

Education

2007 **Ph.D. in Chemistry**, University of Toronto, Toronto, Canada
Advisor: Prof. Paul Brumer.
Thesis title: *Coherent control of laser-induced symmetry breaking: from fundamentals to applications.*

2002 **Diploma in Theoretical Condensed Matter Physics**, The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy (1 year M.Sc.)
Advisor: Dr. Sergei Tretiak.
Thesis title: *Conformational dynamics of photoexcited conjugated molecules.* Grade: Passed with honors (highest mark)

2001 **B.Sc. in Chemistry**, National University of Colombia, Bogotá, Colombia, Summa cum Laude (5 year program)
Advisors: Profs. Victor Tapia and Edgar Daza.
Thesis title: *Atomic contributions to molecular optical activity: an approach through Atoms in Molecules theory.* Grade: Laureated (highest mark)

Professional Experience

Nov. 2025 – **Senior Editor**, *Journal of Physical Chemistry Letters*, American Chemical Society
present

July 2025 – **Professor of Chemistry, Physics and Optics**, University of Rochester
present

July 2024 – **Professor of Chemistry and Physics**, University of Rochester
July 2025

July 2019 – **Associate Professor of Chemistry and Physics**, University of Rochester
June 2024

July 2015 – **Assistant Professor of Chemistry and Physics**, University of Rochester
June 2019

July 2013 – **Assistant Professor of Chemistry**, University of Rochester
June 2015

Oct. 2011 – **Research Group Leader**, Theory Department, Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Jan. 2008 – **Postdoctoral Fellow**, Chemistry Department, Northwestern University, Evanston, IL
Sep. 2011 Advisors: Profs. Mark A. Ratner and George C. Schatz.

Summer 2002, 2003 **Research Assistant**, Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM, Advisor: Dr. Sergei Tretiak

Awards and Honors

- Chair, Gordon Research Conference on Quantum Control of Light and Matter, 2025.
- Visiting Professor, University of Toronto, Fall 2022.

- College Award for Undergraduate Teaching and Mentorship, U. Rochester, 2021.
- Leonard Mandel Faculty Fellow in Quantum Coherence, U. Rochester, 2019-2021
- Lecturer on Quantum Dynamics, Telluride School on Theoretical Chemistry, 2019.
- G. Graydon Curtis ('58) and Jane W. Curtis Award for Faculty Teaching Excellence, U. Rochester, 2019.
- ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry, Fall 2017.
- NSF CAREER Award, 2016-2021.
- Humboldt Research Fellowship, 2012-2013.
- Lachlan Gilchrist Fellowship in Fundamental Physics, University of Toronto, 2006/07.
- Ontario Graduate Scholarship, 2003/04, 2004/05 and 2005/06.
- University of Toronto Fellowship, 2002/03 and 2006/07 (teaching reduction).
- The F. E. Beamish Prize in Physical Chemistry 2006/07.
- The Michael J. Dignam Graduate Travel Award 2004/05.
- Winner of the “2001-02 Otto de Greiff National Undergraduate Theses Contest”, Natural Sciences Area, October 2002. Distinction to the best undergraduate thesis in Natural Sciences in Colombia.
- Winner of the “2001 Best Dissertation Award”, Theoretical Physics Area, National University of Colombia, November 2001. This prize is awarded on a yearly basis to the best undergraduate thesis in Theoretical Physics at the National University of Colombia.
- Summa cum Laude, National University of Colombia, 2001.
- “Best High School Graduates Admission and Scholarship Contest” recipient, National University of Colombia, 1995.

Publications

○ [ORCID: 0000-0002-0802-8185](#) ○ [Google Scholar](#) ○ [Scopus](#)

* denotes corresponding author

76. I. Gustin, C.W. Kim and I. Franco*, “General framework for quantifying dissipation pathways in open quantum systems. III. Off-diagonal system-bath coupling” (*J. Chem. Phys.*, **164**, 034105 (2026) (20 pages).
75. X. Chen and I. Franco*, “Comparison Between Explicit and Implicit Discretization Strategies for a Dissipative Thermal Environment” *J. Chem. Phys.*, **164**, 024112 (2026) (13 pages).
74. V. Tiwari, L. Sierra-Ossa, P. Wojcik and I. Franco*, “Transition from the Nanoscale to Bulk in the Nonequilibrium Optical Response of Laser-Dressed Materials” *J. Phys. Chem. Lett.*, **17**, 214 (2026) (7 pages).
73. I. Gustin, C.W. Kim and I. Franco*, “Dissipation Pathways in a Photosynthetic Complex” *J. Phys. Chem. Lett.*, **16**, 13093 (2025) (9 pages).
72. V. Tiwari and I. Franco*, “Robust purely optical signatures of Floquet states in crystals” *Phys. Rev. Lett.*, **135**, 186901 (2025) (6 pages).

71. X. Chen and I. Franco*, “Tree tensor network hierarchical equations of motion based on time-dependent variational principle for efficient open quantum dynamics in structured thermal environments” *J. Chem. Phys.*, **163**, 104109 (2025) Editor’s Choice. (Cover Article, 20 pages).
70. V. Tiwari and I. Franco*, “First-principle based Floquet engineering of solids in the velocity gauge” , *Phys. Rev. B*, **112**, 085139 (2025) (14 pages).
69. L. S. X. Huffman, A. Seshadri, C.D. Hastings, W. W. Brennessel, I. Franco and B. R. Barnett*, “Assessing structure and dynamics of iron complexes supported by tris(amidate)amine ligands” , *Dalton Trans.*, **54**, 10719 (2025) (6 pages).
68. S. Shen, M. Shiri, P. Mahalingavelar, C. Tang, T. Bills, A. J. Bushnell, L. Mejía, H. Zhang, B. Xu, I. Franco,* J. Azoulay,* K. Wang*, “Ultra-Long-Range Resonant Transport Through Open-Shell Donor-Acceptor Macromolecules”, *J. Am. Chem. Soc.*, **147**, 20310 (2025) Press release. (Cover article, 8 pages)
67. R. Korol, X. Chen and I. Franco*, “High-Frequency Tails in Spectral Densities” *J. Phys. Chem. A*, **129**, 3587-3596 (2025) (10 pages).
66. I. Gustin, X. Chen and I. Franco*, “Decoherence dynamics in molecular qubits: Exponential, Gaussian and beyond” *J. Chem. Phys.*, **162**, 064106 (2025) (11 pages).
65. X. Chen and I. Franco*, “Bexcitonics: Quasiparticle approach to open quantum dynamics” *J. Chem. Phys.*, **160**, 204116 (2024) (13 pages).
64. C.W. Kim* and I. Franco*, “General Framework for Quantifying Dissipation Pathways in Open Quantum Systems. II. Numerical Validation and the Role of Non-Markovianity” *J. Chem. Phys.*, **160**, 214112 (2024) (15 pages).
63. C.W. Kim* and I. Franco*, “General Framework for Quantifying Dissipation Pathways in Open Quantum Systems. I. Theoretical Formulation” *J. Chem. Phys.*, **160**, 214111 (2024) (13 pages).
62. I. Gustin, C.W. Kim, D. W. McCamant and I. Franco*, “Mapping Electronic Decoherence Pathways in Molecules” *Proc. Natl. Acad. Sci. U.S.A.*, **120**, e2309987120 (2023) (9 pages).
61. L. Mejía, P. Cossio and I. Franco*, “Microscopic Theory, Analysis, and Interpretation of Conductance Histograms in Molecular Junctions” *Nat. Comm.*, **14**, 7646 (2023) (12 pages)
60. V. Tiwari, B. Gu and I. Franco*, “Floquet theory and computational method for the optical absorption of laser-dressed solids”, *Phys. Rev. B*, **108**, 064308 (2023) (16 pages)
59. A. Garzón-Ramírez and and I. Franco*, “Stark Control of Electrons Across the Molecule-Semiconductor Interface” *J. Chem. Phys.*, **159**, 044704 (2023) (9 pages).
58. M. Deffner, M.P. Weise, H. Zhang, M. Mücke, J. Proppe, I. Franco, C. Herrmann*, “Learning Conductance: Gaussian Process Regression for Molecular Electronics” *J. Chem. Theory Comput.*, **19**, 992-1002 (2023) (10 pages).
57. W. Hu, I. Gustin, T. D. Krauss, and I. Franco*, “Tuning and enhancing quantum coherence time scales in molecules via light-matter hybridization” *J. Phys. Chem. Lett.*, **13**, 11503 (2022) (9 pages).
56. C.W. Kim, J. M. Nichol, A. N. Jordan and I. Franco*, “Analog Quantum Simulation of the Dynamics of Open Quantum Systems with Quantum Dots and Microelectronic Circuits” *PRX Quantum*, **3**, 040308 (2022) (20 pages). Editor’s choice.

