**—2008.
TTU College of Arts and Sciences **Tribute to Teachers Award**—2005 recipient.
U.S. Department of Energy **Early Career Award**—2002.
Research Corporation **Research Innovation Award**—2001.

First Place Award for Best Poster Presentation,
Atomic and Molecular Interactions Gordon Research Conference—2000.
Outstanding Graduate Student Instructor Award**,** UC Berkeley—1994.

RESEARCH AND ADMINISTRATIVE EXPERIENCE:

Interim Department Chair—Department of Chemistry and Biochemistry, Texas Tech University
May 2021 to September 2022

Oversaw numerous aspects of the TTU Dept. of Chemistry and Biochemistry—a highly research-active department within the College of Arts & Sciences, with 29 faculty, ~25 staff, 100+ graduate students, ~$8M annual budget, and ~$6.3M endowment.

Chairs are expected to develop the strengths of their department by: working to increase the visibility and research profile of the department; providing a wholesome and fulfilling educational experience for students; enhancing diversity within the department; promoting the Dept. Strategic Plan, and broader institutional initiatives.

Duties include: budget management; faculty and staff hiring and annual evaluation; tenure and promotion; scheduling and coordination of all classes and labs; space allocation and renovation; mentoring of junior and mid-career faculty; infrastructure plans and coordination; program development and review; donor outreach and engagement.

During my time as Interim Dept. Chair, I managed six tenure and promotion cases, and six regular departmental faculty searches, at all ranks. I also pursued diversity hires, and other special faculty hiring opportunies, e.g. through the VPR's Strategic Research Group program, as well as the Endowed Robert A. Welch Chair program. In my first year as Chair, departmental faculty published 119 peer-reviewed publications, and spent over $3M in restricted research expenditures.

I oversaw the expansion of the department into new space in the Experimental Sciences Building 2 (ESB2), which required moving about 1/3rd of our faculty and their research labs, presenting both logistical and cultural challenges. I introduced various measures to address the COVID pandemic, including a vaccination clinic. I also led a faculty and staff salary compression and equity program, and engineered several successful retention packages. Other measures I introduced to promote diversity, equity, and inclusion within the department include various town halls and roundtables, as well as a restructuring of our committees. I also conducted a 10-year Graduate Program Review.

Professor—Department of Chemistry and Biochemistry, Texas Tech University
(Graduate Faculty, Joint Professor of Physics) from September 2009

Methods development: New techniques are devised for performing exact quantum dynamics calculations and strongly correlated electronic structure calculations with unprecedented computational efficiency, and for larger systems than ever before. Methods are designed for quantum computers and massively parallel supercomputers, as well as conventional computing platforms.

Applications: rovibrational molecular spectroscopy; reactive scattering; cluster dynamics; environmental chemistry; molecular astrophysics; combustion and atmospheric science; astrobiology and geochemistry; "pre-Born-Oppenheimer" and quantum computing; relativistic quantum mechanics

With collaborators from Harvard U., Los Alamos National Labs, Eötvös Loránd U. (Hungary) and U. College London (UK), I am leading a team to explore: consolidation of the most widely used rovibrational spectroscopy and quantum dynamics codes; establishment of common software standards; dissemination to various user communities. from February 2017

With collaborators from TTU, U. Houston, N. Copernicus U. (Poland), and Industry: Tensor product methods for strongly correlated electronic structure and quantum computing; quantum exponential and Gaussian function evaluation; quantum optimization. from September 2016

With Juergen Eckert: Hydrogen-material interactions; Kubas coordination complexes; hydrogen storage; nanoconfinement; inelastic neutron scattering; selection rules. from September 2013

With collaborators from U. Maryland and U. New Mexico: sulfur mass-independent fractionation (S-MIF) of SO_2 photodissociation is being investigated, to assess S-MIF in the rock record as a proxy for O_2 in the Archean atmosphere, to understand the "oxygen revolution." from February 2013

With collaborators from U. Sao Paulo and ITA (Brazil), Montpellier U. (France), the Weizmann Institute (Israel), Goethe U. (Germany) and U. Texas Austin: Quantum trajectory methods (QTMs) are being developed for molecular and nuclear physics applications. from September 2009

With collaborators from Argonne National Laboratories: Algorithms were developed to enable efficient parallelization of exact quantum dynamics calculations across massively parallel supercomputers. January 2003 to January 2007 (DoE) ; July 2010 to July 2022 (NSF)

Associate Professor—Department of Chemistry and Biochemistry, Texas Tech University
(see above). September 2006 to August 2009

Assistant Professor—Department of Chemistry and Biochemistry, Texas Tech University
(see above). August 2001 to August 2006

Research Associate—Professor Tucker Carrington, Jr. (advisor), Université de Montréal
High resolution molecular spectroscopy for highly rovibrationally excited molecules. Customized calculations for high-lying energy windows of interest, using spectral transform techniques, in conjunction with optimized numerical preconditioning. H_2O and HCO. August 2000 to July 2001

Research Associate—Professor John C. Light (advisor), University of Chicago
Rovibrational molecular spectroscopy. Optimized spectral collocation or basis set methods, using a quasiclassical phase space model to generate a highly efficient correlated representational basis, tailored to a specific Hamiltonian and energy range. October 1997 to August 2000

Graduate Student Researcher—Professor William H. Miller (advisor), UC Berkeley
Quantum reaction dynamics. Reactive scattering of molecules in the gas phase. Development and application of the optimal separable basis methodology, used to compute thermal rate constants for $H+H_2$ and O+HCl. January 1994 to September 1997

Advanced Special Student Researcher—Professor Douglas G. Currie (employer), University of Maryland
Nonlinear dynamics. Developed a chaotic attractor model of solar dynamics, based on a time-delay analysis of the Wolf sun spot numbers and information theory. August 1989 to August 1990
August 1988 to January 1989

Artificial Intelligence Researcher—AI Department, Software Works, Hitachi Ltd., Totsuka, Japan
Machine learning; expert systems. Meta-Object implementation of the Common LISP Object System (CLOS). January 1989 to August 1989

PUBLICATIONS

M. Reddiger and B. Poirier, "The One-Body Born Rule on Curved Spacetime," *Rev. Math. Phys.* (submitted).

M. Aarabi, A. Pandey, and B. Poirier, "On-the-fly Crystal: How to reliably and automatically characterize and construct potential energy surfaces," **invited contribution**, special issue in honor of Elfi Kraka, *J. Comput. Chem.* (submitted).

B. Poirier, "Efficient Evaluation of Exponential and Gaussian Functions on a Quantum Computer, with Application to Quantum Computational Chemistry and Quantum Finance," *Phys. Rev. X Quantum* (final revision stage).

N. A. Coleta da Conceição, B. V. Carlson, and B. Poirier, "Quantum Trajectories and the Nuclear Optical Model," *Physica Scripta A* **98** (11), 115303 (2023) (*13 pages*). doi:10.1088/1402-4896/acfe5d.

M. Aarabi, J. Sarka, A. Pandey, R. Nieman, A. J. A. Aquino, J. Eckert, and B. Poirier, "Quantum Dynamical Investigation of Dihydrogen-hydride Exchange in a Transition Metal Polyhydride Complex," *J. Phys. Chem. A* **127** (31), 6385–6399 (2023). doi:10.1021/acs.jpca.3c01863.

L. Dupuy, G. Parlant, B. Poirier, and Y. Scribano, "Making Sense of Transmission Resonances and Smith Lifetimes in One-dimensional Scattering: The extended phase space quantum trajectory picture," *Chem. Phys.* **572**, 111952 (2023) (*11 pages*). doi:10.1016/j.chemphys.2023.111952.

M. Reddiger and B. Poirier, "Towards a Mathematical Theory of the Madelung Equations: Takabayasi's quantization condition, quantum quasi-irrotationality, weak formulations, and the Wallstrom phenomenon," **topical review**, *J. Phys. A: Math. Theor.* **56**, 193001 (2023) (*63 pages*). doi:10.1088/1751-8121/acc7db.

M. Reddiger and B. Poirier, "The Differentiation Lemma and the Reynolds Transport Theorem for Submanifolds with Corners," *Int. J. Geom. Methods Mod. Phys.* **20** (8), 2350137 (2023) (*44 pages*). doi:10.1142/S0219887823501372.

C. A. Bowesman, I. I. Mizus, N. F. Zobov, O. L. Polyansky, J. Sarka, B. Poirier, M. Pezzella, S. N. Yurchenko, and J. Tennyson, "ExoMol Line Lists – L: High-resolution line lists of H_3^+, H_2D^+, D_2H^+ and D_3^+," *Mon. Notices Royal Astron. Soc.* **519** (4), 6333-6348 (2023). doi:10.1093/mnras/stad050.

L. Dupuy, G. Parlant, B. Poirier, and Y. Scribano, "Direct and Accurate Calculation of Dwell Times and Time Delays Using Quantum Trajectories," *Phys. Lett. A* **456**, 128548 (2022) (*6 pages*). doi:10.1016/j.physleta.2022.128548.xz

L. Dupuy, F. Talotta, F. Agostini, D. Lauvergnat, B. Poirier, and Y. Scribano, "Adiabatic and Nonadiabatic Dynamics with Interacting Quantum Trajectories," *J. Chem. Theory Comput* **18** (11), 6447-6462 (2022). doi:10.1021/acs.jctc.2c00744.

J. Sarka and B. Poirier, "Assigning Quantum Labels and Improving Accuracy for the Rovibrational Eigenstates of H_3^+ Calculated Using ScalIT," **invited contribution**, research topic in structure and dynamics of atmospheric, plasma and astrochemical molecular processes, *Front. Phys.* **10**, (2022) (*14 pages*). doi:10.3389/fphy.2022.996001.

L. A Poveda, L. Grave de Peralta, J. Pittman, and B. Poirier, "A Non-relativistic Approach to Relativistic Quantum Mechanics: The case of the harmonic oscillator," *Found. Phys.* **52**, 29 (2022) (*20 pages*). doi.org/10.1007/s10701-022-00541-5.

B. Poirier and J. Jerke, "Full-Dimensional Schrödinger Wavefunction Calculations using Tensors and Quantum Computers: the Cartesian component-separated approach," part of themed collections on "Quantum Computing and Quantum Information Storage" and "Quantum Computing and Quantum Information Storage: Celebrating the 2022 Nobel Prize in Physics," *Phys. Chem. Chem. Phys.* **24**, 4437-4454 (2022). doi: 10.1039/D1CP02036F.

J. Sarka and B. Poirier, "Hitting the Trifecta: How to Simultaneously Push the Limits of Schrödinger Solution with Respect to System Size, Convergence Accuracy, and Number of Computed States," *J. Chem. Theory Comput.* **17** (12), 7732-7744 (2021). doi:10.1021/acs.jctc.1c00824.

L. Grave de Peralta, L. A Poveda, and B. Poirier, "Making Relativistic Quantum Mechanics Simple, *Euro. J. Phys.* **42**, 055404 (2021) (*13 pages*). doi:10.1088/1361-6404/ac0ecc.

B. Poirier, "Effect of Confinement on the Translation-Rotation Motion of Molecules: The inelastic neutron scattering selection rule," **invited book chapter**, *Chemical Reactivity in Confined Systems: Theory, Modelling and Applications*, ed. P. Chattaraj and D Chakraborty, Chapter 1, 1-24 (John Wiley & Sons, Oxford, UK, 2021).

M. S. Hussein and B. Poirier, "Quantum Trajectory Description of the Time-Independent (Inverse) Fermi Accelerator," **invited contribution**, special issue in honor of Mahir Saleh Hussein, *Braz. J. Phys.* **51**, 193-203 (2021). doi:10.1007/s13538-020-00825-z.

J. Sarka, B. Poirier, V. Szalay, and A. G. Császár, "On Neglecting Coriolis and Related Couplings in First-principles Rovibrational Spectroscopy: Considerations of symmetry, accuracy, and simplicity. II. Case studies for H_2O isotopologues, H_3^+, O_3 and NH_3", *Spectrochim. Acta A* **250**, 119164 (2021) (*32 pages*). doi:10.1016/j.saa.2020.119164.

J. Sarka, D. Das, and B. Poirier, "Calculation of rovibrational eigenstates of H_3^+ using ScalIT," *AIP Advances*, **11**, 045033 (2021) (*28 pages*). doi:10.1063/5.0047823.

B. Poirier and H.-M. Tsai, "Trajectory-based Conservation Laws for Massive Spin-zero Relativistic Quantum Particles in 1 + 1 Spacetime," **invited contribution**, *Symmetries in Science XVIII*, ed. D. Schuch and M. Ramek, *Journal of Physics: Conference Series*, IOP Publishing, **1612**, 012022 (2020). doi:10.1088/1742-6596/1612/1/012022.

A. Pandey and B. Poirier, "Plumbing Potentials for Molecules with Up To Tens of Atoms: How to Find Saddle Points and Fix Leaky Holes," *J. Phys. Chem. Lett.* **11**, 6468-6474 (2020). doi:10.1021/acs.jpclett.0c01435.

A. Pandey and B. Poirier, "An Algorithm to Find (and Plug) "Holes" in Multi-dimensional Surfaces," *J. Chem. Phys.* **152**, 214102 (2020). doi:10.1063/5.0005681.

J. Sarka and B. Poirier, "Comment on "Calculated Vibrational States of Ozone up to Dissociation" [J. Chem. Phys. 144, 074302 (2016)]," *J. Chem. Phys.* **152**, 177101 (2020). doi:10.1063/5.0002762.

J. Sarka, B. Poirier, V. Szalay, and A. G. Császár, "On Neglecting Coriolis and Related Couplings in First-principles Rovibrational Spectroscopy: Considerations of symmetry, accuracy, and simplicity," *Sci. Rep.* **10**, 4872 (2020). doi:10.1038/s41598-020-60971-x.

J. Sarka, C. Petty, and B. Poirier, "Exact Bound Rovibrational Spectra of the Neon Tetramer," *J. Chem. Phys.* **151**, 174304 (2019). doi:10.1063/1.5125145

A. Pandey and B. Poirier, "Using phase-space Gaussians to compute the vibrational states of $OCHCO^+$," *J. Chem. Phys.* **151**, 014114 (2019). doi:10.1063/1.5096770

P. Kumar, J. Klos, B. Jiang, M. H. Alexander, B. Poirier, and H. Guo, "Accurate Characterization of the Lowest Triplet Potential Energy Surface of SO_2 with a Coupled Cluster Method," *J. Chem. Phys.* **150**, 144303 (2019). doi:10.1063/1.5088959

P. Kumar and B. Poirier, "The *J*-dependent rotational Hamiltonian method for analyzing rovibrational spectra: Application to HO_2, H_2O, and O_3," *Chem. Phys. Lett.* **733**, 136700 (2019). doi:10.1016/j.cplett.2019.136700

P. Kumar and B. Poirier, "Isotope shifts and band progressions in SO_2 rovibrational energy levels: using quantum theory to extract rotational constants," *Mol. Phys.* **117**, 2456-2469 (2019). doi:10.1080/00268976.2019.1567850

J. Jerke, J. Karwowski, and B. Poirier, "Exact matrix elements for general two-body central-force interactions, expressed as sums of products," **invited contribution**, special issue in memory of Dieter Cremer, *Mol. Phys.* **117**, 1264-1275 (2019). doi:10.1080/00268976.2018.1538541

Y. Scribano, G. Parlant, and B. Poirier, "**Communication**: Adiabatic quantum trajectory capture for cold and ultra-cold chemical reactions," *J. Chem. Phys.* **149**, 021101 (2018). doi:10.1063/1.5041091

C. Petty, R. F. Spada, F. B. Machado, and B. Poirier, "Accurate rovibrational energies of ozone isotopologues up to $J = 10$ utilizing artificial neural networks," *J. Chem. Phys.* **149**, 024307 (2018). doi:10.1063/1.5041091

M. E. Gonzalez, J. Eckert, A. J. Aquino, and B. Poirier, "A quantum dynamical study of the rotation of the dihydrogen ligand in the $Fe(H)_2(H_2)(PEtPh_2)_3$ coordination complex," *J. Chem. Phys.* **148**, 154303 (2018). doi:10.1063/1.5026637

J. Jerke, B. Poirier, "Two-body Schroedinger Wave Functions in a Plane-wave Basis via Separation of Dimensions," *J. Chem. Phys.* **148**, 104101 (2018). doi:10.1063/1.5017621

R. Tóbiás, T. Furtenbacher, A. G. Császár, O. V. Naumenko, J. Tennyson, J.-M. Flaud, P. Kumar, and B. Poirier, "Critical Evaluation of Measured Rotational-Vibrational Transitions of Four Sulphur Isotopologues of SO_2," *J. Quant. Spect. Rad. Transfer* **208**, 152-163 (2018). doi:10.1016/j.jqsrt.2018.01.006

B. Poirier, "Large Scale Exact Quantum Dynamics Calculations: Using phase space to truncate the basis effectively," **invited contribution**, special issue in memory of John C. Light, *Adv. Chem. Phys.* **163**, 245-271 (2018). doi:10.1002/9781119374978.ch9

