

Ignacio Franco

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

- July 2019 – **Associate Professor**, *University of Rochester*, Rochester, NY.
- July 2013 – **Assistant Professor**, *University of Rochester*, Rochester, NY.
June 2019 Primary appointment in Chemistry. Secondary appointments in Physics and Material Science.
- Oct. 2011 – **Research Group Leader**, *Theory Department, Fritz Haber Institute of the Max Planck Society*, Berlin, Germany.
June 2013
- 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

- Vice Chair/Chair-elect, Gordon Research Conference on Quantum Control of Light and Matter, 2023-2025.
- College Award for Undergraduate Teaching and Mentorship, U. Rochester, 2021.
- Leonard Mandel Faculty Fellow in Quantum Coherence, U. Rochester, 2019-
- 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.

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- 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

Citation metrics: <https://goo.gl/McAAZ4>. * denotes corresponding author

59. C.W. Kim, A. N. Jordan, J. Nichol and I. Franco*, "Quantum Analog Simulation of the Dynamics of Open Quantum System" (to be submitted, 2021)
58. A. Garzón-Ramírez and I. Franco*, "SCELI across the molecule-semiconductor interface" (to be submitted, 2021)
57. W. Hu and I. Franco*, "Quantifying the role of electronic transitions in electronic decoherence" (to be submitted, 2021)
56. L. Mejía, U. Kleinekathöfer and I. Franco*, "Coherent and Incoherent Contributions to Molecular Electron Transport" (to be submitted, 2021)
55. T. Boolake, C. Heide, A. Garzón-Ramírez, H. Weber, I. Franco* and P. Hommelhoff*, "Light-field control of real and virtual charge carriers" (submitted, 2021)
54. 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" (submitted, 2021)
53. W. Hu, T. D. Krauss, and I. Franco*, "Protecting molecular quantum coherences by hybridization with light" (submitted, 2021)
52. L. Mejía, D. Garay-Ruiz, and I. Franco*, "Diels-Alder Reaction in a Molecular Junction", *J. Phys. Chem. C*, **125**, 14599 (2021)
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)
50. C.W. Kim and I. Franco*, "Theory of dissipation pathways in open quantum systems", *J. Chem. Phys.*, **154**, 084109 (2021)
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](#))

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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)
47. W. Hu, B. Gu and I. Franco*, "Toward the laser control of electronic decoherence", *J. Chem. Phys.*, **152**, 184305 (2020)
46. G. Cabra, I. Franco and M. Galperin*, "Optical properties of periodically-driven open nonequilibrium quantum systems", *J. Chem. Phys.*, **152**, 094101 (2020)
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).

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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).

Before Rochester:

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).

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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).

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Invited Talks

92. Dec. 16-21, 2021. ACS Pacificchem, Symposium on "Quantum Coherence in Energy Transfer" and "Modeling exciton and charge dynamics in molecules and clusters toward optoelectronic applications", 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.

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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.

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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.

Before Rochester:

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.

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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 the 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:

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 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.

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Before Rochester:

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:

- **Physical Chemistry I**, CHM251/CHM441. Fall 2016, 2018, 2019, 2020, 2021. 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.

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- **Quantum Chemistry I**, CHM451. 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**, CHM455. 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**, CHM452. Spring 2020, 2021. This course introduces 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

- Xinxian Chen, Ph.D. Student, Jan. 1, 2020– present. Expected defense date Summer 2024.
- Vishal Tiwari, Ph.D. Student, Jan. 1, 2020– present. Expected defense date Summer 2024.
- Ignacio Gustín, Ph.D. Student, Jan. 1, 2021– present. Expected defense date Summer 2025.
- Anjana Seshradi, Undergraduate Student, May 24, 2021– present.
- Aditi Seshradi, Undergraduate Student, May 24, 2021– present.
- Yueheng Min, Undergraduate Student, May 24, 2021– present.
- Luis Delgado, Undergraduate Student, May 24, 2021– present.