55. T. Boolake, C. Heide, A. Garzón-Ramírez, H. Weber, I. Franco* and P. Hommelhoff*, “Light-field control of real and virtual charge carriers” *Nature*, **605**, 251-255 (2022) (4 pages + 15 pages extended methods). Press release. News and Views.
54. L. Mejía, U. Kleinekathöfer and I. Franco*, “Coherent and Incoherent Contributions to Molecular Electron Transport” *J. Chem. Phys.*, **156**, 094302 (2022) (15 pages).
53. C. Heide, T. Eckstein, T. Boolakee, C. Gerner, H. B. Weber, I. Franco and P. Hommelhoff*, “Electronic coherence and coherent dephasing in the optical control of electrons in graphene”, *Nano Lett.*, **21**, 9403 (2021) (6 pages).
52. L. Mejía, D. Garay-Ruiz, and I. Franco*, “Diels-Alder Reaction in a Molecular Junction”, *J. Phys. Chem. C*, **125**, 14599 (2021) (7 pages).
51. A. J. Garzón-Ramírez, F. Fernández Villoria, and I. Franco*, “Screening and band bending effects in the Stark control of electrons at interfaces (SCELI)”, *Phys. Rev. B*, **103**, 235304 (2021) (9 pages).
50. C.W. Kim and I. Franco*, “Theory of dissipation pathways in open quantum systems”, *J. Chem. Phys.*, **154**, 084109 (2021) (15 pages).
49. Z. Li, L. Mejía, J. Marrs, H. Jeong, J. Hihath, and I. Franco*, “Understanding the Conductance Dispersion of Single-Molecule Junctions”, *J. Phys. Chem. C*, **125**, 3406 (2021) (Cover article, 8 pages).
48. A. J. Garzón-Ramírez and I. Franco*, “Symmetry Breaking in the Stark Control of Electrons at Interfaces (SCELI)”, *J. Chem. Phys.*, **153**, 044704 (2020) (11 pages).
47. W. Hu, B. Gu and I. Franco*, “Toward the laser control of electronic decoherence”, *J. Chem. Phys.*, **152**, 184305 (2020) (16 pages).
46. G. Cabra, I. Franco and M. Galperin*, “Optical properties of periodically-driven open nonequilibrium quantum systems”, *J. Chem. Phys.*, **152**, 094101 (2020) (9 pages).
45. B. Gu and I. Franco*, “When can quantum decoherence be mimicked by classical noise?”, *J. Chem. Phys.*, **151**, 014109 (2019) (9 pages). Special Issue on Open Quantum Systems.
44. Z. Li and I. Franco*, “Molecular electronics: Toward the atomistic modeling of conductance histograms”, *J. Phys. Chem. C*, **123**, 9693 (2019) (9 pages). A. Nitzan Festschrift.
43. L. Mejía and I. Franco*, “Force-conductance spectroscopy of a single-molecule isomerization reaction”, *Chem. Sci.*, **10**, 3249-3256 (2019) (8 pages).
42. B. Gu and I. Franco*, “Electronic interactions do not affect electronic decoherence in the pure-dephasing limit”, *J. Chem. Phys.*, **149**, 174115 (2018) (4 pages).
41. B. Gu and I. Franco*, “Optical absorption properties of laser-dressed matter”, *Phys. Rev. A*, **98**, 063412 (2018) (15 pages).
40. A. Garzón-Ramírez and I. Franco*, “Stark control of electrons across interfaces”, *Phys. Rev. B*, **98**, 121305(R) (2018) (5 pages).
39. M. Koch*, Z. Li, C. Nacci, T. Kumagai, I. Franco and L. Grill “How structural defects affect the mechanical and electrical properties of single molecular wires”, *Phys. Rev. Lett.*, **121**, 047701 (2018) (5 pages). Editor’s choice: “How Defects Alter Graphene Nanoribbons”, Physics Synopsis, July 24, 2018 ([link](#)).