C. Xie, B. Jiang, J. Klos, P. Kumar, M. H. Alexander, B. Poirier, and H. Guo, "Final State Resolved Quantum Predissociation Dynamics of $SO_2(\tilde{C}\,^1B_2)$ and Its Isotopomers via a Crossing with a Singlet Repulsive State," *J. Phys. Chem. A*, **121** (26), 4930-4938 (2017). doi:10.1021/acs.jpca.7b04629

B. Jiang, P. Kumar, J. Klos, M. H. Alexander, B. Poirier, and H. Guo, "First-principles C band absorption spectra of SO_2 and its isotopologues," *J.Chem. Phys.*, **146** (15), 154305 (2017). doi:10.1063/1.4980124

P. Kumar, B. Jiang, H. Guo , J. Klos, M. H. Alexander, and B. Poirier, "Photoabsorption Assignments for the $\tilde{C}^1B_2 \leftarrow \tilde{X}^1A_1$ Vibronic Transitions of SO_2, Using New Ab Initio Potential Energy and Transition Dipole Surfaces," *J. Phys. Chem. A*, **121** (5), 1012-1021 (2017). doi:10.1021/acs.jpca.6b12958

H.-M. Tsai and B. Poirier, "Exploring the propagation of relativistic quantum wavepackets in the trajectory-based formulation," **invited contribution**, *EmQM15: Emergent Quantum Mechanics 2015*, ed. G. Grössing, *Journal of Physics*, IOP, **701**(1), 012013 (2016). doi:10.1088/1742-6596/701/1/012013

J. Klos, M. H. Alexander, P. Kumar, B. Poirier, B. Jiang, and H. Guo, "New *ab initio* Adiabatic Potential Energy Surfaces and Bound State Calculations for the Singlet Ground $\tilde{X}\,^1A_1$ and excited $\tilde{C}\,^1B_2$ ($2^1A'$) states of SO_2," *J. Chem. Phys.*, **144** (17), 174301 (2016). doi:10.1063/1.4947526

T. Halverson and B. Poirier, "One Million Quantum States of Benzene," **invited contribution**, special issue on "Dynamics of Molecular Collisions XXV, 50 Years of Chemical Reaction Dynamics," *J. Phys. Chem. A*, **119**, 12417-12433 (2015). doi:10.1021/acs.jpca.5b07868

B. Poirier, "Quantum Mechanics Without Wavefunctions," **invited contribution**, Report No. 27/2015, *Mathematical Methods in Quantum Molecular Dynamics*, ed. G. A. Hagedorn, C. Lasser, and C. Le Bris, 42-45 (Mathematisches Forschungsinstitut Oberwolfach, 2015). doi:10.1021/acs.jpca.5b07868

B. Poirier, "**Communication**: The $H_2@C_{60}$ Inelastic Neutron Scattering Selection Rule: Expanded, and explained," *J. Chem. Phys.*, **143**, 101104 (2015). doi:10.1063/1.4930922

P. Kumar and B. Poirier, "Rotational bound states of SO_2 isotopologues. II: Total angular momentum J=11-20," *Chem. Phys.*, **461**, 34-46 (2015). doi:10.1016/j.chemphys.2015.08.025

T. Halverson and B. Poirier, "Large Scale Exact Quantum Dynamics Calculations: Ten thousand quantum states of acetonitrile," **Editor's Choice**, *Chem. Phys. Lett.*, **624**, 37-42 (2015). doi:10.1016/j.cplett.2015.02.004

P. Kumar, J. Ellis, and B. Poirier, "Rovibrational Bound States of SO_2 Isotopologues. I: Total angular momentum J = 0–10," *Chem. Phys.*, **450-451**, 59-73 (2015) (*15 pages*).

T. Halverson and B. Poirier, "Calculation of Exact Vibrational Spectra for P_2O and CH_2NH Using a Phase Space Wavelet Basis," *J. Chem. Phys.*, **140**, 204112, (2014).

B. Poirier, "The Many Interacting Worlds Approach to Quantum Mechanics," A Commentary on: "Quantum Phenomena Modelled by Interactions Between Many Classical Worlds," **invited contribution,** *Phys. Rev. X*, **4**, 040002 (2014). doi:10.1103/PhysRevX.4.040002

D. Brandon and B. Poirier, "Accurate calculations of Bound Rovibrational States for Argon Trimer," *J. Chem. Phys.*, **141** (3), 034302 (2014). doi:10.1063/1.4887459

C. Petty and B. Poirier, "Comparison of J-shifting Models for Rovibrational Spectra as Applied to the HO_2 Molecule," **Editor's Choice**, *Chem. Phys. Lett.*, **605-606**, 16-21 (2014). doi:10.1016/j.cplett.2014.05.003

C. Petty and B. Poirier, "Using ScalIT for Performing Accurate Rovibrational Spectroscopy Calculations for Triatomic Molecules: A practical guide," **invited contribution**, special issue on iterative methods and applications, *Appl. Math.*, **5**, 2756-2763 (2014).

C. Petty, W. Chen, and B. Poirier, "Quantum Dynamical Calculation of Bound Rovibrational States of HO_2 up to Largest Possible Total Angular Momentum, $J \leq 130$," **invited contribution**, special issue to honor Joel Bowman, *J. Phys. Chem. A*, **117** (32), 7280-7297 (2013). doi:10.1021/jp401154m

B. Yang and B. Poirier, "Rovibrational Bound States of the Ar_2Ne Complex," *J. Theoret. Comput. Chem.*, **12** (1), 1250107 (2013) (*22 pages*).

T. Halverson and B. Poirier, "Accurate Quantum Dynamics Calculations Using Symmetrized Gaussians on a Doubly Dense Von Neumann Lattice," *J. Chem. Phys.*, **137** (22), 224101 (2012) (*15 pages*).

J. Schiff and B. Poirier, "Sech Wave Packets, their Wigner Functions and Bohmian Trajectories," *J. Phys. A*, **45** (40), 405302 (2012) (*10 pages*).

B. Yang and B. Poirier, "Quantum Dynamical Calculation of Rovibrational Bound States of Ne_2Ar," *J. Phys. B*, **45** (13), 135102 (2012) (*15 pages*).

B. Poirier and D. Tannor, "An Action Principle for Complex Quantum Trajectories," **invited contribution**, special issue to honor Bill Miller, *Mol. Phys.*, **110** (9-10), 897-908 (2012).

G. Parlant, Y.-C. Ou, K. Park and B. Poirier, "Classical-like Trajectory Simulations for Accurate Computation of Quantum Reactive Scattering Probabilities," **invited contribution, lead article,** special issue to honor Jean-Claude Rayez, *Comput. Theoret. Chem*., **990**, 3-17 (2012).

J. Schiff and B. Poirier, "**Communication**: Quantum Mechanics Without Wavefunctions," *J. Chem. Phys.*, **136** (3), 031102 (2012). [**One of Most Read Articles in JCP History, with over 22,000 downloads. Number One Most Read JCP for six months; number four or higher for thirteen months**], doi:10.1063/1.3680558, **selected for joint publication in:** *Science and Education Publishing*

J. B. Maddox and B. Poirier, "Bipolar Reaction Path Hamiltonian Approach for Reactive Scattering Problems," *J. Chem. Theory Comput.*, **7** (9), 3484-3504 (2011).

B. Yang, W. Chen, and B. Poirier, "Rovibrational Bound States of Neon Trimer: Quantum dynamical calculation of all eigenstate energy levels and wavefunctions," *J. Chem. Phys.*, **135** (9), 094306 (2011) (*17 pages*).

B. Poirier, "Trajectory-Based Derivation of Classical and Quantum Mechanics," **invited contribution**, *Quantum Trajectories*, ed. K. H. Hughes and G. Parlant, 6-8 (CCP6, Daresbury Laboratory, 2011).

J. B. Maddox and B. Poirier, "The Bipolar Reaction Path Hamiltonian (BRPH) Approach for Multi-dimensional Reactive Scattering Calculations," **invited contribution**, *Quantum Trajectories*, ed. K. H. Hughes and G. Parlant, 9-12 (CCP6, Daresbury Laboratory, 2011).

J. L. McAfee and B. Poirier, "Quantum Dynamics of Hydrogen Interacting with Single-walled Carbon Nanotubes: Multiple H-atom adsorbates," *J. Chem. Phys.*, **134** (7), 074308 (2011) (*19 pages*), **selected for joint publication in:** *Virtual Journal of Nanoscale Science and Technology*, **23** (8), (2011).

W. Chen and B. Poirier, "Quantum Dynamics on Massively Parallel Computers: Efficient numerical implementation for preconditioned linear solvers and eigensolvers," *J. Theoret. Comput. Chem.*, **9** (5), 825-846 (2010).

B. Poirier, "Bipolar Quantum Trajectory Methods," **invited book chapter**, *Quantum Trajectories*, ed. P. Chattaraj, Chapter 15, 235-250 (Taylor & Francis/CRC Press, Boca Raton, 2010).

K. Park and B. Poirier, "Quantum Trajectory Calculations for Bipolar Wavepacket Dynamics in One Dimension: Synthetic single-wavepacket propagation," *J. Theoret. Comput. Chem.*, **9** (4), 711-734 (2010).

W. Chen and B. Poirier, "Quantum Dynamical Calculation of All Rovibrational States of HO_2 for Total Angular Momentum J=0 to 10," *J. Theoret. Comput. Chem.*, **9** (2), 435-469 (2010).

W. Chen and B. Poirier, "Parallel Implementation of Efficient Preconditioned Linear Solver for Grid-based Applications in Chemical Physics: III. Improved parallel scalability for sparse matrix-vector products," *J. Parallel Dist. Comput.*, **70** (7), 779-782 (2010).

B. Poirier, "Bohmian Mechanics without Pilot Waves," **invited contribution**, **lead article**, special issue in honor of Eli Pollak, "Dynamics of Molecular Systems, from Quantum to Classical Dynamics," *Chem. Phys.*, **370** (1-3), 4-14 (2010). [**#15 Most Read CP Article in 2014**]. https://dl.dropboxusercontent.com/u/70088177/NOWAVE.pdf

J. B. Maddox and B. Poirier, "The Bipolar Derivative Propagation Method for Calculating Stationary States for High-dimensional Reactive Scattering Systems," **invited contribution**, *Multidimensional Quantum*

Mechanics with Trajectories, ed. D. V. Shalashilin and M. P. de Miranda, 166-173 (CCP6, Daresbury Laboratory, 2009).

J. B. Maddox and B. Poirier, "Bipolar Quantum Trajectory Simulations: Trajectory surface hopping and path integral Monte Carlo," **invited contribution**, *Multidimensional Quantum Mechanics with Trajectories*, ed. D. V. Shalashilin and M. P. de Miranda, 145-165 (CCP6, Daresbury Laboratory, 2009).

J. L. McAfee and B. Poirier, "Quantum Dynamics of Hydrogen Interacting with Single-walled Carbon Nanotubes," *J. Chem. Phys.*, **130** (6), 064701 (2009) (*16 pages*), **selected for joint publication in:** *Virtual Journal of Nanoscale Science and Technology*, **19** (8), (2009).

K. Park, B. Poirier, and G. Parlant, "Quantum Trajectory Calculations for Bipolar Wavepacket Dynamics in One Dimension," *J. Chem. Phys.*, **129** (8), 194112 (2008) (*16 pages*).

B. Poirier, "Reconciling Semiclassical and Bohmian Mechanics: VI. Multidimensional dynamics," *J. Chem. Phys.*, **129** (8), 084103 (2008) (*18 pages*).

B. Poirier, "Reconciling Semiclassical and Bohmian Mechanics: V. Wavepacket dynamics," *J. Chem. Phys.*, **128** (16), 164115 (2008) (*15 pages*).

B. Poirier, "Flux Continuity and Probability Conservation in Complexified Bohmian Mechanics," *Phys. Rev. A*, **77** (2), 022114 (2008) (*9 pages*).

B. Poirier and G. Parlant, "Reconciling Semiclassical and Bohmian Mechanics: IV. Multisurface Dynamics," **invited contribution**, special issue to honor Bob Wyatt, *J. Phys. Chem. A*, **111** (41), 10400-10408 (2007).

Y. Xiao and B. Poirier, "Using Discrete Variable Representation Path Integral Monte Carlo with Metropolis Sampling to Compute Ground State Wavefunctions," *J. Theoret. Comput. Chem.*, **6** (2), 309-321 (2007).

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W. Chen and B. Poirier, "Parallel Implementation of Efficient Preconditioned Linear Solver for Grid-based Applications in Chemical Physics: II. QMR linear solver," *J. Comput. Phys.*, **219** (1), 198-209 (2006).

W. Chen and B. Poirier, "Parallel Implementation of Efficient Preconditioned Linear Solver for Grid-based Applications in Chemical Physics: I. Block-Jacobi diagonalization," *J. Comput. Phys.*, **219** (1), 185-197 (2006).

R. Lombardini and B. Poirier, "Parallel Subspace Iteration Method for the Sparse Symmetric Eigenvalue Problem," *J. Theoret. Comput. Chem.*, **5** (4), 801-818 (2006).

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R. Lombardini and B. Poirier, "Rovibrational Spectroscopy Calculations of the Neon Dimer Using a Phase Space Truncated Weyl-Heisenberg Wavelet Basis," *J. Chem. Phys.*, **124** (14), 144107 (2006) (*12 pages*).

Y. Xiao and B. Poirier, "Fully Quantum Rovibrational Calculation of the He(H_2) Bound and Resonance States," **invited contribution**, special issue, *J. Phys. Chem. A*, **110** (16), 5475-5480 (2006).

C. Trahan and B. Poirier, "Reconciling Semiclassical and Bohmian Mechanics: III. Scattering states for continuous potentials," *J. Chem. Phys.*, **124** (3), 034116 (2006) (*14 pages*).

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J. Xie, B. Poirier, and G. Gellene, "A Quantum Dynamical Treatment of Symmetry Induced Kinetic Isotope Effects in the Formation of He_2," *J. Am. Chem. Soc.*, **127** (48), 16969-16975 (2005). doi:10.1021/ja0517419

J. Xie, B. Poirier, and G. Gellene, "Accurate, Two-state *ab initio* Study of the Ground And First Excited States of He_2^+, Including Exact Treatment of All Born-Oppenheimer Terms," *J. Chem. Phys.*, **122** (18), 184310 (2005) (*12 pages*).

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B. Poirier, "Analytical Treatment of Coriolis Coupling for Three-Body Systems," **invited contribution**, special issue on dynamics of gas phase reactions, *Chem. Phys.*, **308** (3), 305-315 (2005).

B. Poirier, "Reconciling Semiclassical and Bohmian Mechanics: I. Stationary states," *J. Chem. Phys.*, **121** (10), 4501-4515 (2004).

W. Bian and B. Poirier, "Accurate and Highly Efficient Calculation of the Highly Excited Pure OH Stretching Resonances of O(^1D)HCl, Using a Combination of Methods," *J. Chem. Phys.*, **121** (10), 4467-4478 (2004).

B. Poirier and A. Salam, "Quantum Dynamics Calculations Using Symmetrized, Orthogonal Weyl-Heisenberg Wavelets with a Phase Space Truncation Scheme: III. Representations and Calculations," *J. Chem. Phys.*, **121** (4), 1704-1724 (2004). **selected for joint publication in:** *Virtual Journal of Nanoscale Science and Technology*, **10** (3), (2004).

B. Poirier and A. Salam, "Quantum Dynamics Calculations Using Symmetrized, Orthogonal Weyl-Heisenberg Wavelets with a Phase Space Truncation Scheme: II. Construction and optimization," *J. Chem. Phys.*, **121** (4), 1690-1703 (2004).

W. Bian and B. Poirier, "Accurate and Highly Efficient Calculation of the O(^1D)HCl Vibrational Bound States, Using a Combination of Methods," **invited contribution**, special issue on iterative methods, *J. Theoret. Comput. Chem.*, **2** (4), 583-597 (2003).

J. Xie, B. Poirier, and G. Gellene, "A Quantum Dynamical Study of the $He^+ + 2He \rightarrow He_2^+ + He$ Reaction," *J. Chem. Phys.*, **119** (20), 10678-10686 (2003).

J. Montgomery and B. Poirier, "Eigenspectra Calculations Using Cartesian Coordinates and a Rotational Symmetry Adapted Lanczos Method," *J. Chem. Phys.*, **119** (13), 6609-6619 (2003).

B. Poirier, "Exploiting Both C_{3v} Symmetry and Sparsity in Vibrational Calculations of Methane like Molecules," *J. Chem. Phys.*, **119** (1), 90-93 (2003).

B. Poirier and Tucker Carrington, Jr., "Semiclassically Optimized Complex Absorbing Potentials of Polynomial Form. II. Complex case," *J. Chem. Phys.*, **119** (1), 77-89 (2003).

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B. Poirier and Tucker Carrington, Jr., "Semiclassically Optimized Complex Absorbing Potentials of Polynomial Form. I. Pure imaginary case," *J. Chem. Phys.*, **118** (1), 17-28 (2003).

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B. Poirier and Tucker Carrington, Jr., "A Preconditioned Inexact Spectral Transform Method for Calculating Resonance Energies and Widths, as applied to HCO." *J. Chem. Phys.*, **116** (4), 1215-1227 (2002).

B. Poirier, "Phase Space Optimization of Quantum Representations: Non-Cartesian coordinate spaces," *Found. Phys.*, **31** (11), 1581-1610 (2001).

