



# Xiaosong Li

LARRY R. DALTON ENDOWED CHAIR IN CHEMISTRY

ASSOCIATE DEAN FOR RESEARCH, COLLEGE OF ARTS & SCIENCES

DIRECTOR OF EARLY CAREER NETWORK, IDREAM, DEPARTMENT OF ENERGY ENERGY FRONTIER RESEARCH CENTER

ADJUNCT PROFESSOR OF MATERIALS SCIENCE & ENGINEERING

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## Professional Experience

### University of Washington

ASSOCIATE DEAN FOR RESEARCH, COLLEGE OF ARTS & SCIENCES	<i>Seattle, WA</i>
ASSOCIATE VICE PROVOST FOR RESEARCH CYBERINFRASTRUCTURE	2024 - present
LARRY R. DALTON ENDOWED CHAIR IN CHEMISTRY	2022 - 2024
HARRY AND CATHERINE JAYNE BOARD ENDOWED PROFESSOR OF CHEMISTRY	2022 - present
ASSOCIATE CHAIR OF GRADUATE PROGRAM	2017 - 2022
EXECUTIVE DIRECTOR OF EDUCATION AND OUTREACH, MOLECULAR ENGINEERING MATERIALS CENTER	2018 - 2023
DIRECTOR, MASTER OF SCIENCE IN APPLIED CHEMICAL SCIENCE AND TECHNOLOGY	2020 - 2024
ADJUNCT PROFESSOR OF MATERIALS SCIENCE AND ENGINEERING	2019 - 2022
PROFESSOR OF CHEMISTRY	2018 - present
ASSOCIATE PROFESSOR OF CHEMISTRY	2015 - present
ASSISTANT PROFESSOR OF CHEMISTRY	2012 - 2015
	2005 - 2012

### Pacific Northwest National Laboratory

LAB FELLOW (DUAL APPOINTMENT)	2020 - present
DIRECTOR OF EARLY CAREER NETWORK, IDREAM, DEPARTMENT OF ENERGY ENERGY FRONTIER RESEARCH CENTER	2021 - present

### American Institute of Physics

EDITOR-IN-CHIEF, APL COMPUTATIONAL PHYSICS	2025 - present
ASSOCIATE EDITOR, CHEMICAL PHYSICS REVIEWS	2020 - 2024

## Education

### Yale University

POSTDOCTORAL RESEARCH ASSOCIATE	<i>New Haven, CT</i>
ADVISOR: PROF. JOHN C. TULLY	Aug. 2003 - Jul. 2005

### Wayne State University

PH. D., THEORETICAL CHEMISTRY	<i>Detroit, MI</i>
ADVISOR: PROF. H. BERNHARD SCHLEGEL	Aug. 1999 - Jul. 2003

### University of Science and Technology of China

B.S., CHEMICAL PHYSICS	<i>Hefei, China</i>
ADVISOR: PROF. QINQIANG GUO	Aug. 1994 - Jul. 1999

## Honors & Awards

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- 2025 **Fellow**, American Association for the Advancement of Science (AAAS)
- 2024 **Jack Simons Award in Theoretical Chemistry**, American Chemistry Society
- 2023 **Fellow**, Royal Society of Chemistry
- 2022 **Elected Member**, Washington State Academy of Sciences
- 2022 **Nominee, Distinguished Graduate Mentor Award**, University of Washington
- 2021 **Fellow**, American Physical Society
- 2020 **Distinguished Teaching Award**, University of Washington
- 2020 **Lab Fellow**, Pacific Northwest National Lab
- 2018 **Zhang Dayu Young Investigator Lectureship**, Dalian Institute of Chemical Physics
- 2017 **Harry and Catherine Jayne Boand Endowed Professor of Chemistry**, University of Washington
- 2017 **Department of Chemistry Faculty Lectureship**, University of Washington
- 2017 **Commute Champion**, University of Washington
- 2012 **Outstanding Junior Faculty Award in Computational Chemistry**, American Chemical Society
- 2011 **Sloan Research Fellowship**, Alfred P. Sloan Foundation
- 2011 **Phi Lambda Upsilon Faculty Mentor Award**, University of Washington
- 2009 **CAREER Award**, National Science Foundation