38. L. Chen, Y. Zhang, G. Chen and I. Franco*, “[Stark control of electrons along nanojunctions](#)”, *Nature Comm.*, **9**, 2070 (2018) (12 pages). In the news: “[Laser bursts generate electricity faster than any other method](#)” PHYSorg, June 21, 2018 ([link](#)).
37. W. Hu, B. Gu and I. Franco*, “[Lessons on electronic decoherence in molecules from exact modeling](#)”, *J. Chem. Phys.*, **148**, 134304 (2018) (11 pages).
36. Z. Li, A. Tkatchenko and I. Franco*, “[Modeling Non-Reactive Molecule-Surface Systems on Experimentally Relevant Time and Length Scales: Dynamics and Conductance of Polyfluorene on Au\(111\)](#)” *J. Phys. Chem. Lett.*, **9**, 1140 (2018) (6 pages).
35. B. Gu and I. Franco*, “[Generalized theory for the timescale of molecular electronic decoherence in the condensed phase](#)” *J. Phys. Chem. Lett.*, **9**, 773 (2018) (6 pages).
34. L. Mejía, N. Renaud and I. Franco*, “[Signatures of conformational dynamics and electrode-molecule interactions in the conductance profile during pulling of single-molecule junctions](#)”, *J. Phys. Chem. Lett.*, **9**, 745 (2018) (6 pages).
33. A. Pirrotta, G. C. Solomon, I. Franco and A. Troisi*, “[Excitonic coupling modulated by mechanical stimuli](#)” *J. Phys. Chem. Lett.*, **8**, 4326 (2017) (7 pages).
32. B. Gu and I. Franco*, “[Quantifying early-time quantum decoherence dynamics through fluctuations](#)” *J. Phys. Chem. Lett.*, **8**, 4289 (2017) (6 pages).
31. A. Kar and I. Franco*, “[Quantifying fermionic decoherence in many-body systems](#)” *J. Chem. Phys.*, **146**, 214107 (2017) (12 pages).
30. B. Gu and I. Franco*, “[Partial hydrodynamic representation of quantum molecular dynamics](#)” *J. Chem. Phys.* **146**, 194104 (2017) (8 pages).
29. R. Carey, L. Chen, B. Gu and I. Franco*, “[When can time-dependent currents be reproduced by the Landauer steady-state approximation?](#)” *J. Chem. Phys.* **146**, 174101 (2017) (8 pages).
28. A. Pirrotta, L. De Vico, G.C. Solomon and I. Franco*, “[Simulated force-conductance spectroscopy of hydrogen-bonded molecular complexes](#)” *J. Chem. Phys.*, **146**, 092329 (2017) (9 pages). Special Issue on “[Frontiers in Molecular Scale Electronics](#)”.
27. A. F. Izmaylov and I. Franco*, “[Entanglement in the Born-Oppenheimer Approximation](#)”, *J. Chem. Theory Comput.*, **13**, 20 (2017) (9 pages).
26. A. Pirrotta, G. C. Solomon and I. Franco*, “[Hydrogen-bonding in tight environments: simulated force spectroscopy of nanoconfined hydrogen bonded complexes](#)” *J. Phys. Chem. C*, **120**, 19470 (2016) (8 pages).
25. A. Kar, L. Chen and I. Franco*, “[Understanding the fundamental connection between electronic correlation and decoherence](#)”, *J. Phys. Chem. Lett.*, **7**, 1616 (2016) (6 pages).
24. L. Chen, T. Hansen and I. Franco*, “[Simple and accurate method for time-dependent transport along nanoscale junctions](#)”, *J. Phys. Chem. C*, **118**, 20009-20017 (2014) (8 pages).
23. S. M. Parker, M. Smeu, I. Franco, M. A. Ratner* and T. Seideman*, “[Molecular junctions: can pulling influence optical controllability?](#)” *Nano Lett.*, **14**, 4587-4591 (2014) (4 pages).
22. G. Albareda, H. Appel, I. Franco, A. Abedi and A. Rubio*, “[Correlated electron-nuclear dynamics with conditional wave functions](#)” *Phys. Rev. Lett.*, **113**, 083003 (2014) (5 pages).

21. I. Franco and H. Appel, “Reduced purities as measures of decoherence in many-electron systems”, *J. Chem. Phys.* **139**, 094109 (2013) (9 pages).
20. I. Franco, A. Rubio and P. Brumer, “Long-lived oscillatory incoherent electron dynamics in molecules: *trans*-polyacetylene oligomers”, *New J. Phys.* **15**, 043004 (2013) (16 pages).
19. I. Franco and P. Brumer, “Electronic coherence dynamics in *trans*-polyacetylene oligomers”, *J. Chem. Phys.* **136**, 144501 (2012) (10 pages).
18. I. Franco, M. A. Ratner and G. C. Schatz, “Single-molecule pulling: Phenomenology and Interpretation”, In: *Nano and Cell Mechanics: Fundamentals and Frontiers*, edited by H.D. Espinosa and G. Bao (Wiley, Microsystem and Nanotechnology Series, 2013), Chap. 14 (29 pages).
17. J. Hutcheson, I. Franco, N. Renaud, M. Carignano, M. A. Ratner and G. C. Schatz “TRANSpull: computes pulling coupled to transport properties of single molecules.” DOI: 10254/nanohub-r11739.1 (2011).
16. L. Felberg, I. Franco, M. McCullagh, M. A. Ratner, G. C. Schatz and M. Carignano, “MOLpull: A tool for molecular free energy reconstruction along a pulling coordinate”, DOI: 10254/nanohub-r9583.2 (2011).
15. M. McCullagh, I. Franco, M.A. Ratner and G.C. Schatz, “Defects in DNA: Lessons from Molecular Motor Design”, *J. Phys. Chem. Lett.* **3**, 689-693 (2012) (5 pages).
14. I. Franco, G.C. Solomon, G.C. Schatz and M.A. Ratner, “Tunneling currents that increase with molecular elongation”, *J. Am. Chem. Soc.*, **133**, 15714-15720 (2011) (7 pages). In the news: “Stretching livens up electron transport”, *C&EN*, September 26, 2011.
13. I. Franco, M.A. Ratner, G.C. Schatz, “Coulombic interactions and crystal packing effects in the folding of donor-acceptor oligorotaxanes”, *J. Phys. Chem. B*, **115**, 2477-2484 (2011) (8 pages).
12. M. McCullagh, I. Franco, M.A. Ratner and G.C. Schatz, “DNA-based optomechanical molecular motor”, *J. Am. Chem. Soc.*, **133**, 3452-3459 (2011) (8 pages). In the news: “Researchers turn photons into work using DNA” *PHYSorg*, March 10, 2011.
11. I. Franco, C.B. George, G.C. Solomon, G.C. Schatz and M.A. Ratner, “Mechanically activated molecular switch through single-molecule pulling”, *J. Am. Chem. Soc.*, **133**, 2242-2249 (2011) (8 pages).
10. I. Franco, M. Spanner and P. Brumer, “Quantum interferences and their classical limit in laser-driven coherent control scenarios”, *Chem. Phys.*, **370**, 143-150 (2010) (8 pages).
9. I. Franco, G.C. Schatz and M.A. Ratner, “Single-molecule pulling and the folding of donor-acceptor oligorotaxanes: phenomenology and interpretation”, *J. Chem. Phys.* **131**, 124902 (2009) (13 pages).
8. M. Spanner, I. Franco and P. Brumer, “Coherent control in the classical limit: Symmetry breaking in an optical lattice” *Phys. Rev. A* **80**, 053402 (2009) (7 pages).
7. I. Franco, M. Shapiro and P. Brumer, “Laser-induced currents along molecular wire junctions”, *J. Chem. Phys.* **128**, 244906 (2008) (14 pages).
6. I. Franco, M. Shapiro and P. Brumer, “Femtosecond dynamics and laser control of charge transport in *trans*-polyacetylene”, *J. Chem. Phys.* **128**, 244905 (2008) (13 pages).

5. I. Franco and P. Brumer, “Minimum requirements for laser-induced symmetry breaking in quantum and classical mechanics”, *J. Phys. B* **41**, 074003 (2008) (5 pages).
4. I. Franco, M. Shapiro and P. Brumer, “Robust ultrafast current in molecular wires through Stark shifts”, *Phys. Rev. Lett.* **99**, 126802 (2007) (4 pages). In the news: “Light-Driven Femtosecond Electricity” Physics News in 2007, *APS News*, February 2008 ; *The SPS Observer*, AIP, **41** (3) (2007); “Molecular electronics: Ultrafast stop and go”, *Nature Nanotech.*, **2**, 675-676 (2007); “Molecular electronics: Fast blast”, *Nature Nanotech.*, Sep. 2007 (doi:10.1038/nnano.2007.330).
3. I. Franco and P. Brumer, “Laser-induced spatial symmetry breaking in quantum and classical mechanics”, *Phys. Rev. Lett.* **97**, 040402 (2006) (4 pages). Cover article
2. I. Franco and S. Tretiak, “Electron-vibrational dynamics of photoexcited polyfluorenes”, *J. Am. Chem. Soc.* **126**, 12130-40 (2004) (11 pages).
1. I. Franco and S. Tretiak, “Electron-vibrational relaxation of photoexcited polyfluorenes in the presence of chemical defects: a theoretical study”, *Chem. Phys. Lett.* **372**, 403-408 (2003) (6 pages).