B. Poirier and Tucker Carrington, Jr., "Accelerating the Calculation of Energy Levels and Wave- functions, Using an Efficient Preconditioner with the Inexact Spectral Transform Method," *J. Chem. Phys.*, **114** (21), 9254-9264 (2001).

B. Poirier and J. C. Light, "Phase Space Optimization of Quantum Representations: Three-body systems, and the bound states of HCO," *J. Chem. Phys.*, **114** (15), 6562-6571 (2001).

B. Poirier, "Efficient Preconditioning Scheme for Block Partitioned Matrices with Structured Sparsity," **invited contribution**, special issue, *Numer. Linear Algebra Appl.*, **7** (7-8), 715-726 (2000).

B. Poirier, "Algebraically Self-Consistent Quasiclassical Approximation on Phase Space," *Found. Phys.*, **30** (8), 1191-1226 (2000). **Figure 1 reprinted in:** D. Tannor, *Introduction to Quantum-Mechanics: A Time-dependent Perspective*, (University Science Books, Sausalito, 2006).

B. Poirier and J. C. Light, "Efficient Distributed Gaussian Basis for Rovibrational Spectroscopy Calculations," *J. Chem. Phys.*, **113** (1), 211-217 (2000).

B. Poirier, "Wigner-Weyl Correspondence and Semiclassical Quantization in Spherical Coordinates, *J. Math. Phys.*, **40** (12), 6302-6318 (1999).

B. Poirier and J. C. Light, "Phase Space Optimization of Quantum Representations: Direct-product basis sets," *J. Chem. Phys.*, **111** (11), 4869-4885 (1999).

B. Poirier, "Comment on the Van Vleck Method and Three-Body Kinetic Energies," *Faraday Discuss.*, **110**, 230-231 (1998).

B. Poirier, "Quantum Reactive Scattering for Three-Body Systems via Optimized Preconditioning, as Applied to the O+HCl Reaction," *J. Chem. Phys.*, **108** (13), 5216-5224 (1998).

B. Poirier, "Optimal Separable Bases and Series Expansions," *Phys. Rev. A*, **56** (1), 120-130 (1997).

B. Poirier and W. H. Miller, "Optimized Preconditioners for Green's Function Evaluation in Quantum Reactive Scattering Calculations," *Chem. Phys. Lett.*, **265** (1-2), 77-83 (1997).

BOOKS:

J. Terning, B. Poirier, Y. Nomura, *Quantum Physics, Mini Black Holes and the Multiverse: Debunking Common Misconceptions in Theoretical Physics*, (**invited**) (Springer, 2018).
Highly Recommended by *Choice Magazine*, American Library Association, **56** (2) October, 2018
#8 on BookAuthority's **11 Best New Cosmology Books To Read in 2019** December, 2018
#7 on BookAuthority's **11 Best New Particle Physics Books To Read in 2019** December, 2018

B. Poirier, *A Conceptual Guide to Thermodynamics* (Wiley, 2014).
(formal offers received from three separate publishers)
Recommended by *Choice Magazine*, American Library Association, **52** (8) April 1, 2015
Number one featured physical chemistry title on *Chemistry Amazon* Fall 2015

EXTERNAL FUNDING (RECEIVED; SOLE PI UNLESS OTHERWISE STATED):

Texas Advanced Computing Consortium, Frontera Pathways Allocation
"SwitchIT: Pushing the Limits of Computational Rovibrational Molecular Spectroscopy Simultaneously with Respect to System Size, Convergence Accuracy and Number of Computed States."
192,768 node hours September 2023 to August 2024

Lubbock Economic Development Agency
"Quantum Galaxies Corporation: Proposal for Prototype Grant Fund"
$5,000 November 2022 to August 2023

Creative Destruction Labs, Quantum Bootcamp & Incubator Programs
"Quantum Galaxies Corporation: IBM Hackathon Challenge."
$4,000 August 2022

São Paulo Science Funding Agency (FAPESP), TTU SPRINT Program
"Riding Quantum Trajectories beyond Born-Oppenheimer: Building better methods for reaction dynamics."
$20,000 (one of two co-I's; Poirier share is $10K) June 1, 2022 to May 31, 2025

Texas Advanced Computing Consortium, Frontera Pathways Allocation
"SwitchIT: Pushing the Limits of Computational Rovibrational Molecular Spectroscopy Simultaneously with Respect to System Size, Convergence Accuracy and Number of

Computed States."
224,964 node hours March 2022 to December 2022

National Science Foundation
"SUPPLEMENT II: CDS&E: Massively Parallel Quantum Dynamics: Computing many accurate quantum states for real molecular applications."
$33,400 August 2021 to July 2022

Molecular Sciences Software Institute (MolSSI)
"MolSSI Seed Postdoctoral Fellowship for János Sarka"
$25,000 January 2020 to June 2020

Robert A. Welch Foundation Grant (invited renewal)
"New Methodologies for Accurate Quantum Calculations of the Dynamics of Atomic Nuclei."
$195,000 June 2019 to January 2023

Molecular Sciences Software Institute (MolSSI)
"Rovibrational Molecular Spectroscopy: Setting standards for software packages and toolkits."
$20,000 April 2019 to December 2019

U.S. Army Research Office
"Canonical Tensors Applied to Ab Initio Electronic Structure: Exact electron correlation via full-dimensional calculation."
$60,000 December 10, 2018 to December 9, 2019

National Science Foundation
"SUPPLEMENT I: CDS&E: Massively Parallel Quantum Dynamics: Computing many accurate quantum states for real molecular applications."
$30,998 August 2018 to July 2020

Max Planck Institute: Physics Of Complex Systems.
MPIPKS Guest Scientist Program—Research Proposal (Poirier) (Competitive)
$15,400 March to August, 2018

Max Planck Institute: Physics Of Complex Systems.
MPIPKS Workshop Scientific Coordinator—Research Proposal (Poirier) (Competitive)
"QuSeT: Interdisciplinary Focus Workshop on Quantum and Semiclassical Trajectories
$17,500 February to July, 2018

National Science Foundation
"CDS&E: Massively Parallel Quantum Dynamics: Computing many accurate quantum states for real molecular applications."
$498,009 August 2017 to July 2022

São Paulo Science Funding Agency (FAPESP), TTU SPRINT Program
"Fermi Accelerators, Inverse Fermi Accelerators, Nonadiabatic Dynamics, and Quantum Trajectories: Towards a method for electron dynamics."
$40,000 (one of two co-I's; Poirier share is $20K) July 2017 to December 2019

Hungarian Academy of Sciences Distinguished Guest Scientist Fellowship
$53,000 January to June 2017

Robert A. Welch Foundation Grant (invited renewal, including $10K supplement)
"New Methodologies for Accurate Quantum Calculations of the Dynamics of Atomic Nuclei."
$250,000 (plus $37,500 TTU trip matching funds) June 2016 to May 2019

Robert A. Welch Foundation Grant (invited renewal)
"New Methodologies for Accurate Quantum Calculations of the Dynamics of Atomic Nuclei."
$225,000 (plus $22,500 TTU trip matching funds) June 2013 to May 2016

National Aeronautics and Space Administration, Astrobiology Program,
"A Collaborative Experimental-Theoretical Investigation of Key Pathways In Photochemistry Related to the Origin of Sulfur Mass-Independent Fractionation."
$1,341,895 (one of four co-I's; Poirier share is $300K) April 2013 to April 2017

National Science Foundation,
"Joint NASA-NSF Workshop: Origins, Carriers, and Implications of Mass-Independent Fractionation of Sulfur Isotopes (S-MIF)"
$10,200 (plus $40,500 NASA matching funds) June 2011 to May 2013

National Science Foundation,
"Massive Parallelization of Exact Quantum Dynamics Calculations: Computing (ro)vibrational states for real molecular applications."
$468,715 July 2010 to July 2015

Robert A. Welch Foundation Grant (invited renewal, various supplements)
"New Methodologies for Accurate Quantum Calculations of the Dynamics of Atomic Nuclei."
$215,000 (plus $31,000 TTU TRIP matching funds) June 2010 to May 2013

United States–Israel Binational Science Foundation,
"Solution of the Time-dependent Schroedinger Equation via Quantum Trajectories."
$68,000 (one of three co-PI's) September 2009 to August 2014

National Science Foundation,
Chemistry Research Instrumentation and Facilities, Multi-User,
"A Cluster for Cyber-enabled Research and Education in Computational Chemistry."
$525,325 (dept. instrumentation; co-PI; chief author) February 2009 to July 2013

American Chemical Society Petroleum Research Fund Grant, Type ND,
"Accurate Quantum Dynamical Exploration of Fundamental Interactions between Hydrogen and Carbon Nanotubes."
$100,000 January 2009 to August 2012

National Science Foundation,
"Workshop on Quantum Trajectory Methods."
$5,500 July 2008 to July 2009

Quantum Institute, Los Alamos National Laboratories,
"New Mexico Workshop on Quantum Trajectories."
$5,000 May 2008

New Mexico Institute for Advanced Studies,
"New Mexico Workshop on Quantum Trajectories."
$5,000 April 2008

Center for Nonlinear Studies, Los Alamos National Laboratories,
"New Mexico Workshop on Quantum Trajectories."
$5,000 March 2008

Theoretical Division, Los Alamos National Laboratories
"New Mexico Workshop on Quantum Trajectories."
$5,000 March 2008

National Science Foundation, Small Grant for Exploratory Research
"Bipolar Quantum Trajectory Simulations."
$173,418 August 2007 to August 2009

Robert A. Welch Foundation Grant (invited renewal at $60,000 per year for three years)
"New Methodologies for Accurate Quantum Calculations of the Dynamics of Atomic Nuclei."
$180,000 (plus $12,500 TTU Trip Matching funds) June 2007 to May 2010

Robert A. Welch Foundation Grant (renewal)
"New Methodologies for Accurate Quantum Calculations of the Dynamics of Atomic Nuclei."
$150,000 June 2004 to May 2007

U.S. Department of Energy, Early Career Principal Investigator Program
"Efficient Iterative Linear Solvers and Eigensolvers for Terascale Computing."
$324,813 January 2003 to December 2006

Research Corporation, Research Innovation Award
"Using Symmetrized Orthogonal Wavelets to Customize Quantum Dynamics Calculations of Atomic Nuclei in Molecules."
$35,000 May 2002

American Chemical Society Petroleum Research Fund Grant, Type G
"Accurate Dynamics Calculations for Atomic Nuclei in Molecular Systems, Using New Theoretical Techniques."
$25,000 August 2001 to July 2003

Robert A. Welch Foundation Grant
"New Methodologies for Accurate Quantum Calculations of the Dynamics of Atomic Nuclei."
$150,000 June 2001 to May 2004

ENDOWMENTS AND GIFTS:

TRIP Matching Fund for Robert A. Welch Foundation
$37,500 October 2017

TRIP Matching Fund for Robert A. Welch Foundation
$75,000 October 2016

TRIP Matching Fund for Robert A. Welch Foundation
$31,000 September 2014

TRIP Matching Fund for Robert A. Welch Foundation
$22,500 September 2013

TRIP Matching Fund for Robert A. Welch Foundation
$12,500 January 2013

INTERNAL FUNDING:

TTU National Science Foundation Regional I-Corps Program
"Quantum Galaxies Corporation: Proposal for TTU NSF I-Corps Funding"
$2,000 April 2022 to June 2022

Texas Tech University— Office of the Vice President for Research—Match for:
Army Research Office: Short-term Innovative Research
"Canonical Tensors Applied to Ab Initio Electronic Structure: Exact Electron Correlation via Full-dimensional Calculation."
$20,000 December 10, 2018 to September 9, 2019

Texas Tech University—Three-year research professorship grant
$180,000 May 2016 to April 2019

TECHNOLOGY TRANSFER:

<u>Patents:</u>

"Methods and Systems in Quantum Computing."
Submitted: November 2, 2021; Application: November 2, 2022.
US Provisional Patent: 63/274,877 (TTU-1061USUTIL)

"Methods and Systems for Quantum Computational Chemistry."
Submitted: August 16, 2019; Application: April 15, 2020; Approved: October 12, 2022.
US Patent: US-2023-0169383-A1 Publication Date: 06/01/2023
Canadian Patent: CA3175359A1

"Wide-Field Three-Dimensional Viewing System."
US Patent: US-5357369-A Publication Date: 10/18/94

Start-up Companies:

Quantum Galaxies Corporation (10% shareholder) Incorporated 2022
Quantum Galaxies Corporation seeks to be the premier provider of "quantum benchmarking" services, offering reliably accurate benchmark data for extremely challenging computational applications of interest to quantum computing hardware and software vendors.

INVITED PROFESSIONAL ACTIVITIES:

Advisory Board:

Telluride Science Research Center	(from January 2016)
Quantum Atomic and Molecular Tunneling in Solids	(from July 2012)
Southwest Theoretical and Computational Chemistry	(from October 2009)
Biannual Workshop on Quantum Trajectories	(July 2008 to July 2013)

Consultant:

John Wiley & Sons Publishers; physical chemistry course materials	(from August 2022)

Meeting Organizer:

Workshop Organizer:	Mini-mini-symposium on Quantum Trajectories	(2022)
Workshop Organizer:	Mini-symposium on Quantum Trajectories	(2022)
Symposium Organizer:	Symposium to Honor Bill Hase	(2020)
Conference Organizer:	MolSSI Workshop on Rovibrational Molecular Spectroscopy	(2019)
Conference Organizer:	Quantum and Semiclassical Trajetories (QuSeT)	(2018)
Award Committee:	72nd Southwest Regional ACS Meeting	(2017)
Symposium Organizer:	72nd Southwest Regional ACS Meeting	(2017)
Conference Organizer:	Telluride Workshop on Mass-Independent Fractionation of Sulfur Isotopes: Possible molecular origins"	(2016)
Organizing Committee:	Quantum Atomic and Molecular Tunneling in Solids	(2015, 2017, 2019)
Conference Organizer:	Quantum Atomic and Molecular Tunneling in Solids	(2012)
Conference Organizer:	Joint NASA/NSF Workshop: "Origins, Carriers, and Implications of Mass-Independent Fractionation of Sulfur Isotopes."	(2011)
Conference Organizer:	New Mexico Workshop on Quantum Trajectories	(2008)
Publicity and Printing Chair:	63rd Southwest Regional ACS Meeting	(2007)
Symposium Organizer:	63rd Southwest Regional ACS Meeting	(2007)
Organizer and Session Chair:	Symposium to Honor Purnendu K. "Sandy" Dasgupta	(2006)
Conference Organizer:	Southwest Theoretical and Computational Chemistry	(2003, 2017)
Session Chair:	TPMSCM21 workshop, MPIPKS, Dresden, Germany	(2021)
	QAMTS workshop, Borovets, Bulgaria	(2019)
	72nd Southwest Regional ACS Meeting, Southwest Theoretical and Computational Chemistry Symposium	(2016)
	QAMTS workshop, Beatenberg, Switzerland	(2015)

	GCURS, Houston, TX	(2014)
	Telluride Workshop on New Challenges for Theory in Chemical Dynamics	(2010, 2014, 2018)
	EUROMAT Meeting	(2011)
	CCP6 Workshop on Quantum Trajectories	(2010)
	Southwest Theoretical Chemistry Conference	(2006, 2008, 2016, 2017)
Poster Judge:	Texas Tech Department of Physics, Society of Physics Student Poster Competition	(2017)
	Texas Tech University Graduate Poster Competition	(2013, 2014, 2015)
	Southwest Theoretical Chemistry Conference	(2009)
Concluding Discussion Leader:	IMA Workshop on Chemical Dynamics	(2009)
Summer School Instructor:	Presqu'ile de Giens, France	(2007)
Lecture Series Organizer:	Argonne National Laboratories	(2003)

NASA Advisory Group (one of three members):

Authors of NASA Summary Report: (2012)
"Mass-Independent Fractionation of Sulfur Isotopes: Carriers and Sources"
initial distribution: NASA and NSF program officers and administrators
final release: seven targeted scientific communities

NASA website url: http://is.gd/s_mif

Editorial Service:

Frontiers in Chemistry, Journal Editor	(from August 2022)
Symmetry, Journal Editor	(from August 2020)
Reports in Theoretical Chemistry, Honorary Editorial Board	(2011-2014)

Interviews:

Living with Long Covid: A Conversation with Dr. Bill Poirier	*Humanities Now Podcast*	(May 2023)
Professors' Reactions to COVID-19	*TTU Daily Toreador*	(August 2021)
Physics of the Observer: Quantum Physics	*Multiversal Journeys*	(September 2017)
Misconceptions in Quantum Physics	*Multiversal Journeys*	(July 2015)
Upgrades, growth for UT supercomputer center	*Austin-American Statesman*	(July 2015)
Quantum Quandary	*Texas Tech Discoveries*	(Spring 2015)
Weltanschauung	*KPFT Houston Public Radio*	(November 2014)
Many Interacting Worlds	*Cosmos Magazine*	(October 2014)
Ghost Universes Kill Schrödinger's Quantum Cat	*New Scientist*	(October 2014)
Admissions Advisor	*Graduate School Life*	(January 2012)

Panel Member:

Advances in Hydrogen Molecular Ions H_3^+, H_5^+ and beyond:	Final Panel	(January 2019)
Multiversal Journeys:	Physics of the Observer—A Documentary	(September 2017)
National ACS Meeting:	Graduate School Reality Check	(March 2011)

Reviewer and Referee:

Research Proposal Panel Member: National Science Foundation (8x)

Research Proposal Reviewer:
American Chemical Society Petroleum Research Fund (G, AC)
American Chemical Society Petroleum Research Fund ND (3x)
Canada Research Chair
German Israeli Foundation for Scientific Research
Israeli Science Foundation (2x)
National Aeronautics and Space Administration (NASA)

National Science and Engineering Research Council of Canada
National Science Foundation (76x)
Research Corporation (Cottrell College Science Award) (5x)
Research Corporation (Cottrell Scholar Award)
U.S. Department of Energy (3x)
U.S. Department of Energy (Energy Frontiers Research Center)
U.S.–Israel Binational Science Foundation

Journal Reviewer Arbiter:

Journal of Chemical Physics
Journal of Chemical Physics, COMMENT
Journal of Physical Chemistry A
Journal of Physics, Conference Proceedings EmQM13
Physics Letters A
Physical Review Letters (2x)
Physical Review X

Journal Referee:

Advances in Chemical Physics (John Light Memorial Issue)
Annals of Physics
Canadian Journal of Chemistry
Canadian Journal of Physics
Chemical Physics (5x)
Chemical Physics Letters (3x)
Computational Materials Science
European Journal of Operations Research
European Physics Letters
Foundations of Physics (5x)
Frontiers in Chemistry (2x)
International Journal of Hydrogen Energy
International Journal of Theoretical Physics
Journal of Chemical Education
Journal of Chemical Physics, regular article (38x)
Journal of Chemical Physics, RAPID COMMUNICATION (8x)
Journal of Computational Physics (3x)
Journal of Parallel and Distributed Computing
Journal of Physical Chemistry A (14x)
Journal of Physical Chemistry C
Journal of Physical Chemistry Letters (2x)
Journal of Physics A
Journal of Quantitative Spectroscopy and Radiative Transfer
Journal of Theoretical and Computational Chemistry (4x)
Molecular Physics (4x)
Monthly Notices of the Royal Astronomical Society (3x)
Parallel Computing
Physica Scripta
Physical Chemistry Chemical Physics (4x)
Physical Review A (4x)
Physical Review E
Physical Review Letters
Proceedings of the Royal Society A (2x)
Quantum Studies: Mathematics and Foundations
Results in Physics
Symmetries in Science Proceedings
Theoretical Chemistry Accounts

Theoretical Chemistry Accounts (special issue, 50th anniversary)

Book Reviewer: *Chasing the Quantum Dragon*, W. H. Madden (CreateSpace, 2013)
Foundations of Chemical Engineering Thermodynamics; R. Ravi (Wiley, not published)
Introductory Chemistry, 4th edition, Steve Russo and Michael Silver (Pearson, New York, 2010).
Quantum Trajectories, ed. P. Chattaraj (Taylor & Francis/CRC Press, Boca Raton, 2010).

Invited Professorships, and Faculty Development Leaves (sabbaticals):

Invited Professor: Dresden, Germany (Max Planck Institute: Physics of Complex Systems) March 2020

Faculty Development Leave/Invited Professor:
Dresden, Germany (Max Planck Institute: Physics of Complex Systems) Spring/Summer 2018

Distinguished Guest Scientist: Budapest, Hungary (Eötvös Loránd University) Spring/Summer 2017

Invited Professor: Dresden, Germany (Max Planck Institute: Physics of Complex Systems) October 2015

Invited Professor: Budapest, Hungary (Eötvös Loránd University) May 2015

Professeur Invité: Montpellier France (Centre national de la recherche scientifique)
Une nouvelle méthode de simulation pour la chimie: November 2015
les Trajectoires Bohmiennes August 2011

Faculty Development Leave: Montpellier France (Montpellier II University) Fall 2011

Invited Workshop Participant:

Advances in Hydrogen Molecular Ions H_3^+, H_5^+ and Beyond, London UK January 2019

John Light Memorial Symposium, University of Chicago, IL May 2016

International Workshop on Martin Gutzwiller's Scientific Universe: November 2015
From Wavefunctions Over Periodic Orbits to Sun, Moon and Earth.
Max Planck Institute, Dresden, Germany

NSF Exploratory Workshop on Scientific Software Innovation Institutes: August 2010
Atomistic modeling and simulation, Arlington, VA

IMA Workshop on Chemical Dynamics: Challenges and Approaches, January 2009
Minneapolis, MN

Invited Posters, Publications, Book Chapters, and Books:

Poster: Defense TechConnect Innovation Summit (2022).
Dynamics of Molecular Collisions Conference (2007).
Chemical Dynamics Symposium (2001).

Publications: B. Poirier, A. Pandey, and B. Poirier, *J. Comput. Chem*. special issue (submitted).
J. Sarka and B. Poirier, *Front. Phys.* **10**, special issue (2022)
M. S. Hussein and B. Poirier, *Braz. J. Phys.* **51**, 193-203 special issue (2021).
B. Poirier and H.-M. Tsai, *Symmetries in Science XVIII*, ed. D. Schuch and M. Ramek, (Journal of Physics, IOP, 2020).
J. Jerke, J. Karwowski, and B. Poirier, *Mol. Phys*. **117**, 1264-1275 special issue (2019).
B. Poirier, *Adv. Chem. Phys.* **163**, 245-271 special issue (2018).
H.-M. Tsai and B. Poirier, *J. Phys.*, **701**, 012013 (2016).
T. Halverson and B. Poirier, *J. Phys. Chem. A,* **119**, 12417-12433 special issue (2015).
B. Poirier, *Mathematical Methods in Quantum Molecular Dynamics*, 42-45, (Mathematisches Forschungsinstitut Oberwolfach, 2015)
H.-M. Tsai and B. Poirier, *EmQM15: Emergent Quantum Mechanics 2015*, ed. G.

Grössing, (Journal of Physics, IOP, 2016).
B. Poirier, *Phys. Rev. X*, **4**, 040002 (2014)
C. Petty and B. Poirier, *Appl. Math.*, **5**, 2756-2763 special issue (2014).
C. Petty, W. Chen and B. Poirier, *J. Phys. Chem. A*, **117** (32), special issue (2013).
B. Poirier and D. Tannor, *Mol. Phys.*, **110** (9-10), special issue (2012).
G. Parlant, Y.-C. Ou, K. Park and B. Poirier, *Comput. Theoret. Chem.*, **990** special issue, **lead article** (2012).
J. Maddox and B. Poirier, *CCP6 Workshop Proc*. (2x), (2011).
J. L. McAfee and B. Poirier, *Virt. J. of Nano Sci. and Tech.*, **23** (8), (2011).
Poirier, *Chem. Phys*., **370** (1-3) special issue, **lead article** (2010).
J. L. McAfee and B. Poirier, *Virt. J. of Nano Sci. and Tech.*, **19** (8), (2009).
J. Maddox and B. Poirier, *CCP6 Workshop Proc*. (2x), (2009).
B. Poirier, *J. Phys. Chem. A*, **111** (41), special issue (2007).
B. Poirier, *J. Phys. Chem. A*, **110** (16), special issue (2006).
B. Poirier, *Chem. Phys.*, **308** (3), special issue (2005).
B. Poirier and A. Salam, *Virt. J. of Nano Sci. and Tech.*, **10** (3), (2004).
W. Bian and B. Poirier, *J. Theo. Comput. Chem.*, **2** (4), special issue (2003).
B. Poirier, *Num. Lin. Alg. with Appl.* **7** (7), special issue (2000).

Book Chapter: B. Poirier, "Effect of Confinement on the Translation-Rotation Motion of Molecules: The inelastic neutron scattering selection rule," Chap. 1, pp. 1-24, *Chemical Reactivity in Confined Systems: Theory, Modelling and Applications*, ed. P. Chattaraj and D. Chakraborty (John Wiley & Sons, Oxford, UK, 2021).
B. Poirier, "Bipolar Quantum Trajectory Methods," *Quantum Trajectories*, ed. P. Chattaraj (Taylor & Francis/CRC Press, Boca Raton, 2010).

Book: J. Terning, B. Poirier, Y. Nomura, *Quantum Physics, Mini Black Holes and the Multiverse: Debunking Common Misconceptions in Physics*, (Springer, 2018).

Invited Lectures:

Department of Mathematics and Statistics, Texas Tech University — April 2023
"Quantum Mechanics Without Wavefunctions"

Department of Computer Science, Texas Tech University — April 2023
"Efficient Evaluation of Exponential and Gaussian Functions on a Quantum Computer."

28th Austin Symposium on Molecular Structure and Dynamics — February 2023
Southern Methodist University, Dallas, TX
"Full-dimensional Schrödinger Wavefunction Calculations Using Tensors and Quantum Computers: the Cartesian component-separated approach."

TTU Department of Physics and Astronomy, Special Seminar, — November 2022
"Entangled States: A Special Seminar on This Year's Nobel Prize in Physics."

International Workshop on Quantum Reactive Scattering: QRS 2022, — September 2022
Balatonfõldvar, Hungary
"Hitting the Trifecta: How to simultaneously push the limits of Schroedinger solution with respect to system size, convergence accuracy, and number of computed states," (delivered by post-doc).

25th International Workshop on Quantum Chemistry, Physics, and Biology — June 2022
University of Torun, Poland
"Full-dimensional Schroedinger Wavefunction Calculations using Tensors and Quantum Computers: the Cartesian component-separated approach."

Telluride Workshop on Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems, Telluride, Colorado — June 2022

"Hitting the Trifecta: How to simultaneously push the limits of Schroedinger solution with respect to system size, convergence accuracy, and number of computed states."

18th International Workshop on Quantum Atomic and Molecular Tunneling in Solids and Other Phases (QAMTS), Calgary, Canada — May 2022

"Hitting the Trifecta: How to simultaneously push the limits of Schroedinger solution with respect to system size, convergence accuracy, and number of computed states."

"Quantum Dynamical Study of the Hydrogen Exchange Reaction in the $[FeH(H_2)(PH_3)_4]^+$ Coordination Complex," (delivered by post-doc).

"Resonant Tunneling in Chemistry from Quantum Trajectory Based Method," (delivered by student).

Goldman Sachs Quantum Algorithms Pod Seminar, New York, NY (virtual) — November 2021
"Efficient Evaluation of Exponential and Gaussian Functions on a Quantum Computer."

A Quantum Lunch Seminar, Los Alamos National Labs, NM — September 2021
"Freeing Andromeda: A gateway to the quantum realm."

IUPAC Canadian Chemistry Conference, Toronto, Canada — August 2021
"Hitting the Trifecta: How to simultaneously push the limits of Schroedinger solution with respect to system size, convergence accuracy, and number of computed states."

American Chemical Society National Meeting, San Francisco, CA — April 2021
"Plumbing Potentials for Molecules with Up to Tens of Atoms: How to Find Saddle Points and Fix Leaky Holes," A Symposium in Honor of Professor William L. Hase

TTU Workshop on Quantum Information and Quantum Computation, Lubbock, TX — August 2020
"Efficient Evaluation of Exponential and Gaussian Functions on a Quantum Computer."

Centro Brazileiro de Pesquisas Físicas, Rio de Janeiro, Brazil — January 2020
"Quantum Mechanics Without Wavefunctions"

MolSSI Workshop on Rovibrational Molecular Spectroscopy, Blacksburg, VA — November 2019
"Accurate Calculations of Rovibrational Bound States Using ***ScalIT***."

Southwest Theoretical and Computational Chemistry Conference, Norman, OK — October 2019
"Tensor product methods for exact Schrödinger solutions in electronic structure."

TTU Vice President for Research Office, Lubbock, TX — October 2019
"Report on Texas Tech University and its Involvement in the Texas Quantum Institute."

Texas Quantum Institute Kickoff Meeting, College Station, TX — October 2019
"Texas Tech Quantum Research."

Utah Workshop on Quantum Methods in Molecular and Solid-State Theory, Park City, UT — September 2019
"Tensor product methods for exact Schrödinger solutions in electronic structure: geminals, quantum computing, and periodic boundary conditions."

Department of Chemistry, University of North Texas, Denton, TX — September 2019
"Exact Quantum Dynamical Treatment of Hydrogen-material Interactions: Kubas complexes, and entanglement-induced selection rules"

Symmetries in Science: SiS XVIII, Bregenz, Austria — August 2019
"Hidden symmetries in quantum mechanics—revealed, by the trajectory-based formulation."

International Workshop on Quantum Reactive Scattering: QRS 2019, Saitama, Japan — July 2019
"Adiabatic Quantum Trajectory Capture Method for Ultra-cold Chemical Reactions."

17th International Workshop on Quantum Atomic and Molecular Tunneling In Solids and other Phases (QAMTS), Borovets, Bulgaria, — June 2019
"Exact Quantum Dynamical Treatment of Hydrogen- material Interactions: $Fe(H)_2(H_2)(PEtPh_2)_3$ and $[FeH(H_2)(PH_3)_4]^+$"

US Army Research Office Contractors Meeting, Durham, NC June 2019
"Lifting the Curse of Dimensionality: Ewald, diatomic pre-born Oppenheimer, and 3-electron computations"
(delivered by Jonathan Jerke)

Telluride Workshop on Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems, Telluride, Colorado June 2019
"The crystal algorithm: Finding – and fixing – leaky `holes' in potential energy surfaces."

International Symposium on Quantum Effects in Chemistry and Biology, Shanghai, China May 2019
"Adiabatic Quantum Trajectory Capture Method for Ultra-cold Chemical Reactions."

Quantum Computing Seminar Series, Texas Tech University March 2019
"Entanglement and the EPR(B) Paradox."

Southwest Theoretical and Computational Chemistry Conference, Edinburg, TX October 2018
"Sulfur Mass Independent Fractionation (S-MIF): How quantum dynamics is answering fundamental questions about the origins of life."

Department of Chemistry, Frankfurt Am Main Goethe University, Frankfurt, Germany July 2018
"Quantum Mechanics Without Wavefunctions"

Interdisciplinary Focus Workshop on Quantum and Semiclassical Trajectories (QuSeT), Max Plank Institute for the Physics of Complex Systems, Dresden, Germany June 2018
"Trajectory-based Theory of Relativistic Quantum Particles."
"Adiabatic Quantum Trajectory Capture Method for Ultra-cold Chemical Reactions" (delivered by Yohann Scribano)

Max Plank Institute for the Physics of Complex Systems, Dresden, Germany, Quantum Dynamics Seminar April 2018
"Quantum Mechanics Without Wavefunctions."

Anharmonicity in Medium-Sized Molecules and Clusters (AMOC), Budapest, Hungary April 2018
"Large Scale Vibrational Spectroscopy Calculations: Massive parallelization and the classical phase space picture"
"Eugene Wigner: Man of Science" (after dinner talk)

Department of Chemistry, University of Chicago March 2018
"Application of Data Science technologies to chemical and physics computations" (delivered by Jonathan Jerke)

27th Austin Symposium on Molecular Structure and Dynamics, Dallas, TX March 2018
In honor of Dieter Cremer.
"Trajectory-based Theory of Relativistic Quantum Particles"

Instituto de Fisica, University of São Paulo, São Paulo, Brazil February 2018
"Quantum Mechanics Without Wavefunctions"

Telluride Workshop on New Challenges for Theory in Chemical Dynamics January 2018
"Rovibrational States for Free: The *J*-dependent rotational Hamiltonian method"

Department of Chemistry & Biochemistry, Baylor University, Waco, TX December 2017
"New Methods in Quantum Dynamics, Molecular Applications and Experimental Validation."
"Chalk Talk."

American Chemical Society Southwest Regional Meeting, Lubbock, TX October 2017
Southwest Theoretical and Computational Chemistry Symposium
"Trajectory-based Theory of Relativistic Quantum Particles."

Perimeter Institute, Quantum Foundations Seminar, Waterloo, Ontario October 2017
"Quantum Mechanics Without Wavefunctions"

Department of Chemistry, University of Waterloo October 2017
"Sulfur Mass Independent Fractionation: How quantum dynamics will answer fundamental questions about the origins of life."

Stem Across Continents Workshop, Texas Tech University September 2017
"Fermi Accelerators and Quantum Trajectories:
Theory across continents, and across disciplines."

Physics of the Observer—A Documentary, Ondine, Sausalito, CA, September 2017
"Physics of the Observer—Quantum Physics"

Telluride Workshop on Spectroscopy and Dynamics of Coupled Anharmonic July 2017
Vibrations of Floppy Molecular Systems
"Rovibrational States for Free: The *J*-dependent rotational Hamiltonian method"

Department of Quantum Optics and Quantum Information June 2017
Wigner Research Center, Budapest, Hungary
"Quantum Mechanics Without Wavefunctions"
"Quantum Mechanics Without Wavefunctions II: Measurement, Collapse, and the Relativistic Formulation"

MOLIM Workshop: Time dependent Methods, ETH Zurich, Switzerland April 2017
"Exact Quantum Dynamical Treatment of Hydrogen-material Interactions"

Ortvay Kollokvium Talk, Institute of Physics, Eötvös Loránd University March 2017
"Quantum Mechanics Without Wavefunctions"

Institute for Solid State Physics and Optics, Hungarian Academy of Sciences February 2017
Wigner Research Center, Budapest, Hungary
"Exact Quantum Dynamical Treatment of Hydrogen-material Interactions"

American Chemical Society Southwest Regional Meeting, Galveston, TX November 2016
Southwest Theoretical and Computational Chemistry Symposium
"The $H_2@C_{60}$ Inelastic Neutron Scattering Selection Rule: Expanded, and explained."