Alumni

- Dr. Chang Woo Kim, Postdoctoral Fellow, Sep. 2019– Aug. 2021. Currently: Assistant Professor, Chonnam National U. (Korea)
- Garrett Beals, Undergraduate Student, Jan. 1, 2020– May 2021. Currently: Ph.D. student at Columbia. [Recipient of a NSF Graduate Research Fellowship 2021.](#)
- Dr. Leopoldo Mejía, Ph.D. Student, Jan. 1, 2017– August 18, 2021. Currently: PDF at Berkeley (Rabani). [Recipient of the 2021 ACS Graduate Award in Theoretical Chemistry.](#)
- Dr. Wenxiang Hu, Ph.D. Student, Feb. 1, 2016 – May 6, 2021. Currently: Data Scientist at Amazon.
- Dr. Antonio Garzón, Ph.D. Student, Jan. 1, 2016– Feb. 25, 2021. Currently: PDF at McGill (Simine).
- Dr. Bing Gu, Postdoctoral Fellow, September 1, 2016– October 30, 2018. Currently: PDF at UC Irvine (Mukamel). [Recipient of the 2018 ACS Physical Chemistry Young Investigator Award.](#)
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- Dr. Liping Chen, Postdoctoral Fellow, July 1, 2013– March 1, 2016. Currently: Researcher at Zhejiang U.
- Dr. Arnab Kar, Postdoctoral Fellow, July 1, 2014– July 1, 2016. Currently: Engineer at Intel.
- Dr. Zhi Li, Ph.D. Student, Jan. 1, 2014– Jan 5, 2019. Currently: Data scientist at ApartmentList.
- Dr. Alessandro Pirrotta, Ph.D. Student, U. Copenhagen, 2013–2017 (co-supervised with Prof. G.C. Solomon). Currently: Data science Engineer at PFA Pension, Copenhagen.
- Daniel Carstairs, Undergraduate Student, U. Rochester. Fall 2020.
- Francisco Fernández, M.Sc. Student, U. Madrid. Summer 2019. Currently: Ph.D. student at UAM.
- Yuly Chamorro, Visiting M.Sc. Student, Jan 15, 2019– May 15, 2019. Currently: Ph.D. student at Groningen.
- Rachel Carey, M.Sc. Student, Jan. 1, 2014– April 1, 2017. Now candidate at Sisters of Saint Joseph.
- Diego Garay, Undergraduate Student, U. Barcelona. Summer 2018. Currently: Ph.D. student at U. Barcelona.
- Pawel Wojcik, Undergraduate Student, U. Warsaw, Poland. Summer 2017. Currently: Ph.D. student with Anna Krylov at USC.
- Reshmi Dani, Undergraduate Student, IIT-Guwahati, India. Summer 2016. Currently: Ph.D. student with Nancy Makri at U. Illinois.
- Ulises Torres, Undergraduate Student, UNAM, Mexico. Summer 2015. Now Ph.D. student at UNAM.

Departmental and Professional Service:

Conference organizer/advisor:

- Co-organizer, Biennial Telluride workshop on “Quantum Frontiers in Molecular Science”, June 26-30, 2018 and June 22-26, 2020.
- 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.

University Service:

- Founding Member, Diversity, Equity and Inclusion Committee, Chem. Dept., U. Rochester, 2020–.
- Coordinator and Founder, Summer Research Fellowship Program for International Students, Chem. Dept., U. Rochester, 2015–2018.
- Member, Executive Committee, Center for Coherence and Quantum Optics, U. Rochester. 2014–.

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- Other U. Rochester Departmental Committees: Awards, 2018–; Development/News-Promotion, 2018–, Colloquium/Distinguished Lecturers & Seminars, 2016–2018; Graduate Recruiting, 2013–2018; Graduate Studies, 2015–2016, 2018–2019; Faculty Recruiting, 2014–2015, 2019–2020, Services/Space: 2020–2021, Undergraduate Studies: 2020–, Faculty Senate Sub-Committee on Faculty Club, 2017–.

Professional Service:

- *Reviewer for the following scientific journals:* Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Journal of Chemical Physics, Nature, Nature Chemistry, Nature Communications, Journal of Chemical Theory and Computation, Nanoscale, NanoLetters, ACS Nano, Journal of the American Chemical Society, Scientific Reports, Optica, ACS Applied Materials & Interfaces, Chemical Physics, JSTAT, Angewante Chemie, Chemical Science, ACS Sensors
- *Reviewer for the following funding agencies:* Petroleum Research Fund, NSF (ad-hoc and panelist), NSF CCI, DOE, Center for Integrated Nanotechnologies, Netherlands Organisation for Scientific Research, CECAM.
- Member, Board of Directors, Newman School, Bogotá, Colombia. 2007–.

Other

- *Languages:* Fluent in Spanish (native) and English. Basic communication skills in Italian.
- *Professional memberships:* American Chemical Society, American Physical Society.

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