Invited Talks

138. February 11, 2026. Seminar, Virtual International Seminar on Theoretical Advancements (VISTA).
137. January 5-9, 2026. Lecturer on Open Quantum Systems, Texas School on Open Quantum Dynamics and Quantum Information in the Chemical Sciences, Wimberley, TX.
136. December 15-20, 2025. Session on “Modern Methods for Strong Light-Matter Interactions in Complex Chemical Systems”, Pacificchem 2025, Honolulu, Hawaii.
135. December 15-20, 2025. Session on “Quantum Dynamics of Complex Systems”, Pacificchem 2025, Honolulu, Hawaii.
134. November 12-14, 2025. Optica Incubator on Petahertz Electronics, Optica Global Headquarters, Washington, DC.
133. November 5, 2025. Physical Chemistry Seminar, Purdue University.
132. October 16, 2025. Condensed Matter Physics Seminar, University of Texas at Austin.
131. Jan. 31, 2025. Colloquium, Physics Department, Queen’s University, Canada.
130. Dec. 16-20, 2024. Workshop on Molecular Quantum Technology III, Puerto Varas, Chile.
129. Oct. 14, 2024. Physical Chemistry Seminar, Department of Chemistry, Caltech.
128. July 28-Aug. 2, 2024. Quantum Frontiers in Molecular Science, Mexico City.
127. June 10, 2024. Telluride workshop on ”Emerging Phenomena in the Strong Light-Matter Coupling Regime”, Telluride, CO
126. June 3, 2024. Colloquium, Chemistry Department, UCLA.
125. May 28-30, 2024. Photonics-North , Session on “Quantum Light-Matter Interactions”, Vancouver, CA
124. May 24, 2024. Atto Fridays, University College London.
123. March 25-29, 2024. Telluride workshop on “Quantum Computing for Quantum Chemistry, Molecular Dynamics, and Beyond”, Telluride, CO

122. March 8, 2024. Workshop on “Open Quantum Dynamics”, CUNY Graduate Center, New York, NY.
121. Feb. 12, 2024. Keynote speaker, NSF/UKRI Bilateral Workshop on Quantum Information Science in Chemistry, Washington D.C.
120. Jan. 22, 2024. Colloquium, Chemistry Department, University of Utah.
119. Oct. 25, 2023. 13th International Conference on Excitonic and Photonic Processes in Condensed Matter and Nano Materials. Santa Fe, NM.
118. Oct. 17-19, 2023. International Workshop on Frontiers in Ultrafast Science, Lam, Germany
117. Oct. 16, 2023. Colloquium, Department of Physics and Engineering Physics, Tulane University.
116. Aug. 28, 2023. US-Ukraine Quantum Forum
115. June 23, 2023. Colloquium, Niels Bohr Institute, University of Copenhagen, Denmark.
114. June 11, 2023. Workshop on Exciton/Photon Interactions for Quantum Systems, Telluride, CO.
113. May 24, 2023. International Workshop on Dynamical Control of Quantum Materials, Dresden, Germany
112. April 20, 2023. Quantum Meeting, University of Rochester.
111. March 22, 2023. STEM days, Anglo Colombian School, Bogotá, Colombia.
110. Feb. 27, 2023. Colloquium, Institute of Optics, University of Rochester.
109. Jan. 9, 2023. Ultrafast Coffee House, University of Pittsburgh.
108. Nov. 22, 2022. Quantum Research Seminar Toronto.
107. Nov. 13, 2022. ACS Career Kick-Starter Workshop for ACS Bridge Fellows, Washington D.C.
106. Nov. 7-11, 2022. XI Photodynamics Conference, Havana, Cuba.
105. Oct. 28, 2022. Colloquium, Department of Physics, Mississippi State University
104. Oct. 7, 2022. Colloquium, Center for Quantum Information and Quantum Control, University of Toronto.
103. Oct. 5, 2022. Seminar, Aspuru-Guzik Group, University of Toronto.
102. July 27, 2022. Colloquium, Department of Physics, Friedrich-Alexander-Universität, Erlangen, Germany.
101. July 26, 2022. Seminar, Chair of Laser Physics, Friedrich-Alexander-Universität, Erlangen, Germany.
100. July 21, 2022. Colloquium, Department of Physics, Technical University, Berlin, Germany.
99. July 19, 2022. Colloquium, Dahlem Center for Complex Quantum Systems, Department of Physics, Free University, Berlin, Germany.
98. July 14, 2022. Colloquium, Department of Chemistry, University of Hamburg, Germany.
97. July 6, 2022. Colloquium, Department of Physics, Jacobs University, Bremen, Germany.
96. July 5, 2022. Computational Materials Science Group, University of Bremen, Germany.
95. June 13-17, 2022. Canadian Chemistry Conference and Exhibition, Symposium on “Charge and Energy Transport in Open Quantum Systems”, Calgary, Canada.

94. June 6-10, 2022. Workshop on Quantum Frontiers in Molecular Science, Telluride, CO.
93. April 4-6, 2022. Theory Division, Los Alamos National Laboratory.
92. Dec. 16-21, 2021. Symposium on “Quantum Coherence in Energy Transfer” and “Modeling exciton and charge dynamics in molecules and clusters toward optoelectronic applications”, ACS Pacificchem, Honolulu, Hawaii.
91. August 23-25, 2021. Session on “Synthesizing Quantum Coherence”, ACS Fall 2021, Atlanta, GA.
90. July 19-23, 2021. Workshop on Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, CO.
89. April 18-24, 2021. Symposium on “Koopman Methods in Classical and Classical-Quantum Mechanics”, Germany
88. April 5-16, 2021. Symposium on “Chemistry of Molecular Electronics”, Spring 2021 ACS Meeting (virtual)
87. April 9, 2021. Computing Seminar, Department of Chemical and Biological Engineering at the University of Wisconsin-Madison.
86. Dec. 17, 2020. (Bio)Molecular Electronics Colloquia, virtual seminar series, U. Liverpool.
85. Dec. 9, 2020. Theory and Simulation of Electronic and Optical Processes in Molecules and Materials, virtual seminar series, U. Kansas.
84. Nov. 12, 2020. Quantum Information Division of the Mexican Physical Society, virtual seminar series.
83. Oct. 26, 2020. Physics Department, University of Delaware. Virtual seminar.
82. July 20-24, 2020. Quantum Frontiers in Molecular Science, Telluride, CO. Virtual seminar.
81. Aug. 25-29, 2019. Symposium on “Nanoscale and molecular assemblies: Designing matter to control energy transport”, Fall 2019 ACS Meeting, San Diego, CA.
80. Aug. 11-16, 2019. Gordon Research Conference on Quantum Control of Light and Matter, Newport, RI.
79. July 29-Aug. 2, 2019. Quantum Transport in Nanoscale Molecular Systems, Telluride, CO.
78. July 29-Aug. 2, 2019. 5 Lectures on Quantum Dynamics, Telluride Research School in Theoretical Chemistry, Telluride, CO.
77. July 22-24, 2019. Physics and Chemistry Meeting at the Interface, Humboldt Kolleg, Medellín, Colombia.
76. June 7, 2019. Symposium on “Recent Developments in Quantum Molecular Dynamics Algorithms and Applications”, 102nd Canadian Chemistry Conference and Exhibition, Quebec City, Canada.
75. Feb. 22, 2019. Chemistry Department, Dalhousie University.
74. Nov. 14, 2018. Chemistry Department, University of Rochester.
73. Oct. 11, 2018. Chemistry Department, University of Michigan.
72. June 27, 2018. Workshop on “Quantum Frontiers in Molecular Science”, Telluride, CO.
71. May 16, 2018. Chemistry Department, University of Washington.