Stem Across Continents Workshop, Texas Tech University August 31 & September 1 2016
"Experiences in Brazil: Scientific and otherwise"

Departamento de Ciência e Tecnologia Aerospacial at Instituto Technológico June 2016
de Aeronáutica, São José dos Campos, Brazil
"Sulfur Mass Independent Fractionation (S-MIF): How quantum dynamics will answer fundamental questions about the origins of life."
"Quantum Mechanics Without Wavefunctions"

Departamento de Química Universidade Federal de São Carlos, Brazil June 2016
"Quantum Dynamics of Hydrogen Interacting Exohedrally with Single-walled Carbon Nanotubes"

Laboratório de Astroquímica e Astrobiologia at Universidade do Vale do Paraiba, June 2016
São José dos Campos, Brazil
"Sulfur Mass Independent Fractionation (S-MIF): How quantum dynamics will answer fundamental questions about the origins of life."

Telluride Workshop on Mass-Independent Fractionation of Sulfur Isotopes: June 2016
Possible Molecular Origins;
"The Quantum States of SO_2: State labeling, $C \leftarrow X$ vibronic transitions, and ramifications for self-shielding."

Department of Chemistry, Eötvös Loránd University, Budapest, Hungary, May 2015
Ferenc Török Memorial Lecture,
"Large Scale Exact Quantum Dynamics Calculations: One Hundred Thousand Quantum States of Benzene"

26th Austin Symposium on Molecular Structure and Dynamics, Dallas, TX March 2016
"Large Scale Vibrational Spectroscopy Calculations: Massive parallelization and the classical phase space picture."

BIRS Workshop on Exploiting New Advances in Mathematics to Improve January 2016

Calculations in Quantum Molecular Dynamics, Banff, Canada
"Quantum Mechanics Without Wavefunctions."

Telluride Workshop on New Challenges for Theory in Chemical Dynamics January 2016
"One Million Quantum States of Benzene"
"The $H_2@C_{60}$ Inelastic Neutron Scattering Selection Rule: Expanded and explained."

Advances in Quantum Dynamics From Spectroscopy to Dynamics, December 2015
Pacifichem 2015
"Large scale exact quantum dynamics calculations: Massive parallelization and the classical phase space picture"

New Insights from Quantum Dynamics, Pacifichem 2015 December 2015
"Sulfur mass independent fractionation (S-MIF): How quantum dynamics will answer fundamental questions about the origins of life"

Institut Charles Gerhardt, Montpellier, France November 2015
"Quantum Mechanics Without Wavefunctions Applications"

LC2 at Montpellier University, Montpellier, France November 2015
"Quantum Mechanics Without Wavefunctions Foundations"

Max Planck Institute: Physics of Complex Systems, Invited Lecture November 2015
"Phase Space Basis Sets: From Davis & Heller, to One Million Quantum States of Benzene"

Max Planck Institute: Physics of Complex Systems, Invited Lecture November 2015
"Quantum Mechanics Without Wavefunctions"

EmQM15 International Symposium about Quantum Mechanics , October 2015
Technical University, Vienna Austria,
"Quantum Mechanics Without Wavefunctions: When quantum worlds collide"

Mini-conference on Misconceptions in Physics and Cosmology July 2015
Lawrence Hall of Science, University of California, Berkeley, CA, **Plenary Lecture**,
"Misconceptions in Quantum Mechanics"
https://www.youtube.com/watch?v=GrpGPkoZvlc

Brazilian High School Summer Student Camp, Texas Tech University July 2015
"The Mysteries of Quantum Mechanics" and "The Mysteries of Quantum Physics"

Matematisches Forschunginstitut Oberwolfach Workshop on Mathematical Methods June 2015
In Quantum Molecular Dynamics, Oberwolfach, Germany,
"QuantumMechanics Without Wavefunctions"

17th International Workshop on Quantum Atomic and Molecular Tunneling June 2015
In Solids and other Phases (QAMTS) , Interlaken, Switzerland, **Plenary Lecture**
"Exact Quantum Dynamical Treatment of Hydrogen-material Interactions"

Department of Chemistry, Eötvös Loránd University, Budapest, Hungary, May 2015
Ferenc Török Memorial Lecture,
"Large Scale Exact Quantum Dynamics Calculations: One Hundred Thousand Quantum States of Benzene"

Computational Talk at University of Birmingham, Birmingham, UK January 2015
Plenary Lecture,
"Quantum Mechanics Without Wavefunctions"

Workshop on Quantum Trajectories/Hydrodynamics, Aston University, January 2015
Birmingham, UK, **Plenary Lecture,**
"Quantum Mechanics Without Wavefunctions"
http://www.nerukh.aston.ac.uk/trajectories/index.html

Department of Chemistry, Leeds University, Leeds, UK January 2015
"Quantum Mechanics Without Wavefunctions"

Department of Chemistry, University of Houston, Houston, TX — October 2014
"250,000 Quantum States of Benzene: Massive parallelization and the classical phase space picture"

National Science Foundation Center Seminar, Texas Southern University, Houston, TX, — October 2014
"Large Scale Exact Quantum Dynamics Calculations: massive parallelization and the classical phase space picture"

4th Workshop on High Dimensional Quantum Dynamics: Challenges and Opportunities, Mittelwihr, France. — September 2014
"Toward Thirty Thousand Quantum States of Benzene"

American Chemical Society National Meeting, San Francisco, CA — August 2014
"Toward Thirty Thousand Quantum States of Benzene"

Telluride Workshop on Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems — July 2017
"Thirty Thousand Quantum States of Benzene"

CECAM Meeting on Recent Progress on Adiabatic and Non-adiabatic Methods in Quantum Dynamics, Lausanne, Switzerland — May 2014
"Trajectory-based Theory of Relativistic Quantum Particles"

NASA SO2 Group, University of Maryland, College Park, MD — May 2014
"Sulfur Mass Independent Fractionation: How quantum dynamics answer fundamental questions about the origins of life"

Center for Chemical Biology at Texas Tech University, Lubbock, TX — April 2014
"Sulfur Mass Independent Fractionation (S-MIF): How quantum dynamics Will answer fundamental questions about the origins of life

Department of Chemistry, Queen's University, Kingston, Ontario — February 2014
"Quantum Dynamics of Hydrogen Interacting Exohedrally with Single-Walled Carbon Nanotubes"

Telluride Workshop on New Challenges for Theory in Chemical Dynamics — January 2014
"Ten Thousand Quantum States of Acetonitrile"

FQXi Conference on the Physics of Information, Vieques, Puerto Rico — January 2014
"How to Construct a Viable Single-Particle Theory of Relativistic Quantum Mechanics"

American Chemical Society Southwest Regional Meeting, Waco, TX — November 2013
"Ten Thousand Quantum States of Acetonitrile"

29th Waterloo Chemical Physics Symposium, Waterloo, Ontario — November 2013
"Ten Thousand Quantum States of Acetonitrile"

EmQM13 Conference on Emergent Quantum Mechanics — October 2013
Plenary Lecture, Austrian Academy of Sciences, Vienna, Austria
"Trajectory Based Theory of Relativistic Quantum Particles"
http://www.emqm13.org/abstracts/

Department of Physics, Texas Tech University — September 2013
"Trajectory Based Theory of Relativistic Quantum Particles"

Telluride Workshop on Quantum Trajectories: Foundations and Future — July 2013
"Trajectory Based Theory of Relativistic Quantum Particles"

CECAM Workshop on Many-Dimensional Quantum Dynamics with (non) Classical Trajectories, — June 2013
"Exact Quantum Dynamics Calculations Using Phase Space Wavelets"

BIRS Workshop on Mathematical Methods in Quantum Molecular Dynamics — May 2013

"Exact Quantum Dynamics Calculations using Phase Space Wavelets"

Department Mathematics & Statistics, Texas Tech University — February 2012
"Quantum Mechanics Without Wavefunctions" (delivered by Jeremy Schiff)

Department of Physics, Texas Tech University — January 2012
"Quantum Mechanics Without Wavefunctions"

Dept. of Math and Computer Science, Weizmann Institute, Rehovot, Israel — January 2012
"Quantum Mechanics Without Wavefunctions" (delivered by Jeremy Schiff)

Dept. of Atomic, Molecular, and Cluster Physics, CSIC, Madrid, Spain — December 2011
"Quantum Mechanics Without Wavefunctions"

CTMM, Montpellier II University, France — November 2011
"Quantum Dynamics of Hydrogen Interacting Exohedrally with Single-walled Carbon Nanotubes."

Rehovot Symposium on Quantum-Classical Dynamics — November 2011
"Quantum Mechanics Without Wavefunctions I" (**Plenary Lecture)**
"Quantum Mechanics Without Wavefunctions II" (delivered by Jeremy Schiff)

Madrid Workshop on Open Quantum Systems — October 2011
"Classical-like Trajectory Simulation of Quantum Cumulative Reaction Probabilities" (delivered by Gerard Parlant)

Santa Fe Workshop on Quantum Reactive Scattering — July 2011
"Massive Parallelization of Exact Quantum Dynamics Calculations"

NASA/NSF Workshop on Mass-Independent Fractionation of Sulfur Isotopes — June 2011
"Massively Parallel Quantum Dynamics Codes"

Bordeaux Symposium on Molecular Beams — May 2011
"Trajectories-only Computation of Quantum Cumulative Reaction Probabilities" (delivered by Gerard Parlant)

Computational Science Seminar, Texas Tech University — February 2011
"Exact Quantum Dynamics Calculations of Rovibrational Spectra Using Massively Parallel Computers." (delivered by Corey Petty)

Department of Chemistry, Marquette University, Milwaukee, WI — February 2011
"Quantum Dynamics of Hydrogen Interacting Exohedrally with Single-walled Carbon Nanotubes."

Department of Chemistry, New Mexico State University, Las Cruces — January 2011
"Quantum Dynamics of Hydrogen Interacting Exohedrally with Single-walled Carbon Nanotubes."

CECAM Workshop on Adiabatic and Nonadiabatic Methods in Quantum Dynamics, — November 2010
"Classical Bipolar Trajectory Surface Hopping"

International Workshop on Scattering of Atoms and Molecules from Surfaces — October 2010
"Quantum Dynamics of Hydrogen Interacting Exohedrally with Single-walled Carbon Nanotubes"

Department of Chemistry, Weizmann Institute, Rehovot, Israel — October 2010
"Various Aspects of Unipolar and Bipolar Complex Quantum Trajectories"

14th International Workshop on Quantum Atomic and Molecular Tunneling in Solids and Other Condensed Phases, Darmstadt , Germany — September 2010
"Quantum Dynamics of Hydrogen Interacting Exohedrally with Single-walled Carbon Nanotubes"

CCP6 Workshop on Quantum Trajectories — July 2010
"Bohmian Mechanics Without Pilot Waves"

"The Bipolar Reaction Path Hamiltonian (BRPH) Approach for Multi-dimensional Reactive Scattering Systems."(delivered by Jeremy Maddox)

Mesilla Workshop on Electronic Non-Adiabatic Dynamics — February 2010
"Classical Bipolar Trajectory Surface Hopping"

Nanoscience Center, University of South Carolina, Columbia — January 2010
"Quantum Dynamics of Hydrogen Interacting Exohedrally with Single-walled Carbon Nanotubes."

Telluride Workshop on New Challenges for Theory in Chemical Dynamics — January 2010
"Bipolar Quantum Trajectory Simulations."

Canadian Society of Chemistry Meeting (national) — June 2009
"Bipolar Bohmian Mechanics: An overview."

Conference on Computational Molecular Structure and Dynamics (Wyatt 70th) — January 2009
"Bipolar Quantum Trajectory Methods."

Department of Chemistry, University of Texas, Austin (Wyatt group) — November 2008
"Latest Developments in Bipolar Quantum Trajectory Methodologies."

Naval Research Laboratories, Washington, DC — October 2008
"Bipolar Quantum Trajectory Simulations: The bipolar derivative propagation method (BDPM) for calculating stationary states of high-dimensional reactive scattering systems." (delivered by Jeremy Maddox)

CCP6 Workshop on Multidimensional Quantum Mech. with Trajectories — September 2008
"Bipolar Quantum Trajectory Simulations: Trajectory Surface Hopping and Path Integral Monte Carlo."

Department of Chemistry, Texas Tech University — August 2008
"Even Newer Methods in Quantum Dynamics, Molecular Applications, and Experimental Validation."

New Mexico Workshop on Quantum Trajectories — July 2008
"Bipolar Quantum Wavepacket Dynamics for Multidimensional Systems."
"Bipolar Quantum Trajectory Dynamics." (delivered by Gérard Parlant)

Department of Chemistry, Marne-la-Vallée University, France — June 2008
"Bohmian Mechanics and Bipolar Quantum Trajectory Methods."

Department of Chemistry, Paul Sabatier University, Toulouse, France — June 2008
"New Methods in Quantum Dynamics, and Molecular Applications"

LSDMSS, Montpellier II University, France — May 2008
"Quantum Dynamics on Massively Parallel Supercomputers: Methods and Applications."

Southwest France Dynamics Days Colloquium (JDSO) — May 2008
"Bipolar Quantum Trajectory Methods: Wavepacket Dynamics"
"Bipolar Quantum Trajectory Methods: Analytical Solutions" (delivered by Toufik Djama)

Department of Physics, Texas Southern University, Houston — April 2008
"Bohmian Mechanics and Multipolar Quantum Trajectory Methods."

American Chemical Society Southwest Regional Meeting — November 2007
Southwest Theoretical and Computational Chemistry Symposium
"Multipolar Quantum Trajectory Methods."

Department of Chemistry, University of New Mexico, Albuquerque — October 2007
"New Methods in Quantum Dynamics, and Molecular Applications"

Summer School in Chemical Dynamics, Presqu'ile de Giens, France — September 2007
"Wavelet Approach"
"Semiclassical Mechanics"

"Bipolar Quantum Trajectory Methods" (tutored project)

Safed Workshop on the Quantum World in Real Time — June 2007
"Multipolar Quantum Trajectory Methods: Wavepacket, Multisurface and Multidimensional Dynamics"

Department of Chemistry, Weizmann Institute, Rehovot, Israel — June 2007

Questers, Texas Tech University, Lubbock — January 2007
"Einstein's Brain: Understanding Special Relativity."

Austin Workshop on Trajectory Methods in Quantum Dynamics — December 2006
"Multipolar Quantum Trajectory Methods: Wavepacket, Multisurface, and Multidimensional Dynamics"

Third Feynman Festival — August 2006
"Multipolar Quantum Trajectory Methods"

Madrid Workshop on Bohmian Mechanics — May 2006
"Multipolar Quantum Trajectory Methods"

Department of Chemistry, Baylor University — February 2006
"New Methods in Quantum Dynamics, and Molecular Applications"

Department of Chemistry, Texas Tech University — August 2005
"New Methods in Quantum Dynamics, and Molecular Applications"

Sandia National Laboratories — July 2005
"New Computational Methods in Quantum Dynamics, and Molecular Applications"

Canadian Society of Chemistry Meeting (national) — May 2005
"Exact Quantum Dynamics Using Classical Trajectories"

Paris Workshop on Quantum Dynamics of Complex Molecular Systems — May 2005
"Exact Quantum Dynamics Using Classical Trajectories"

Mesilla Workshop on Tex-Mex Theoretical and Computational Chemistry — April 2005
"Exact Quantum Dynamics Using Classical Trajectories"

Department of Chemistry, University of Texas, Austin — March 2005
"Exact Quantum Dynamics Using Classical Trajectories"

Department of Chemistry, University of Houston, Houston — March 2005
"Exact Quantum Dynamics Using Classical Trajectories"

Department of Chemistry, Concordia University, Montreal — March 2005
"New Methods in Quantum Dynamics, and Molecular Applications"

LANL Center for Nonlinear Studies Workshop — July 2004
Quantum and Semiclassical Molecular Dynamics of Molecular Nanoclusters
"Reconciling Semiclassical and Bohmian Mechanics."

Canadian Symposium on Theoretical Chemistry — July 2004
"Reconciling Semiclassical and Bohmian Mechanics."

Argonne National Laboratories (delivered by Dr. Wenwu Chen) — June 2004
"Parallel Implementation of the OSB Package,"
"Chemical Applications of the OSB Package."

Department of Physics, Texas Tech University — April 2004
"Reconciling Semiclassical and Bohmian Mechanics."

Mini-Meeting on Quantum Trajectories — March 2004
"Reconciling Semiclassical and Bohmian Mechanics."

Department of Chemistry, University of Chicago — June 2003
"Phase Space Optimized Wilson-Daubechies Wavelets in Quantum Dynamics Calculations."

Argonne National Laboratories — June 2003
"Parallel Calculations in Cartesian Coordinates,"
"Rovibrational Symmetry Adapted Lanczos,"
"Optimal Separable Basis Plus Wyatt Preconditioning."

American Chemical Society Meeting (National) — March 2003
"Using Optimized Preconditioning to Greatly Reduce the Number of Iterations for Quantum Calculations at High Energies."

Department of Computer Science, Texas Tech University — October 2002
"Using Optimized Preconditioning to Greatly Improve Performance of Quantum Calculations at High Energies."

CECAM Workshop on Quantum Dynamics — September 2002
"Phase Space Optimized Wilson-Daubechies Wavelets in Quantum Dynamics Calculations."

Department of Chemistry, University of Chicago — August 2002
"Using Optimized Preconditioning to Greatly Improve Performance of Quantum Calculations at High Energies."

Chemistry Division, Argonne National Laboratory — August 2002
"Using Optimized Preconditioning to Greatly Improve Performance of Quantum Calculations at High Energies."

Department of Physics, Texas Tech University — September 2001
"A Simple Classical Picture for Optimizing Quantum Calculations for Small Molecules."

Department of Chemistry, Texas Tech University — November 2000
"A Simple Classical Picture for Optimizing Quantum Calculations for Small Molecules."

Chemistry Division, Argonne National Laboratory — July 2000
"Optimized Preconditioning in Quantum Green's Function Calculations."

Department of Chemistry, University of Chicago — February 2000
"Quasiclassical Phase Space Approaches for Optimizing Exact Quantum Calculations for Small Molecules."

Department of Physics, Northern Arizona University — January 2000
"A Simple Classical Picture for Optimizing Quantum Calculations for Small Molecules."

National Research Council of CANADA — August 1997
"Optimized Quantum Reactive Scattering for Three-Body Systems, as Applied to the O+HCl —> OH+Cl Reaction."

Department of Chemistry, University of Utah — August 1997
"Three-body Quantum Reactive Scattering via Coriolis Coupling Minimization and Optimized Preconditioning."

Department of Chemistry, Brown University — June 1996
"Optimized Preconditioning for Quantum Reactive Scattering Calculations."

CONFERENCES:

2024 Association of Academic Physiatrists Annual Meeting (Physiatry '24), Orlando, FL (contributed poster, with physician colleagues, addressing my long covid experiences).

2024 Mesilla Workshop in honor of Bill Hase, Mesilla, NM (**invited lecture**).

2023 Southwest Regional ACS Meeting, Stillwater, OK (poster, by student).

2023 Physics Dept. Student Poster Competition, TTU, Lubbock, TX (poster, by student).

2023 TACCSTER 2023 Symposium for Texas Researchers, Austin, TX (contributed lecture and poster, delivered by post-doc).

2023 Quantum Effects in Gravitational Fields, Leipzig University, Germany (contributed poster, by student).

2023 National Spring APS Meeting, virtual (contributed lecture, delivered by colleague).

2023 Royal Society of Chemistry Poster Twitter Conference, virtual (contributed lecture, delivered by post-doc).

2023 28th Austin Symposium on Molecular Structure and Dynamics, Southern Methodist University, Dallas, TX (**invited lecture**).

2022 November Mini-mini-symposium on Quantum Trajectories, TTU, Lubbock, Texas (two contributed lectures by colleagues, one contributed lecture by student).

2022 TTU TrUE Symposium, Lubbock, TX (contributed lecture, by student).

2022 Defense TechConnect Innovation Summit, Washington, DC (invited poster).

2022 QRS workshop, Balatonfõldvar, Hungary, **invited lecture** (delivered by post-doc).

2022 Departmental Graduate Poster Competition, TTU, Lubbock, TX (**best poster physical division**, by student).

2022 Vibrational Spectroscopy Gordon Research Conference, Smithfield, Rhode Island (**invited lecture**, not delivered due to COVID).

2022 7th High-Dimensional Quantum Dynamics Conference, Groningen, The Netherlands (**invited lecture**, not delivered due to COVID).

2022 25th International Workshop on Quantum Chemistry, Physics, and Biology, Torun, Poland (**invited lecture**).

2022 ISMS, University of Illinois, Urbana-Champaign, Illinois, (contributed talk, delivered by post-doc).

2022 Telluride Workshop on Floppy Molecular Systems, Telluride, CO, (**invited lecture**).

2022 Mini-Symposium on Quantum Trajectories, TTU, Lubbock, TX (contributed lecture, two contributed lectures delivered by colleagues, contributed lecture delivered by post-doc, two contributed lectures delivered by students).

2022 QAMTS workshop, Calgary, Canada (**invited lecture**, two contributed lectures delivered by student and post-doc).

2022 Joint Mathematics Meeting of the AMS, virtual (contributed lecture, by student).

2021 Midwest Relativity Meeting, Urbana-Champaign, IL (contributed lecture, by student).

2021 IUPAC Canadian Chemistry Conference, Toronto, Canada, virtual (**invited lecture**, delivered by post-doc).

2021 National Summer APS Meeting, virtual (poster, by student).

2021 ACS National Meeting, virtual (**invited lecture**).

2021 National Spring APS Meeting, virtual (poster, delivered by colleague).

2021 AMS Spring Eastern Section Meeting, Providence, RI (contributed lecture, by student).

2021 Tensor Product Methods for Strongly Correlated Molecular Systems, MPIPKS, Dresden, Germany, virtual (contributed lecture).

2020 Midwest Relativity Meeting, Notre Dame, IN (contributed lecture, by student).

2020 TACCSTER 2020 Symposium for Texas Researchers, Austin, TX (contributed lecture, delivered by post-doc).

2020 TTU Workshop on Quantum Information and Quantum Computation, Lubbock, TX (**invited lecture**).

2020 Texas Section APS Meeting, Lubbock, TX (two contributed lectures, by students).

2019 MolSSI Workshop on Rovibrational Molecular Spectroscopy, Blacksburg, VA (**organizer**, invited lecture).

2019 TACCSTER 2019 Symposium for Texas Researchers, Austin, TX (one post-doc poster).

2019 Texas Section APS Meeting, Lubbock, TX (two student and post-doc posters).

2019 Southwest Theoretical and Computational Chemistry Conference, Norman, OK (invited lecture, contributed lecture by postdoc, two student and post-doc posters).

2019 Texas Quantum Institute Kickoff Meeting, College Station, TX (invited lecture).

2019 Utah Workshop on Quantum Methods in Molecular and Solid-State Theory (contributed lecture).

2019 Symmetries in Science: SiS XVIII, Bregenz, Austria (invited lecture).

2019 QRS workshop, Saitama, Japan (invited lecture).

2019 QAMTS workshop, Borovets, Bulgaria (invited lecture, session chair).

2019 US Army Research Office Contractors Meeting, Durham, NC (invited lecture, presented by postdoc).

2019 Telluride Workshop on Floppy Molecular Systems, Telluride, CO (invited lecture).

2019 International Symposium on Quantum Effects in Chemistry and Biology, Shanghai, China (invited lecture).

2019 Rice University Oil & Gas HPC Conference, Houston, TX (contributed poster, presented by postdoc).

2019 ACS National Meeting, Orlando, FL (contributed lecture, presented by postdoc).

2019 Advances in Hydrogen Molecular Ions H_3^+, H_5^+ and Beyond, London UK (participant, panelist).

2018 Welch Conference, Houston, TX (invited, attend banquet).

2018 Southwest Theoretical and Computational Chemistry Conference, Edinburg, TX (**invited lecture**, contributed lecture by postdoc, two student and post-doc posters).

2018 TACCSTER 2018 Symposium for Texas Researchers, Austin, TX (four student and post-doc posters).

2018 MPIPKS Interdisciplinary Focus Workshop on Quantum and Semiclassical Trajectories (QuSeT), Dresden, Germany (**scientific coordinator, invited lecture**, plus one **invited lecture** by collaborator).

2018 Anharmonicity in Medium-Sized Molecules and Clusters (AMOC), Budapest, Hungary (**invited lecture**, one post-doc poster).

2018 27th Austin Symposium on Molecular Structure and Dynamics, Dallas, TX (**invited lecture**).

2018 Telluride Workshop on New Challenges for Theory in Chemical Dynamics, Telluride, CO (**invited lecture**).

2017 Southwest Regional ACS Meeting, Lubbock, TX (**Symposium organizer,** Award committee member, Graduate recruitment fair). (contributed lecture, plus four contributed lectures by postdocs and collaborators).

2017 STEM Across Continents Workshop, Lubbock, TX (**invited lecture**).

2017 Telluride Workshop on Floppy Molecular Systems, Telluride, CO (**invited lecture**).

2017 High Resolution Molecular Spectroscopy, Helsinki, Finland (poster).

2017 MOLIM Workshop on Time dependent Methods, ETH Zurich, Switzerland (**invited lecture**).

2016 Southwest Regional ACS Meeting, Galveston, TX (**invited lecture**, Graduate recruitment fair, session chair).

2016 STEM Across Continents Workshop, Lubbock, TX (**invited lecture**).

2016 Telluride Workshop on Sulfur Mass-Independent Fractionation, Telluride, CO (**organizer**).

2016 John C. Light Symposium, University of Chicago, Chicago, IL (invited participant).

2016 ACS National Meeting, San Diego, CA (graduate recruitment fair, council meeting).

2016 26th Austin Symposium on Molecular Structure and Dynamics, Dallas, TX (**invited lecture**, one post-doc poster).

2016 BIRS Workshop on Exploiting New Advances in Mathematics to Improve Calculations in Quantum Molecular Dynamics, Banff, Alberta (**invited lecture**).

2016 Telluride Workshop on New Challenges for Theory in Chemical Dynamics, Telluride, CO (**invited lecture**).

2015 Pacifichem 2015, Advances in Quantum Dynamics from Spectroscopy to Dynamics, and ab initio Potentials in High Dimensional Systems, Honolulu, Hawaii, (**invited lecture**).

2015 Pacifichem 2015, New Insights from Quantum Dynamics, Honolulu, Hawaii, (**invited lecture**).

2015 EmQM15 Conference, on Symposium on Quantum Mechanics, Technical University in Vienna Austria, (**invited lecture**).

2015 International Workshop on Martin Gutzwiller's Scientific Universe: From Wavefunctions Over Periodic Orbits to Sun, Moon and Earth. Max Planck, Dresden, Germany, (participant).

2015 ACS National Meeting Boston, MA (graduate recruitment fair, council meeting).

2015 Mini-conference on Misconceptions in Physics and Cosmology; University of California, Berkeley, CA, (**Plenary Lecture**).

2015 Mathematical Methods in Quantum Molecular Dynamics, Oberwolfach, Germany, (**invited lecture**).

2015 QAMTS workshop, Beatenberg, Switzerland, (**invited lecture,** session chair).

2015 Bohmian Mechanics and Hydrodynamics Nonlinearity and Complexity workshop, Astor University, Birmingham, UK (**Plenary lecture**).

2014 Welch Conference, Houston, TX (invited, attend banquet).

2014 Gulf Coast Undergraduate Research Symposium, Houston, TX (session chair, judge, contributed lecture by Joe Ellis, Eric Sikma, undergraduates).

2014 ACS National Meeting, San Francisco, CA (**invited lecture**, graduate recruitment fair, council meeting).

2014 Telluride Workshop on Floppy Molecular Systems, Telluride, CO (**invited lecture**).

2014 4th Workshop on High Dimensional Quantum Dynamics, Mittelwihr, France (**contributed lecture**).

2014 Workshop on Nanotechnology Applied to Clean and Renewable Energy, Rio de Janeiro, Brazil (**invited lecture**, graduate recruiting).

2014 Telluride Workshop on New Challenges for Theory in Chemical Dynamics, Telluride, CO (**invited lecture**).

2014 FQXi Conference on the Physics of Information, Vieques, Puerto Rico (**invited lecture**).

2013 Southwest Regional ACS Meeting, Waco, TX (**invited lecture**, contributed lecture by postdoc, two student posters, graduate recruitment fair, governance meeting).

2013 Chemical Physics Symposium, Waterloo, Ontario (**invited lecture**).

2013 EmQM13 Conference on Emergent Quantum Mechanics, **Austrian Academy of Sciences**,Vienna, Austria (**plenary lecture,** Nobel Laureate keynote speaker).

2013 ACS National Meeting, Indianapolis, IN (**contributed lecture**, graduate recruitment fair, council meeting).

2013 Telluride Workshop on Quantum Trajectories, Telluride, CO (**invited lecture**, two contributed lectures by postdoc and student).

2013 CECAM Workshop on Many-Dimensional Quantum Dynamics with (non)Classical Trajectories, Lausanne, Switzerland (**invited lecture**).

2013 Ohio State University International Symposium on Molecular Spectroscopy, Columbus, OH (contributed lecture by student).

2013 BIRS Workshop on Mathematical Methods in Quantum Molecular Dynamics, Banff, Alberta (**invited lecture**).

2013 ACS National Meeting, New Orleans, LA (graduate recruitment fair, council meeting).

2013 Western Spectroscopy Association Conference, Asilomar, CA (student poster).

2012 Texas Section APS Meeting, Lubbock, TX (**contributed lecture** by postdoc, one student poster).

2012 Southwest Theoretical Chemistry Conference, College Station, TX (**contributed lecture**, one student poster).

2012 Workshop on Quantum Atomic and Molecular Tunneling in Solids and Other Condensed Phases, Santa Fe, New Mexico (**organizer,** two student posters).

2012 ACS National Meeting, San Diego, CA (**contributed lecture** delivered by Jeremy Maddox, graduate recruitment fair, council meeting).

2011 One-day Symposium on Quantum-Classical Dynamics, Rehovot, Israel [**two invited lectures (one plenary)**].

2011 Southwest Theoretical Chemistry Conference, Lubbock, TX (one poster by student and postdoc).

2011 EUROMAT Meeting, Montpellier, France (**contributed lecture**).

2011 11th International Workshop on Quantum Reactive Scattering, Sante Fe, New Mexico (**invited lecture**, student poster).

2011 Joint NASA/NSF Workshop: "Origins, Carriers, and Implications of Mass-Independent Fractionation of Sulfur Isotopes," Washington, DC (**organizer, invited lecture**).

2011 ACS National Meeting, Anaheim, CA (graduate recruitment fair, council meeting, **panel member**).

2010 CECAM Workshop on Adiabatic and Nonadiabatic Methods in Quantum Dynamics, Lausanne, Switzerland (**invited lecture**).

2010 International Workshop on Scattering of Atoms and Molecules from Surfaces, Rehovot, Israel (**invited lecture**).

2010 Workshop on Quantum Atomic and Molecular Tunneling in Solids and Other Condensed Phases, Darmstadt, Germany (**invited lecture**).

2010 NSF Exploratory Workshop on Scientific Software Innovation Institutes, Arlington, VA (**invited participant**).

2010 CCP6 Workshop on Quantum Trajectories, Bangor, Wales (**invited lecture**).

2010 ACS National Meeting, San Francisco, CA (postdoctoral poster, graduate recruitment fair, council meeting).

2010 Mesilla Workshop on Electronic Non-Adiabatic Dynamics, Mesilla, NM (**invited lecture**).

2010 Telluride Workshop on New Challenges for Theory in Chemical Dynamics, Telluride, CO (**invited lecture**).

2009 Southwest Theoretical Chemistry Conference, Houston, TX (**contributed lecture** by student, poster judge).

2009 ACS National Meeting, Washington, DC (graduate recruitment fair, council meeting).

2009 CSC Symposium on Quantum Chemical Dynamics, Hamilton, Ontario (**invited lecture**).

2009 ACS National Meeting, Salt Lake City, UT (**contributed lecture**, graduate recruitment fair, council meeting).

2009 IMA Workshop: Chemical Dynamics, Minneapolis, MN (invited participant).

2009 Computational Molecular Structure and Dynamics, Austin, TX (**invited lecture**).

2008 1st ACS Workshop for Postdoctoral Scholars, Clemson, SC (invited postdoctoral attendee).

2008 Southwest Theoretical Chemistry Conference, El Paso, TX (**contributed lecture**, one **contributed lecture** by student, and one poster by postdoc).

2008 Southwest Regional ACS Meeting, Little Rock, AR (student poster, graduate recruiting).

2008 CCP6 Workshop on Multidimensional Quantum Mechanics with Trajectories, Leeds, UK (**invited lecture** and **invited publication**).

2008 New Mexico Workshop on Quantum Trajectories, Los Alamos, NM (**organizer**). (two **invited lectures** and three postdoctoral and student posters).

2008 American Conference on Theoretical Chemistry, Chicago, IL (postdoctoral poster).

2008 Southwest France Dynamics Days Colloquium (JDSO), Montpellier, France (two **invited lectures**, one by student, and one poster by colleague).

2008 ACS National Meeting, New Orleans, LA (graduate recruitment fair).

2007 Southwest Regional ACS Meeting, Lubbock, TX (**Symposium organizer**). (three **contributed lectures** and one poster, by students and postdocs).