70. May 15, 2018. Chemistry Department, University of California, Irvine.
69. April 30, 2018. Chemistry Department, Princeton University.
68. April 26, 2018. Institute for Advanced Computational Science, Stony Brook University.
67. April 24, 2018. Chemistry Department, Yale University.
66. April 16, 2018. Chemistry Department, University of Oregon.
65. April 3, 2018. Chemistry Department, University of Chicago.
64. March 27, 2018. Chemistry Department, University of Toronto.
63. March 13-15, 2018. Theochem, U. Boston, MIT and Harvard.
62. March 2, 2018. Chemistry Department, Duke University.
61. Feb. 27, 2018. Chemistry Department, NYU.
60. Feb. 15, 2018. Chemistry Department, Cornell University.
59. Feb. 8, 2018. Chemistry Department, Northwestern University.
58. Feb. 7, 2018. Chemistry Department, University of Illinois at Urbana Champaign.
57. Jan. 23, 2018. Chemistry Department, University of California, San Diego.
56. Jan. 18, 2018. Chemistry Department, University of Pennsylvania.
55. Nov. 6, 2017. Chemistry Department, University of Southern California.
54. Nov. 2, 2017. Workshop on “Quantum conductance and forces across molecular junctions”, CUNY Graduate Center, New York, NY.
53. Oct. 16, 2017. Department of Condensed Matter Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany.
52. Oct. 9 - 13, 2017. CECAM-Psi-k Workshop on “Charge carrier dynamics in nanostructures: optoelectronic and photo-stimulated processes”, Bremen, Germany.
51. Sep. 25 - 29, 2017. International conference on “Transport at the Nanoscale”, Centro Internacional de Ciencias, Cuernavaca, Mexico
50. Aug. 22, 2017. ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry, Washington, D.C.
49. Aug. 7, 2017. Gordon Research Conference on Quantum Control of Light and Matter. Hot topic talk.
48. July 17-21, 2017. Workshop on “Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy”, Telluride, CO.
47. June 4-6, 2017. Symposium on “Theory and Computation: Toward Electronic Properties of Molecular Materials”, ACS Mid Atlantic Regional Meeting, Hershey, PA.
46. May 3-5, 2017. IX Int. Conference in Education and Modeling in Basic Sciences. Medellín, Colombia.
45. April 20, 2017. Department of Chemistry, Colorado State University.
44. Feb. 8, 2017. Department of Chemistry, Purdue University.
43. Oct. 7, 2016. “Spectroscopy” and “Theoretical Chemistry” sessions, ACS northeast regional meeting, Binghamton, NY.
42. Sep. 16, 2016. CIRC Symposium. University of Rochester, Rochester, NY.

41. June 1-3, 2016. Workshop on “Theoretical challenges simulating materials out of equilibrium”, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany.
40. May 9-13, 2016. “9th Int. Conference on Photodynamics and Related Aspects”, Mendoza, Argentina.
39. April 11, 2016. Physics Department, Binghamton University SUNY, Binghamton, NY.
38. March 30, 2016. Department of Physics, University of Rochester, Rochester, NY.
37. March 16-17, 2016. Session on “Time-dependent dynamics and electronic excited states”, ACS March Meeting, San Diego.
36. Feb. 11, 2016. Department of Chemistry, University of Notre Dame.
35. Dec. 18-20, 2015. PACIFICHEM 2015, “Quantum Coherence in Energy Transfer”, Honolulu, Hawaii.
34. Oct. 14, 2015. Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM.
33. Aug. 24-26, 2015. International workshop on “Charge, Heat and Energy Transport in Molecular Junctions”, Copenhagen, Denmark.
32. July 20-24, 2015. Workshop on “Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy”, Telluride, CO.
31. May 27, 2015. International workshop on “Modeling Many-Body Interactions 2015”, Lake Garda, Italy.
30. May 21, 2015. Nanoscience Seminar, Department of Chemistry, University of Copenhagen, Denmark.
29. May 20, 2015. P. Chem. Seminar, Department of Chemistry, University of Hamburg, Germany
28. May 18, 2015. P. Chem. Department, Fritz Haber Institute of the Max Planck Society, Berlin, Germany.
27. May 5, 2015. The Graduate Center, City University of New York, New York, NY.
26. Dec. 4, 2014. Hunter College, City University of New York, New York, NY.
25. Aug. 27, 2014. International workshop on “Quantum coherence and decoherence II”, Medellín, Colombia.
24. Aug. 14, 2014. International workshop on “Coherence and Control in the Quantum World: the Legacy of Moshe Shapiro”, University of British Columbia, Canada.
23. Apr. 21, 2014. Center for Coherence and Quantum Optics Seminar, University of Rochester, NY.
22. Mar. 24, 2014. Department of Physics, Stony Brook University.
21. July 22, 2013. Telluride Workshop on “Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy”, Telluride, CO.
20. Jan. 21, 2013. Theory Seminar, Chemistry Department, University of Rochester, Rochester, NY.
19. Nov. 9, 2012. CECAM Workshop on “Vibrational coupling: most important, often ignored, and a challenge for ab-initio theory”, CECAM-HQ, Lausanne, Switzerland.



18. Aug. 30, 2012. Department of Chemistry, Universidad Nacional de Colombia, Bogotá, Colombia.
17. Aug. 31, 2012. Department of Chemistry, Universidad de Antioquia, Medellín, Colombia.
16. Aug. 28, 2012. Department of Chemistry, Universidad del Valle, Cali, Colombia.
15. July 18-21, 2012. Frontiers in Computational Material Science, Ringberg Castle, Germany.
14. June 15, 2012. Cross Border Workshop on Laser Science 2012, McGill University, Montreal, Canada.
13. Jan. 31, 2012. Max Planck Institute of Quantum Optics, Garching, Germany.
12. Jan. 23, 2012. University of the Basque Country, San Sebastián, Spain.
11. Jan. 16, 2012. Department of Chemistry, University of Rochester, Rochester, NY
10. Dec. 8, 2011. Theory Department, Fritz Haber Institute of the Max Planck Society, Berlin, Germany.
9. Nov. 17, 2011. Nanoscience Group, Fritz Haber Institute of the Max Planck Society, Berlin, Germany
8. Feb. 18, 2011. Department of Chemistry, University of Copenhagen, Copenhagen, Denmark.
7. Feb. 8, 2011. Department of Chemistry, University of Utah, Salt Lake City, UT.
6. Jan. 31, 2011. Department of Chemistry, University of Nevada-Reno, Reno, NV.
5. Jan. 17, 2011. Department of Chemistry, Princeton University, Princeton, NJ.
4. Nov. 28, 2010. Department of Chemistry, Cornell University, Ithaca, NY
3. Nov. 18, 2010. Department of Chemistry, University of North Carolina-Chapel Hill, Chapel Hill, NC
2. Dec. 10, 2009. Department of Chemistry, Texas A&M University, College Station, TX.
1. Nov. 30, 2009, Department of Chemistry, University of Utah, Salt Lake City, UT

Other Oral Presentations, Posters and Meetings:

30. August 6-11, 2023. Gordon Research Conference on Quantum Control of Light & Matter, Newport, RI
29. March 6-10, 2023. APS March Meeting, Las Vegas.
28. August 25-29, 2019. ACS Fall Meeting, San Diego.
27. March 4-8, 2019. APS March Meeting, Boston, MA.
26. Aug. 5-10, 2018. Gordon Research Conference on Electron Donor-Acceptor Interactions. Salve Regina University.
25. Aug. 6-11, 2017. Gordon Research Conference on Quantum Control of Light & Matter, Mount Holyoke College.
24. Aug. 7-12, 2016. Gordon Research Conference on Electron Donor-Acceptor Interactions. Salve Regina University.
23. March 13-18, 2016. ACS National Meeting, San Diego, CA.
22. Dec. 18-20, 2015. PACIFICHEM 2015
21. Aug. 2-7, 2015. Gordon Research Conference on Quantum Control of Light & Matter, Mount Holyoke College.