2007 Welch Foundation Meeting and Awards Banquet, Houston, TX (**invited participant**).

2007 Summer School in Chemical Dynamics, Presqu'ile de Giens, France (**invited instructor**).

2007 Dynamics of Molecular Collisions Conference, Santa Fe, NM (student poster).

2007 Safed Workshop on the Quantum World in Real Time, Safed, Israel (**invited lecture**).

2006 Austin Workshop on Bohmian Mechanics, Austin, TX (**invited lecture**).

2006 Southwest Theoretical Chemistry Conference, Austin, TX (three student and postdoctoral **contributed lectures**).

2006 Southwest Regional ACS Meeting, Houston, TX.

2006 Symposium to Honor Purnendu K. "Sandy" Dasgupta, Lubbock, TX (**organizer**).

2006 Third Feynman Festival, College Park, MD (**invited lecture**).

2006 Madrid Workshop on Bohmian Mechanics, Madrid, Spain (**invited lecture**).

2006 ACS Leaders Conference, Baltimore, MD (**invited attendee**).

2005 CSC Symposium on Illuminating Chemistry, Saskatoon, Saskatchewan (**invited lecture**).

2005 Paris Workshop on Quantum Dynamics, Paris, France (**invited lecture**).

2005 Mesilla Workshop on Tex-Mex Chemistry, Mesilla, NM (**invited lecture**).

2004 Southwest Theoretical Chemistry Conference, Galveston, TX (**contributed lecture**). (four student and postdoctoral posters).

2004 Oklahoma Supercomputing Symposium, Norman, OK (postdoctoral poster).

2004 Canadian Symposium on Theoretical Chemistry, Sainte Adèle, Quebec (**invited lecture**).

2004 LANL CNLS Workshop on Molecular Nanoclusters, Los Alamos, NM (**invited lecture**). (one postdoctoral **contributed lecture**).

2004 54th Meeting of Nobel Laureates and Students, Lindau, Germany (invited student attendee).

2004 Mini-Meeting on Quantum Trajectories, Austin, TX (**invited lecture**).

2004 SIAM Conference on Parallel Processing and Scientific Computation, San Francisco, CA.

2003 Southwest Theoretical Chemistry Conference, Lubbock, TX (**Conference Organizer**).

2003 Regional American Physical Society Meeting, Lubbock, TX

2003 Nat'l ACS Session on Iterative Methods in Chemistry, New Orleans, LA (**invited lecture**).

2002 Southwest Theoretical Chemistry Conference, Houston, TX (**contributed lecture**).

2002 CECAM Workshop on Quantum Dynamics, Lyons, France (**invited lecture**).

2002 Gordon Research Conference, Atomic and Molecular Interactions, Bristol, RI (poster).

2002 Student Research Conference, Portales, NM (poster by Jason Montgomery).

2001 Southwest Theoretical Chemistry Conference, El Paso, TX (**contributed lecture**).

2001 84th Canadian Society of Chemistry Conference, Montreal, CA.

2001 Chemical Dynamics Symposium, Berkeley, CA (**invited poster**).

2000 Chemical Physics Symposium, Waterloo, Ontario (poster, **contributed lecture**).

2000 PRAHA 2000: 16th International Conference on High Resolution Molecular Spectroscopy, Prague, Czech Republic (**contributed lecture**).

2000 Gordon Research Conference, Atomic and Molecular Interactions, New London, NH, **Vice Chairman's Award for Best Poster Presentation**.

1999 Dynamics of Molecular Collisions Conference, Lake Harmony, PA (poster).

1999 Gordon Research Conf., Dyn. of Simple Systems, Newport, RI (poster).

1999 SIAM Sparse 99: International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Industrial Applications, Minn., MN (poster).

1999 Midwest Theoretical Chemistry Conference, South Bend, IN (poster).

1998 Faraday Discussion 110, Royal Soc. of Chem., St. Andrews, UK (poster).

1997 Dynamics of Molecular Collisions Conference, Brainerd, MN (poster).

1997 West Coast Theoretical Chemistry Conference, Berkeley, CA.

1997 American Chemical Society Meeting, San Francisco, CA (poster).

1996 American Conference on Theoretical Chemistry, Park City, UT (poster).

1996 West Coast Theoretical Chemistry Conference, Las Vegas, NV (poster).

1995 Dynamics of Molecular Collisions Conference, Asilomar, CA (poster).

TEACHING EXPERIENCE:

Guest Professor–Eötvös Loránd University Spring 2017
CHEM 5104 Time Dependent Quantum Dynamics

Assistant, Associate and Full Professor—Texas Tech University, Dept. of Chemistry and Biochemistry (assistant professor from fall, 2001; tenured associate from fall, 2006; full professor from fall, 2009).

For all courses taught to date except CHEM 1107: performed all lectures, office hours, review sessions, homework, exams, proctoring, and (except for CHEM 1307 and 3307) discussion sections and grading.

Undergraduate Courses:
CHEM 1107, Principles of Chemistry Laboratory I 2 semesters

CHEM 1307, Principles of Chemistry I	2 semesters
CHEM 3307/5340, Physical Chemistry I	20 semesters

Graduate Courses:

CHEM 5010/5104, Time-Dependent Quantum Dynamics	3 semesters
CHEM 5344/5104, Chemical Kinetics	8 semesters
CHEM 5345, Molecular Spectroscopy	6 semesters
CHEM 5346, Statistical Mechanics	6 semesters
CHEM 5101/5102, Graduate Seminar	7 semesters

Student Mentoring:

CHEM 3000, Undergraduate Research	8 semesters
CHEM 4300, Undergraduate Research	4 semesters
CHEM 7000, Graduate Research	45 semesters
CHEM 6000, Master's Thesis	9 semesters
CHEM 8000, Doctoral Dissertation	31 semesters
PHYS 6000, Master's Thesis	1 semesters
PHYS 7000, Graduate Research	15 semesters
PHYS 8000, Doctoral Dissertation	9 semesters

Graduate Student Instructor (GSI)—UC Berkeley Physics Department:

20 hrs./wk.: discussion and reading sections., labs, office hours, review sessions, grading of homework, labs, and exams.

Physics 8A, Mechanics, Waves, and Electrostatics, **Head GSI**	Fall 1993
Physics 7A, Mechanics and Wave Motion for Engineers	Spring 1993
Physics 8A, Mechanics, Waves, and Electrostatics	Fall 1992
Physics 21, Physics of Music	Spring 1991
Physics 7B, Heat, Electricity, and Magnetism for Engineers	Fall 1990

Upper division physical chemistry tutor—UC Berkeley, 1990-1991.

Computer science teaching assistant—Introductory CS, Brown University, 1986-1987.

Undergraduate physics and chemistry tutor—Brown University, 1985-1986.

STUDENTS AND POSTDOCTORAL FELLOWS:

Student Involvement for Non-Research Projects:

Jason Ostermann, Greg Whigham, Sean Peterson, Chris Fielder, Manish Kumar, Jeffrey Ho, Glenn Geron, Srirangam Addepalli, Shravan Vurputoor, Aditya Akula, Jagadeesh Chitikesi, Hao Tang, Dylan Drake-Wilhelm, Hui Li, Yiyi Wei, Walter Wever, Kayla Mendoza, Mingying Xue, Kristy Peck, James Green, Drew Brandon, Joseph Ellis, Robert Lord, Brandon Watson, Yinglei Pu, Ryan Merritt, Megan Gonzalez, Jayani Silva, Sofia Salazar-Miralles

Undergraduate Students Supervised for Research Projects:

Diego Garcia, Department of Physics

Tessa Hoang, Department of Chemistry — May 2022 to December 2022
"A 2-D Potential Energy Surface study of the Dynamical Rotation of the Dihydrogen Ligand in the $[FeH(H_2)(PEtPh_2)^3]^+$ Coordination Complex."
(U. Penn. Graduate School in Chemistry)

Torrey Stubblefield, Department of Chemistry — May 2022 to December 2022
"Using Crystal Code to Create a Potential Energy Surface for Methylene Imine."

Nyandwi Ngembo, Department of Chemistry — January 2022 to May 2022
"Computational Studies in Quantum Dynamics."

Litzy Guevara, Department of Chemistry — June 2021 to May 2022

"Study of the Rotational dynamics of H_2 in the $FeH_3(PH_3)_4$ complex."
(Brown University Graduate School in Chemical and Environmental Engineering)

Jacob Pittman, Department of Chemistry September 2020 to May 2021
"Relativistic Quantum Mechanics."

Colin Guilbeau, Department of Chemistry September 2020 to December 2020
"Potential Energy Surfaces for Kubas Coordination Complexes."

Joseph/Joanna Ellis, Department of Chemistry June 2013 to May 2015
"Rovibrational bound state calculations of sulfer dioxide isotopologues using ***ScalIT***"
Presented at Gulf Coast Undergraduate Research Symposium
Springborn Fellowship at University of Illinois, Urbana-Champaign

Emily Powell, Department of Chemistry June 2011 to August 2011
Outstanding Performance in Physical Chemistry Award, Texas Tech University

Drew Brandon, Department of Chemistry June 2010 to August 2010
Top Graduating Senior Award, Lubbock Christian University

Karl Gillenwater, Department of Chemistry January 2010 to December 2010
"Harmonic Motion."

Matthew Reyes, Department of Chemistry January 2007 to May 2007
"Numerical Investigation of Chlorine Ion Collision with Methyl Chloride
by the Counter-Propagating Wave Method."
4.0 GPA, Dean's List

Nick Miersma, Department of Chemistry September 2004 to December 2004
"Quantum and Classical Trajectory Methods for Scattering Calculations."

<u>Graduate Students Supervised and Degree Programs:</u>

Jhonatas Carvalho, Doctoral Candidate, Department of Chemistry

Brandon Palomo, Masters Candidate, Department of Physics

Seyyed Mahdi Aarabi, Doctoral Candidate, Department of Chemistry

Maik Reddiger, Doctoral Degree, Department of Physics December 2022
"Towards a Probabilistic Foundation for Non-Relativistic and Relativistic Quantum Theory"
David Howe Graduate Fellowship
(Scientific Associate, Anhalt University of Applied Sciences, Germany)

Bhumika Jayee, Doctoral Degree, Department of Chemistry August 2022
"Theoretical Study of Functionalized Carbon-Based Materials and Chemical Dynamics Simulations."

Maik Reddiger, Master's Degree, Non-Thesis, Department of Physics May 2020

Debojyoti Das, Master's Degree, Department of Chemistry December 2020
"Calculations and Labeling of Ro-Vibrational Eigenstates of H_3^+ Ion using ScalIT."
Provost Fellowship

Ankit Pandey, Doctoral Degree, Department of Chemistry, Chancellor's Fellowship May 2020
"Crystal: An Algorithm to Find and Plug "Holes" in Potential Energy Surfaces"

Ankit Pandey, Master's Degree, Department of Chemistry May 2018
"Using wavelets to compute the vibrational states of $OCHCO^+$"

Chaowen Guo, Doctoral Degree, Department of Chemistry May 2017
"Quantum Reactive Scattering Quantities in Molecular Physics:
New computational approaches based on quantum trajectories."
Provost Fellowship
(Postdoctoral Fellow, Texas Tech University, Lubbock, Texas)

Megan Gonzalez, Master's Degree, Department of Chemistry December 2016

"A Quantum Dynamical Study of the Dihydrogen Ligand in the $Fe(H)_2(H_2)(PEEPh_2)_3$ Coordination Complex"
Provost Fellowship
(Doctoral Degree, Department of Chemistry, Texas Tech University, May 2019)
(Staff Scientist, US Army Engineer Research and Development Center, Vicksburg, MS)

Thomas Halverson, Doctoral Degree, Department of Physics December 2015
"Exact Quantum Dynamics Calculations of Large Dimensional Molecules Using Phase Space Basis Truncation."
Provost Fellow, **Sigma Pi Sigma Physics Honor Society**, Doctoral Dissertation Fellow
(Postdoctoral Fellow, University of Waterloo, Ontario, Canada)
(Postdoctoral Fellow, University of Southern California, Los Angeles, CA)
(Applied Research Lead for Strategic Quantum Investment, Booz Allen Hamilton, Inc.)

Corey Petty, Doctoral Degree, Department of Chemistry August 2014
"Exact Quantum Dynamical Calculations of Rovibrational Spectra Using Massively Parallel Computers"
Provost Fellow
(FAPESP Fellow, Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil)
(Analyst, Novetta)
(Analyst, Booz Allen Hamilton, Dark Labs Division)
(Security and Infrastructure Lead, Status.im)

Drew Brandon, Master's Degree, Department of Chemistry December 2013
"Accurate Calculations of Rovibrational Bound States for Argon Trimer using ***ScalIT***."
(Doctoral Degree, Department of Chemistry, Texas Tech University, August 2017)
(Assistant Professor of Chemistry, Cal State University, Bakersfield, California)
(Assistant Professor of Chemistry, Clayton State University, Morrow, Georgia)

Jason McAfee, Doctoral Degree, Department of Chemistry May 2010
"Dynamics of Systems of Carbon and Hydrogen: Quantum and Classical Calculations."
2010 Song Prize Award for Best Dissertation
(Professor, Howard College, Big Spring, Texas)
(Senior Lecturer of Chemistry, University of Texas, Dallas, Texas)
(Adjunct Lecturer of Chemistry, University of North Texas, Denton, Texas)

Yingsheng Xiao, Doctoral Degree, Department of Chemistry August 2007
"Efficient Full Quantum Calculations for Small Molecules Using Novel Phase Space Optimized Discrete Variable Representation Path Integral Monte Carlo Methods."
(Software Quality Engineer at MathWorks, Inc. [creators of MATLAB])

Richard Lombardini, Doctoral Degree, Department of Physics August 2006
"Rovibrational Spectroscopy Calculations Using a Weyl-Heisenberg Wavelet Basis and Classical Phase Space Truncation."
(Assistant Professor and Chair of Physics, Greenville College, Illinois)
(Associate Professor of Physics, St. Mary's University, San Antonio, Texas)

Jason Montgomery, Master's Degree, Department of Chemistry August 2002
"Quantum Mechanical Eigenspectra Calculations of the Neon Dimer, using a Phase Space Optimized Discrete Variable Representation / Symmetry-Adapted Lanczos Method."
(Associate Professor of Chemistry, Florida Southern College, Florida)

<u>Graduate Dissertation Committees:</u>

Bright Mgbeojikwe, Doctoral Candidate, Department of Chemistry

Mengke Tielige, Doctoral Candidate, Department of Physics

Reza Amani, Ph.D., Department of Chemistry December 2022
"Solid-State NMR methods and techniques to characterize large membrane protein complexes."

Samila Muthumuni, Ph.D., Department of Physics December 2021

"Search for Dark Matter from Baryon Number Violation Process in Proton-Proton Collisions at 13 TeV." (Graduate Dean's Representative).

Kamal Lamichhane, Ph.D., Department of Physics December 2020
"Search for New Bosons in Gluon-Gluon and Vector Boson Fusion Processes at the LHC and Development of Silicon Module Assembly Techniques for the CMS High Granularity Calorimeter," (Graduate Dean's Representative).

Yuxuan Yao, Ph.D., Department of Chemistry May 2020
"Wigner Sampling, and Simulations of the Unimolecular Dissociation of the Criegee Intermediate and Intramolecular Relaxation of the N-H Bonds in Protonated Tryptophan."

Eshan Gurung, Ph.D., Department of Chemistry December 2016

James Faulkner, Ph.D., Department of Physics December 2016
"A Search for WWgamma and WZgamma Triboson Production and Anomalous Quartic Gauge Couplings at sqrt[s] = 8 and 13 TeV within the Compact Muon Solenoid."

Austin Privett, Ph.D., Department of Chemistry August 2015
"Electron nuclear dynamics: Resolution of electronic states, extension to direct Ionization, and the irradiation of biomolecules in proton cancer therapy."

Jing Xie, Ph.D., Department of Chemistry May 2015
"Direct dynamics simulation of OH-$(H_2O)_n$ + CH^{31} ion-molecule reactions in gas-phase."

Shawn Horn, Master's Degree, Department of Chemistry December 2014
"A study of the multiradical nature of graphene as affected by the total spin state, modeled by acenes and periacenes."

Daniel Dominguez, Ph.D., Department of Physics December 2014
"Next-generation optical microscope condensers."

Yingying Luan, Master's Degree, Department of Chemistry August 2012
"Desymmetrilizing Organic Molecules via Structural Functionalization."

Patrick McLaurin, Ph.D., Department of Chemistry August 2011
"New applications of the electron nuclear dynamics theory to scattering processes and chemical reactions: tool development, method validation, and computer simulation."

Walter Wever, Master's Degree, Department of Chemistry May 2011
"Chiral and Achiral N-Phosphonyl Imine Chemistry and Microwave-Assisted Reactions."

Kyoyeon Park, Ph.D., Department of Chemistry October 2010
"Developments and applications of the chemical dynamics simulations. Surface-induced dissociation, organic reaction mechanism, and non-adiabatic dynamics."

Dylan Drake-Wilhelm, Ph.D., Department of Chemistry August 2010
"The Investigation of Molecular and Kinetic Properties of H_2^+, HD^+, and $B^+(H_2)$ Through the Development of Highly Accurate Analytical Potential Energy Surfaces Built Upon High Level *ab initio* Calculations."

Srinivas Karra, Ph.D., Department of Chemical Engineering October 2009
"Modeling, Identification, and Control of Complex Systems—A New Paradigm," (Graduate Dean's Representative).