20. March 2-6, 2015. APS March Meeting, San Antonio, TX.
19. June 15-19, 2014. Gordon Research Conference on Multiphoton Processes, Bentley University.
18. July 28-August 2, 2013. Gordon Research Conference on Quantum Control of Light & Matter, Mount Holyoke College.
17. Nov. 6-9, 2012. Vibrational coupling: most important, often ignored, and a challenge for ab-initio theory, CECAM-HQ, Lausanne, Switzerland.
16. June 6-17, 2011. PASI school on electronic properties of complex systems, Cartagena, Colombia.
15. May 25-27, 2011. Energy Frontier Research Center Summit & Forum, Washington D.C.
14. May 29-June 2, 2010. 93rd Canadian Chemistry Conference and Exhibition, Toronto, Canada.
13. March 22-26, 2010. ACS National Meeting, San Francisco, CA.
12. July 6-24, 2009. Boulder School for Condensed Matter and Materials Physics: Nonequilibrium Statistical Mechanics, Boulder, CO.
11. March 2-6, 2009. Workshop on Coherence, Control, and Dissipation, Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, MN.
10. July 19-24, 2008. American Conference on Theoretical Chemistry, Northwestern University, Evanston, IL.
9. Aug. 12-17, 2007. Gordon research conference on quantum control of light and matter, Newport, RI.
8. May 17-19, 2007. Crossborder workshop 07 on laser science, Toronto.
7. Aug. 8-11, 2006. Conference on Quantum Information and Quantum Control II, Toronto, Canada.
6. July 31-August 5, 2005. Gordon research conference on quantum control of light and matter, Waterville, ME.
5. June 7-9, 2004. Building Computational Devices using Coherent Control. University of Michigan, Ann Arbor.
4. July 19-23, 2004. Conference on Quantum Information and Quantum Control, Toronto, Canada.
3. Aug. 11-16, 2003. Excited State Processes in Electronic and Bio Nano-Materials. Los Alamos National Laboratory, Los Alamos, NM.
2. April, 2001. Spring College on Numerical Methods in Electronic Structure Theory, The Abdus Salam International Centre for Theoretical Physics, Trieste.
1. Jan. 1998, 2nd Ibero American School of Computational Chemistry and Molecular Design. Havana University, Havana.

Teaching:

- **General Chemistry for Engineers**, CHEM137. Fall 2024, 2025. This undergraduate course is an introduction to general chemistry specifically for engineering students requiring only one semester of chemistry. The course discusses the microscopic and macroscopic basis for chemical structure and reactivity and is designed to give engineering students a conceptual foundation in the principles of chemistry that are relevant to solving engineering problems. Important topics include the nature of chemical compounds; stoichiometry, properties of gases; the Periodic Table; electrons and atoms; chemical bonding and applications to materials; thermodynamics and energy; rates of chemical reactions; chemical equilibrium; electrochemistry.
- **Physical Chemistry I**, CHEM251/CHEM441. Fall 2016, 2018, 2019, 2020, 2021, 2023. This undergraduate course is an introduction to the quantum theory of matter, with applications to problems of chemical interest. It starts from the basic principles of quantum mechanics using wavefunctions and build up the models that are essential for understanding many molecular properties and processes including vibrations, spectroscopy, chemical bonding, and atomic and molecular structure.
- **Quantum Chemistry I**, CHEM451. Fall 2013, 2014, 2015, 2016 and 2017. This graduate course is a rigorous introduction to non-relativistic Quantum Mechanics. The course develops the mathematical foundations of quantum mechanics, introduces and discusses the postulates, and develops the models and techniques that are essential to understand quantum theory. The goal of this course is to help students develop a graduate-level working knowledge of elementary non-relativistic Quantum Mechanics at the level of Cohen-Tannoudji/Sakurai/Shankar/Messiah.
- **Thermodynamics and Statistical Mechanics**, CHEM455. Spring 2015, 2016, 2019. This graduate course is a rigorous introduction to Thermodynamics and Statistical Mechanics. The goal is to help students develop a graduate-level working knowledge of modern Statistical Mechanics and Thermodynamics with a focus on applications to molecular systems at the level of Callen's "Thermodynamics", and Tuckerman/Pathria/Balescu "Statistical Mechanics". The course starts by developing a solid foundation on Hamiltonian dynamics, ensemble theory, and thermodynamics, and proceeds to develop the statistical basis of thermodynamics. It includes a detailed discussion of the basic ensembles, quantum and classical gases, phase transitions, and linear response theory.
- **Quantum Dynamics**, CHEM452. Spring 2020, 2021, 2022, 2023, 2024, 2025, 2026. This course is designed to help students transition from a first graduate-level course in quantum mechanics to research-level competency in quantum dynamics. The course introduces the basic strategies to capture the quantum dynamics of closed systems and those in interaction with a quantum surrounding. The class covers formal aspects of quantum dynamics, numerical methods for solving the time-dependent Schrödinger equation, excited state molecular dynamics, the theory of quantum control, and the theory of open quantum systems.

Student Supervision

Current Students

- Dr. Michelle Anderson, Postdoctoral Fellow, Nov. 1, 2025 – present.
- Dr. Kwang Hyun Cho, Postdoctoral Fellow, from April 1, 2026.
- Rishabh Dora, Ph.D. Student, Jan. 1, 2023 – present.

- Jhoan Fernández, Ph.D. Student, Jan. 1, 2025 – present.
- Hank Longo, Ph.D. Student, Jan. 1, 2026 – present.
- Juan Camilo Rodríguez, Ph.D. Student, Jan. 1, 2026 – present.
- Vedant Agrawal, Undergraduate Student, Jan. 28, 2026 – present
- Luchang Niu, Undergraduate Student, June 15, 2025 – present
- Anna Spak, Undergraduate Student, Sep. 1, 2025 – present

Alumni

Postdoctoral Fellows

- Dr. Roman Korol, Postdoctoral Fellow, Sep. 1, 2023 – Dec. 31, 2025, Currently: Assistant Professor, U. Sherbrooke (Canada).
- Dr. Chang Woo Kim, Postdoctoral Fellow, Sep. 2019 – Aug. 2021. Currently: Assistant Professor, Chonnam National U. (Korea)
- Dr. Bing Gu, Postdoctoral Fellow, September 1, 2016 – October 30, 2018. [Recipient of the 2018 ACS Physical Chemistry Young Investigator Award](#). Currently: Assistant Professor Westlake U., China.
- Dr. Arnab Kar, Postdoctoral Fellow, July 1, 2014 – July 1, 2016. Currently: Engineer at Intel.
- Dr. Liping Chen, Postdoctoral Fellow, July 1, 2013 – March 1, 2016. Currently: Researcher at Zhejiang U.

Graduate Students

- Dr. Xinxian Chen, Ph.D. Student, Jan. 1, 2020 – Oct. 17, 2025. Thesis title: “*Tensor Network Decomposition of Open Quantum Dynamics for Efficient Simulation of Next-Generation Quantum Systems*”. Current position: Scientist at Huawei.
- Dr. Vishal Tiwari, Ph.D. Student, Jan. 1, 2020 – Aug. 15, 2025. Thesis title: “*Floquet Engineering the Optical Absorption Properties of Materials*”. Current position: Postdoc at WashingtonU (Masiello).
- Dr. Ignacio Gustin, Ph.D. Student, Jan. 1, 2021 – July 31, 2025. Thesis title: “*Mapping Decoherence Pathways in Molecules*”. Current position: Postdoc at UToronto (Aspuru-Guzik).
- Rahul Chourasiya, M.Sc. Student, Jan. 1, 2024 – Aug. 31 2025. Currently: Ph.D. student at Northwestern.
- Dr. Leopoldo Mejía, Ph.D. Student, Jan. 1, 2017 – August 18, 2021. Thesis title: “*Mechanical Control of Charge Transport and Chemical Reactivity in Molecular Junctions*”. [Recipient of the 2021 ACS Graduate Award in Theoretical Chemistry](#). Postdoc at Berkeley (Rabani). Currently: Assistant Professor, Universidad Andrés Bello, Chile
- Dr. Wenxiang Hu, Ph.D. Student, Feb. 1, 2016 – May 6, 2021. Thesis title: “*Modeling and control of quantum decoherence in molecules*”. Currently: Scientist at Amazon.
- Dr. Antonio Garzón, Ph.D. Student, Jan. 1, 2016 – Feb. 25, 2021. Thesis title: “*Ultrafast Control of Electrons Using Few-cycle Laser Pulses*”. Currently: Postdoc at Northwestern (Tempelaar).

- Dr. Zhi Li, Ph.D. Student, Jan. 1, 2014– Jan 5, 2019. Thesis title: “*Frontiers in the Atomistic Modeling of Molecular Junctions: Bringing Theory Closer to Experiment*”. Currently: Scientist at Meta.
- Dr. Alessandro Pirrotta, Ph.D. Student, U. Copenhagen, 2013–2017 (co-supervised with Prof. G.C. Solomon). Thesis title: “*Modulating Pathways for Electron and Energy Transfer Through Molecules*”. Currently: Data science engineer at PFA Pension, Copenhagen.

Undergraduate Students

- Cristóbal Carrió, Undergraduate Student, June 2-Aug. 8, 2026.
- Derek Chien, Undergraduate Student, May 15, 2023 – Dec. 15, 2024. Currently: Churchill Scholar, U. Cambridge.
- Juan Camilo Rodríguez, Undergraduate Student, Summer 2024. Currently: Ph.D. Student at U Rochester.
- Jhoan Fernández, Undergraduate Student, Summer 2023. Currently: Ph.D. Student at U Rochester.
- Rylee Neumann, Undergraduate Student, June 2022– April 2023.
- Junjie Wang, Undergraduate Student, August 2022– April 2023. Currently: Graduate student at Northwestern
- Luis Alejandro Sierra, Undergraduate Student, Summer, 2022. Currently: Ph.D. student at Northwestern (Tempelaar).
- Anjana Seshradi, Undergraduate Student, 2021-2022. Currently: Ph.D. student at Cornell.
- Aditi Seshradi, Undergraduate Student, Summer, 2021. Currently: Ph.D. student at Cornell.
- Luis Delgado, Undergraduate Student, Summer, 2021. Currently: Ph.D. student at UChicago (Mazziotti).
- Yueheng Min, Undergraduate Student, Summer, 2021. Currently: M.Sc. student at U Rochester.
- Garrett Beals, Undergraduate Student, U. Rochester. Jan. 1, 2020– May 2021. Currently: Ph.D. student at Columbia. [Recipient of a NSF Graduate Research Fellowship 2021](#).
- Daniel Carstairs, Undergraduate Student, U. Rochester. Fall 2020. M.Sc. UChicago. 2024. Currently: Chemist at AbbVie.
- Francisco Fernández, M.Sc. Student, U. Madrid. Summer 2019. Ph.D. at UAM 2024 (Palacios). Currently: Data Scientist Naudit
- Yuly Chamorro, Undergraduate Student, U. Antioquia. Jan 15, 2019– May 15, 2019. Currently: Ph.D. student at Groningen.
- Diego Garay, Undergraduate Student, U. Barcelona. Summer 2018. Ph.D. Institut Català d’Investigació Química. Currently: Postdoc at IMN-CNM, CSIC
- Paweł Wojcik, Undergraduate Student, U. Warsaw, Poland. Summer 2017. Ph.D. USC (Krylov). Currently: Quant at nVerses Capital.
- Reshma Dani, Undergraduate Student, IIT-Guwahati, India. Summer 2016. Ph.D. at UIUC (Makri). Currently: Engineer at Intel.

- Ulises Torres, Undergraduate Student, UNAM, Mexico. Summer 2015. Currently: PDF at UNAM.

Departmental and Professional Service:

Conference organizer:

- Co-organizer, Texas Quantum Winter School on Open Quantum Systems and Quantum Information in the Chemical Sciences, Newport, January 4-9, 2026.
- Chair, Gordon Research Conference on Quantum Control of Light & Matter, Newport, RI, August 4-8, 2025.
- Co-organizer, 12th Rochester Conference on Coherence and Quantum Science. Rochester, NY, June 23-27, 2025.
- Co-organizer, Biennial workshop on “Quantum Frontiers in Molecular Science”, June 26-30, 2018 (Telluride); June 22-26, 2020 (online); June 6-10, 2022 (online); July 28-Aug. 2, 2024 (Mexico); July 27-31, 2026.
- Vice-chair, Gordon Research Conference on Quantum Control of Light & Matter, Newport, RI, August 6-11, 2023.
- Co-organizer, Workshop on “Quantum Information in Chemistry”, Initiative for the Theoretical Sciences, CUNY, December 3, 2021.
- Co-organizer, Rochester Conference on Coherence and Quantum Optics XI, August 4-8, 2019.
- Co-organizer, Psi-K workshop on “Modeling Single-Molecule Junctions: Novel Spectroscopies and Control”, October 14-16, 2013. Berlin, Germany.

Departmental Committee Service:

- Colloquium/Distinguished Lecturers and Seminars. Member: 2016-2018. Chair: 2022-present.
- Undergraduate Studies. Member: 2020–present
- Ad-Hoc Committee, Chair Evaluation, Department of Chemistry, 2024.
- Awards. Member: 2018-2022
- Development/News-Promotion Committee. Member: 2018-2021, 2022-2023
- Faculty Recruiting. Member: 2014-2015, 2019-2020, 2021-2022
- Graduate Studies. Member: 2015-2016, 2018-2019, 2023-2024
- Graduate Recruiting. Member: 2013-2018
- Services/Space. Member: 2019-2020

University Service:

- Leadership, Center for Coherence and Quantum Science, U. Rochester. 2014–.
- Member, Executive Committee, Center for Integrated Research Computing, 2025
- Member, ad-hoc tenure committee, 2022.
- Member, Faculty Senate Sub-Committee on Faculty Club, U. Rochester, 2017–2021.