Paulo Machado, Ph.D., Department of Physics, McMaster Univ., Ontario December 2007
"Computational Approach to Bohm's Quantum Mechanics," (External Dissertation Committee Member).

Liwen Yu, Ph.D., Department of Chemistry, Univ. of North Texas, Denton March 2007
"Computational Studies on Group 14 Elements (C, Si, and Ge) in

Organometallic and Biological Compounds,"
(External Dissertation Committee Member).

Abel Diaz, Ph.D., Department of Physics — September 2006
"Using the Dynamics of Satellite Galaxies to Probe Dark Matter,"
(Graduate Dean's Representative).

Kent Chambers, Ph.D., Department of Chemistry — August 2005
"Improving Performance in First Year Chemistry."

Scott R. Franklin, Ph.D., Department of Mathematics — May 2005
"A Computational Three-field Methodology for Non-conforming Finite Elements over Partitioned Domains," (Graduate Dean's Representative).

Daniel Chang, Ph.D., Department of Chemistry — December 2002
"Quantum Dynamical Studies on an *Ab Initio* Potential Energy Surface for the Helium Trimer Ion: Rovibrational States and Helium Dimer Formation."

Thomas Baker, Master's Degree, Department of Chemistry — August 2002
"Classical and Quasiclassical Trajectory Calculations of Ozone Isotopomer Formation in $O+O_2$ collisions."

Postdoctoral Coworkers:

Dr. János Sarka (Hungarian Academy of Sciences Independent Postdoctoral Fellow, Budapest, Hungary)

Dr. Chaowen Guo

Dr. Jonathan Jerke (Quantum Galaxies Corporation, Dallas, TX)

Dr. Vince Grimes (deceased)

Dr. Praveen Kumar (staff scientist, IM Systems Group, Rockville, MD)

Dr. Hung-Ming Tsai (instructor, Physics Department, Texas Tech University, Lubbock, TX)

Dr. Benhui Yang (research associate, Physics Department, University of Georgia, Athens, GA)

Dr. Yong-Cheng Ou

Dr. Kisam Park

Prof. Jeremy Maddox (Associate Professor, Western Kentucky University, Bowling Green, KY)

Dr. Junkai Xie (system administrator, Center for Computationally Assisted Science and Technology, North Dakota State University, Fargo, ND)

Dr. Corey Trahan (staff scientist, Army Corps of Engineers, US Dept. of Defense, Vicksburg, MS).

Prof. Wenwu Chen (Professor of Civil Engineering and Mathematics, Lanzhou University, China).

Prof. Wensheng Bian (**Director of the State Key Laboratory for Molecular Sciences, Chinese Academy of Sciences, Beijing National Laboratory**).

Prof. Akbar Salam (Ollen R. Nalley Fellow, Wake Forest University, Winston-Salem, NC, also **Visiting Fellow, ITAMP, Harvard University**).

Visiting Scholars:

Prof. Attila Császár (visiting scholar, Eötvös Loránd University, Hungary)

Prof. Brett Carlson (visiting scholar, Instituto Tecnológico de Aeronáutica, Brazil)

Lucien Dupuy (visiting graduate student, Montpellier II University, France)

Prof. Richard Lombardini (visiting scholar, St. Mary's University, San Antonio, Texas)

Prof. Jia Fu (visiting scholar, Xihua University, Chengdu, Sichuan, China)

Prof. Mahir Hussein (visiting scholar, University of São Paulo, Brazil)

Dr. Jonathan Jerke, Research Faculty Professor (Collaborator)

Prof. Yohann Scribano (visiting scholar, Montpellier II University, France)

Dr. Gilbert Moultaka (visiting scholar, Montpellier II University, France)

Dr. Juergen Eckert, Research Faculty Professor (Collaborator)
Dr. Jianyi Ma (visiting scholar, University of New Mexico).
Prof. Jeremy Schiff (visiting scholar, Bar-Ilan University, Israel).
Noa Zamstein (visiting graduate student, Weizmann Institute of Science, Israel).
Dr. Gérard Parlant (visiting scholar, Montpellier II University, France).

DEPARTMENTAL AND UNIVERSITY SERVICE:

Committee Service—Department of Chemistry and Biochemistry:

Probationary Committees for Untenured Faculty
- Prof. Ruibin Liang, chair — from October 2022
- Prof. Ben Wylie, chair — October 2020 to May 2021
- Prof. Anthony Cozzolino, member — January 2020 to May 2021
- Prof. John D'Auria, member — February 2014 to August 2020
- Prof. Christopher Bradley, chair — February 2014 to August 2019
- Prof. Dmitri Pappas, member — March 2011 to August 2012

July 2007 to August 2011

Interim Chair — May 2021 to September 2022

Merit and Productivity Committee — August 2020 to May 2021

Dept. Policy Committee — August 2020 to May 2021; October 2017 to May 2018

Physical Chemistry Division Coordinator — August 2020 to May 2021

Executive Committee — (de facto) May 2021 to September 2022; August 2020 to May 2021; January 2016 to September 2017

Biochemistry Faculty Search Committee — August 2018 to April 2019

Dept. Chair Search Committee — April 2015 to October 2015

Dept. Chair Search Mechanism Committee — March 2015

Comprehensive Performance and Evaluation Committee — January 2013, 2014, 2015, 2019

Faculty Awards Committee — from August 2014

Chemistry Degree Plan Coordinator (M.S. and Ph.D.) — October 2012 to January 2018

Graduate Degree Program Assessment Subcommittee — October 2012 to January 2018

Publicity and Strategic Planning Committee — February 2012 to September 2017

Tenure and Promotion Guideline Committee — Spring 2011

Graduate Program Director, Dept. of Chemistry and Biochemistry — August 2007 to January 2018
Supervise all academic aspects of current and prospective graduate students in the dept. Organize and participate in recruiting activities, and design recruiting materials. Evaluate Applications to the graduate programs in Chemistry and Biochemistry

Graduate Affairs Committee, Chair *ex officio* — August 2007 to January 2018
Supervise all academic aspects of current and prospective graduate students in the dept. Organize and participate in recruiting activities, and design recruiting materials. Evaluate Applications to the graduate programs in Chemistry and Biochemistry

Computational Chemistry/Academic IT Support Oversight — August 2007 to May 2012

Department Affairs Committee — September 2006 to August 2007

Theory Lab Renovation Committee (ad hoc), Chair — November 2005 to June 2010
(secured $300,000 from Provost, CFO Anderes, A&S Dean Winer, and VPR Smith)

Awards Committee, Chair — September 2006 to August 2007
Member — August 2008 to August 2014
Member — August 2004 to August 2006

Chemistry Placement Exam Automation Committee — January 2003 to August 2007
Design on-line version of placement exam for large introductory chemistry classes, as well as corresponding demographic database for chemical education research, (to be used in 5000-person pilot study by ACS Exams Institute in Spring 2008).

Departmental Seminar Committee, Chair — August 2002 to August 2007

Information Technology Committee — August 2001 to August 2003

Committee Service—College of Arts and Sciences:

Center for Chemical Biology, founding member — September 2012 to September 2016

Natural and Physical Science Research Council — September 2010 to August 2014
Identify and develop research opportunities.

Dean of Arts and Sciences Advisory Committee — April 2010, Summer 2015
Review applicants for Chair of the Department of Chemistry and Biochemistry

Committee Service—Graduate School

Dean's Graduate Council — August 2013 to December 2017

Graduate Faculty Subcommittee — September 2014 to December 2017

Committee Service—Texas Tech University:

TTU Faculty Success Software Evaluation Core Committee — August 2022 to December 2022
Provost Committee to Evaluate Candidates for Dean of Arts & Sciences — May 2020
College of Engineering Faculty Search Committee, Quantum Sensing — October 2019 to May 2021
Computer Science Full Professor Promotion Committee — September 2018
TTU Ethics Advisory Committee — August 2016 to May 2021
Mentor Tech member — from August 2016
Vice-President for Research NASA Grants Committee — June 2014 to September 2017
Graduate Program Growth Initiative Committee — October 2013 to September 2015
President's Strategic Priority Committee — August 2013 to September 2015
TTU Brazilian Scientific Mobility Program Workshop (panel member) — November 2014
Provost Search Committee — Fall 2013
OP74.08 ad hoc Committee under Associate Vice President for Research Integrity — Fall 2013
Clark Scholars Program Evaluation — April 2013
Advisory Panel, Search Committee, Vice President for Research — April 2013
SACS Reaffirmation for Graduate Education — February 2013 to September 2015
Advisory Panel, Search Committee, — February 2013
Vice Provost for Graduate Affairs and Dean of the Graduate School
Vice President for Research Proposal Stimulus Program Evaluation — January 2013
Chancellor's Distinguished Research Awardee Evaluation — October 2012, 2016
National Academy of Science National Research Council — January 2007
Texas Tech University representative to assess doctoral programs.
Phi Beta Kappa Steering Committee — August 2004 to April 2007
Anti-Terrorism Task Force — September 2001

Other Service:

Presentation to TTU Vice President for Research on TTU Quantum Computing Efforts — November 2019

Special Lecture Series—TTU, Ethics Center & Health Sciences Center Fall 2017
Organized a special visit by Derek Fetzer, Director, Global Public Health, Johnson&Johnson, to discuss the CaringCrowd crowd-funding platform that he pioneered.

Texas Tech University Biochemistry Society October 2017
"Graduate School Admissions: What Biochemistry Programs are looking for."

Presentation to American Chemical Society Student Affiliates at TTU October 2016
"Applying to Graduate School"

Presentation to Brazilian High School Student Summer Camp at TTU (2x) June 2015
"The Mysteries of Quantum Mechanics"

Presentation to Graduate Dean on TTU-Brazil Agreements May 2014

Research Proposal Evaluation—TTU, Center for Chemical Biology October 2012

Seminar Series—TTU, Chemistry Department Spring 2002, 2009, 2012, 2015
Organized the Physical Chemistry Seminar series, and invited guest lecturers. Fall 2006

CheMentor Program—TTU, Chemistry Department Fall 2001
Advise, and sponsor social activities for, undergraduate chemistry majors.

Lecture Series—UC Berkeley, Chemistry Department August 1997
Organized lecture series presented by physics Prof. R. G. Littlejohn, "Gauge Theory of Rotations, Coriolis Forces, and Frame Fixing in Molecules."

Head GSI—UC Berkeley, Physics Department Fall 1993
Recruited GSIs for large (~800 students) premed physics course; organized scheduling of all labs, discussion sections, etc.; designed policies, with professors, for dealing with student grievances and grade appeals.

BROADER SERVICE:

Graduate Student Job Placement Event—Organizer April 2023
Interdisciplinary recruiting event, with industry professionals from quantum computing (Booz Allen Hamilton) and the blockchain networks field (status.im) came to TTU to meet with and recruit graduate students from the physical sciences, computer science, and engineering.

Doctoral Fellowship Reviewer—Austrian Academy of Sciences October 2019

NASA Graduate Fellowship Reviewer (8x)—FINESST
(Future Investigators in NASA Earth and Space Science and Technology) April 2019

General Member—Telluride Science Research Center (TSRC)
Strategic Plan Working Group from November 2016

College of Reviewers for the Canada Research Chairs Program—Member from January 2016
Research Proposal Evaluation November 2015

Research Proposal Evaluation—NSERC Grant November 2015

Research Proposal Evaluation—St. Mary's University Faculty Grant Program March 2015

ScalIT Training Sessions—TTU Chemistry Theory and Computation Lab
July 2012, October 2012, August 2014
Outreach program to train expert quantum dynamicists as well as non-expert users from the broader chemical dynamics community in the use of the ScalIT codes for computing rovibrational spectra of small molecules.

Academic Program External Reviewer
Eötvös Loránd University, Budapest, Hungay January 2022
East Carolina University May 2010

Graduate School Reviewer—Thomson-Reuters Survey April 2011
March 2010

Graduate School Reviewer—US News and World Report December 2009, January 2021, January 2022

Graduate Recruitment and Outreach—Visits to Texas Tech University:
- Graduate Recruiting Weekend March 2008–2011, 2013, 2015–2017
- University of Texas March 2015
- Hardin-Simmons University July 2013, May 2015
- Baylor University March 2014
- New Mexico Tech March 2014
- St Edwards University March 2014
- Texas Tech University (undergrads) November 2012
- Wayland Baptist University November 2012
- Huston-Tillotson College July 2012
- Angelo State University December 2009, August 2011, October 2017

Graduate Recruitment and Outreach—Visits in Brazil
- University of São Paulo February 2018
- Universidade do Vale do Paraiba, São José dos Campos, Brazil June 2016
- Universidade Federal de São Carlos, São Carlos, Brazil June 2016
- Instituto Technológico de Aeronáutica, São José dos Campos, Brazil June 2016
- Federal University of Rio de Janeiro, Rio de Janeiro, Brazil March 2014
- Institute of Military Engineering, Rio de Janeiro, Brazil March 2014
- Sao Paulo State Research Foundation (FAPESP), São Paolo, Brazil March 2014
- Mackenzie Presbyterian University, São Paolo, Brazil March 2014
- The National Council for Scientific and Evaluation of Graduate Education (CAPES) Brasília, Brazil March 2014

Tenure and Promotion Reviewer—National Tsing Hua University of Taiwan March 2017
- National University of Singapore May 2016
- Lamar University November 2015
- Baylor University June 2015
- U Texas Arlington October 2009

Summer Research Academy for Theoretical and Computational Chemistry— June 2012
Outreach program to expose underrepresented students from local high schools to advanced chemistry research, and to motivate them to pursue post-secondary education in science. June 2011, June 2009, June 2008

Focus Group Member—American Chemical Society Roundtable March 2008

Graduate Recruitment and Outreach—Scientific Meetings:
- American Chemical Society, National Meeting
  March 2008, 2009, August 2009, March 2010, 2011, 2012, April 2013, September 2013
  August 2014, 2015, March 2016
- American Chemical Society, Southwest Regional Meeting
  November 2007, October 2008, November 2013, November 2016, October 2017

Summer School Instructor—Chemical Dynamics, Presqu'ile de Giens September 2007

Web-based Quantum Dynamics Tutorial System:
Showcase pedagogical aspects of accurate quantum dynamics methodologies.
Web-based, Java and *Mathematica* player format, for broad dissemination, designed in collaboration with Montpellier II University, France.
funded by the National Science Foundation. August 2007 to August 2009

Lead Judge—New Mexico Northeastern Regional Science and Engineering Fair March 2019, 2021

Grand Awards Judge—INTEL International Science and Engineering Fair May 2007

American Chemical Society, South Plains Local Section (elected):
- Councilor—South Plains Local Section, American Chemical Society 2009–2016
- Chair—South Plains Local Section, American Chemical Society 2007

Chair-Elect—South Plains Local Section, American Chemical Society 2006
Secretary—South Plains Local Section, American Chemical Society 2005

Welch Summer Scholar Program—Texas Tech University, Chemistry Department June 2002
Conduct short research projects with gifted high school students from throughout Texas.

Judge—Texas Tech Graduate School Research Poster Competition March 2013, 2014, 2015
Gulf Coast Undergraduate Research Symposium, Rice University October 2014
South Plains Regional Science and Engineering Fair
March 2002, February 2003, April 2004, March 2006, February 2013

Publicity and Outreach—speaking engagements and media articles for the general public on quantum physics

FQXi podcast (11/29/2014), http://www.fqxi.org/community/podcast/2014.11.29
Houston Public Radio, https://dl.dropboxusercontent.com/u/70088177/kpft-interview.mp3
Huffington Post (PI featured blog), http://www.huffingtonpost.com/bill-poirier/quantum-weirdness-and-many-interacting-worlds_b_6143042.html
Huffington Post (article), http://www.huffingtonpost.com/2014/11/04/parallel-universes-quantum-mechanics-theory_n_6091438.html?utm_hp_ref=science
KTTZ Radio, invited interview, 60 second spot. (1/1/2018 and 1/15/2018), http://www.depts.ttu.edu/artsandsciences/Connect/ASfollowSocial.php
Multiversal Journeys, Misconceptions in Physics and Cosmology (7/9/15), https://www.youtube.com/watch?v=GrpGPkoZvlc
Multiversal Journeys, Physics of the Observer—A Documentary (9/11/17), http://www.mvjs.org/
Nature News, http://www.nature.com/news/a-quantum-world-arising-from-many-ordinary-ones-1.16213
New Scientist, http://www.newscientist.com/article/mg22429944.000-ghost-universes-kill-schrodingers-quantum-cat.html
Reddit, http://redd.it/1xxmfl
Science Daily, http://www.sciencedaily.com/releases/2014/11/141112131927.htm
Sean Carroll Blog, The Preposterous Universe (12/16/14), http://www.preposterousuniverse.com/blog/
"Stranger Things" TV show; expert consultant (8/16) http://www.livescience.com/55883-stranger-things-science-of-parallel-worlds.html
Texas Tech Discoveries, Quantum Quandary (4/6/15), http://www.depts.ttu.edu/vpr/discoveries/spring-2015/multiple-universes.php
Texas Tech Today, Department of Chemistry & Biochemistry Enjoys Record-Breaking Summer (9/29/2017), http://today.ttu.edu/posts/2017/09/chemistry-grants
Yahoo News, http://news.yahoo.com/parallel-worlds-could-explain-wacky-quantum-physics-140403032.html