- Thesis defense chair for: Yang Xu (Optics, 2026), Tyler Mason (ChemE, 2026), Zihao Wang (Physics, 2026), James Young (Physics, 2025), Ali Khourshaei Shargh (Mechanical Engineering, 2023), Margaret Samuels (Material Science, 2022), Gail Jardine (Mathematics, 2022), Rodrigo Gutiérrez (Optics, 2019), Julian Martínez (Physics, 2017), Areeya Chantasri (Physics, 2016), Jin Liu (ChemE, 2016), Dejun Lin (Biophysics, 2015).

Professional Service:

- Member, Editorial Advisory Board, ACS Physical Chemistry Au. 2025–
- Member, Board of Directors, Newman School, Bogotá, Colombia. 2007–.
- Thesis committee member for: Ray Parker (Physics, current), Wenxiang Yin (Chemistry, 2025), Alejandro Alvarez (Materials Science, 2024), Negede Alemayehu (Biophysics, 2024), William Bro-Jorgensen (Chemistry, U. Copenhagen, 2024), Le Hu (Physics, 2024), Tathagata Karmakar (Physics, 2024), Dan Younis (Physics, 2024), Dominik Orlowski (Chemistry, U. Copenhagen, 2023), Spencer Rogers (Physics, 2023), Geemi Wellawatte (Chemistry, 2023), Dalton Hanaway (Chemistry, 2022), Zekai Chen (Physics, 2022), Xinyang Li (Chemistry, 2021), Arkajit Mandal (Chemistry, 2021), Sutirtha Chowdhury (Chemistry, 2021), Jing Yang (Physics, 2021), Chapin Cavender (Biophysics, 2021), Rainier Barrett (ChemE, 2020), Justin Tian (Physics, 2017).
- *Reviewer for the following scientific journals:* Nature, Nature Chemistry, Nature Communications, Angewandte Chemie, Journal of the American Chemical Society, Proc. Natl. Acad. Sci. U.S.A., Journal of Physical Chemistry Letters, Journal of Physical Chemistry, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Nanoscale, NanoLetters, ACS Nano, Scientific Reports, Optica, ACS Applied Materials & Interfaces, Chemical Physics, JSTAT, Chemical Science, ACS Sensors, Results in Physics.
- *Reviewer for the following funding agencies:* National Science Foundation (ad-hoc and panelist), Department of Energy, Petroleum Research Fund, Natural Sciences and Engineering Research Council of Canada, Center for Integrated Nanotechnologies, Netherlands Organisation for Scientific Research, CECAM.
- Member, Selection Committee, Justin Jankunas Doctoral Dissertation Award in Chemical Physics, 2023-2025.

Research Support

Pending

- National Science Foundation, Division of Physics, Quantum Information Science Program. “Analog Quantum Simulation of the Microscopic Dynamics of Two-Level Fluctuators in Silicon Qubits”. Potential award amount: \$720,394.

Current

- National Science Foundation, Division of Chemistry, Chemical Structure and Dynamics Program. “Mapping Electronic Decoherence Pathways in Molecules” Total award amount: \$699,275. CHE-2511834. Award period: 05/01/2025-04/30/2028 (with David McCamant).
- Department of Energy, Quantum Information Science Research in Chemical Sciences, Geosciences, and Biosciences. “Tensor Network Decomposition of Open Quantum Dynamics for Efficient Simulation of Next-Generation Quantum Systems.” Total award amount: \$550,302. DE-SC0025334. Award period: 08/15/2024-08/14/2027.

- National Science Foundation, Division of Physics, Quantum Information Science Program. “Analog Quantum Simulation of the Dynamics of Open Quantum Systems with Quantum Dots and Microelectronic Circuits”. Total award amount: \$350,069. PHY-2310657. Award period: 07/1/2023-06/30/2026.
- National Science Foundation, Division of Chemistry, Chemical Theory, Models and Computation Program. “Theory and Simulation of Laser-Dressed Molecules and Materials” Total award amount: \$529,482. CHE-2416048. Award period: 08/01/2024-07/31/2027.
- University of Rochester, Transdisciplinary Center Award. “Center for Coherence and Quantum Science (CCQS)”. Total award amount: \$540,000. Award period: 07/01/2025-06/30/2027 (PI: Nichol, Role: co-PI).
- Pump Primer II, University of Rochester. “Many-Body Effects in PetaHertz Electronics” Total award amount: \$60,000. Award period: 01/01/2026-12/31/2027.

Completed

- Department of Energy, AMOS Program, “2025 Quantum Control in Light and Matter GRS/GRC”. Total award amount: \$10,000. Award period: 05/01/2025-09/08/2025.
- Army Research Office, Photonics, Electronics, and Quantum Sciences Branch, “2025 Quantum Control in Light and Matter GRS/GRC”. Total award amount: \$10,000. 85270-PE-CF. Award period: 05/02/2025-09/08/2025.
- Air Force Office of Scientific Research, Quantum Information Sciences, “2025 Quantum Control in Light and Matter GRS/GRC”. Total award amount: \$10,370. Award period: 05/01/2025-09/08/2025.
- Pump Primer II, University of Rochester. “Toward the development of a general package to simulate open quantum systems based on tensor network hierarchical equations of motion (TN-HEOM)” Total award amount: \$42,960. Award period: 01/01/2024-12/31/2024.
- National Science Foundation, Division of Chemistry, Chemical Theory, Models and Computation Program. “Theory and Simulation of Laser-Dressed Molecules and Materials” Total award amount: \$462,000. CHE-2102386. Award period: 06/1/2021-05/31/2024.
- Pump Primer II, University of Rochester. “Analog Quantum Simulation With Variable Particle Number” Total award amount: \$33,000. Award period: 01/01/2023-12/31/2023.
- University Research Award, University of Rochester. “Quantum Alchemy: Floquet Engineering of Qutrits Hamiltonians” Total award amount: \$37,500. Award period: 07/01/2022-6/30/2023.
- Pump Primer II, University of Rochester. “Mapping Quantum Decoherence Pathways in Molecules” Total award amount: \$50,000. Award period: 01/01/2022-12/31/2022.
- Research Award, Alexander von Humboldt Foundation. Total award amount: \$3,000. Award period: 7/01/2022-7/31/2022.
- Lewis College Award for Undergraduate Teaching and Research Mentorship. Total award amount: \$20,000. Award period: 07/01/2021-06/30/2022.
- University Research Award, University of Rochester. “Molecules for Quantum Technologies: Tackling the Decoherence Challenge.” Total award amount: \$32,500. Award period: 07/01/2021-06/30/2022.
- Leonard Mandel Faculty Fellowship on Quantum Coherence, University of Rochester. Total award amount: \$30,000. Award period: 07/01/2019-07/01/2021.

- National Science Foundation, “CAREER: Decoherence, non-equilibrium dynamics and Stark control of electrons in the nanoscale.” Total award amount: \$704,952. CHE-1553939. Award period: 02/15/2016-01/31/2021.
- Pump Primer II, University of Rochester. “Toward the development of an experimental simulator of quantum molecular dynamics.” Total award amount: \$50,000. Award period: 03/01/2019-02/28/2020.