## Research Interest

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- **Relativistic Electronic Structure Theory:** We are working on advanced methods to study molecules containing rear-earth and heavy elements and simulate relativistic spectroscopies. Our approach is based on variational treatments of the relativistic Dirac equation, enabling accurate analysis of relativistic interactions, including scalar relativities and spin-orbit coupling. We focus on employing two- and four-component treatments with the Dirac–Coulomb–Breit operator to accurately predict the chemical and spectroscopic characteristics of heavy elements and magnetic systems, as well as dynamic processes involving changes in the molecular spin state. This project is currently funded by
  - DOE Heavy-Element Chemistry supporting the development of relativistic multi-reference many-body theory toward heavy-element chemistry
  - DOE Computational & Theoretical Chemistry supporting the development of quantum field many-body theory
- **Real-Time Time-Dependent Many-Body Theory:** We are developing theories and computational methods to study how many-electron systems respond to external forces like electromagnetic fields and internal interactions involving electron spins. We focus on advanced methods like real-time time-dependent density functional theory (RT-TDDFT), time-dependent equation-of-motion coupled-cluster (RT-EOM-CC), and time-dependent configuration interaction (RT-CI), and extensions of these methods for more complex, relativistic systems. These tools will enhance our understanding of electron dynamics, including ultrafast charge transfer and spin behaviors. This project is currently funded by
  - DOE Computational Chemical Sciences supporting the development of RT-TDDFT beyond the dipole approximation
  - DOE Scientific Discovery through Advanced Computing supporting the development of RT-EOM-CC
- **First-Principles Nonadiabatic Dynamics and Nuclear–Electronic Orbital Theory:** We are developing quantum and mixed quantum-classical methodologies to simulate non-adiabatic dynamics, with a focus on photochemical processes. Our approaches include *ab initio* Ehrenfest dynamics, surface-hopping, and the nuclear-electronic orbital (NEO) theory. These methods are integrated with relativistic electronic structure theory, enabling efficient simulations of spin-driven chemical processes. This project is funded by
  - DOE Computational Chemical Sciences supporting the development of multi-scale NEO method

- NSF Cyberinfrastructure for Sustained Scientific Innovation supporting the development of an open-source software infrastructure for NEO-based methods
- **Computational Spectroscopies and Photochemical Processes:** We are working on developing highly accurate and computationally efficient computational spectroscopy methodologies. These include density functional theory and multi-reference many-body theory, applicable in both relativistic and non-relativistic frameworks, to simulate spectroscopic measurements. Our focus is primarily on relativistic spectroscopies, such as X-ray spectroscopy (XAS, XES, RIXS), magneto-optical photo-absorption (MPA), magnetic circular dichroism (MCD), and magnetic hysteresis. This project is currently funded by
  - NSF Chemical Theory, Models, and Computational Methods supporting the development of computational MPA and MCD methods
  - DOE Computational Chemical Sciences supporting the development of EOM-CC methods for computing polariton chemistry
  - DOE Solar Photochemistry supporting simulations of ultrafast excited state dynamics in transition metal complexes
  - DOD AFSOR Molecular Dynamics and Theoretical Chemistry supporting supporting studies of spin-driven chemical processes
  - DOE IDREAM EFRC supporting studies of radiation driven chemical processes
- **Computational Molecular Sciences:** The program is focused on designing molecular systems and nanocrystals with unique electronic, optical, and magnetic characteristics for potential applications in photonics, spintronics, and photovoltaics. We are particularly interested in how defects and dopants induce magnetism and activate new photochemical processes, and the methods to control their reaction pathways using quantum mechanical processes. Our aim is to understand and harness these properties for advanced technological applications. This project is currently funded by
  - NSF UW MRSEC supporting studies of magnetic defects in nanocrystals to explore new electronic, optical, and magnetic characteristics
  - DOD ONR MURI supporting studies of photodoping in organic semiconductors
  - DOD AFOSR MURI supporting studies of interplays of chirality and spin in chiral assemblies
- **AI and Quantum Information Sciences:** We are exploring innovative solutions to overcome the challenges associated with the quantum information sciences. The noise and errors introduced during the quantum measurement step, particularly with a constrained measurement budget, are hurdles in realizing the full potential of the quantum computing technology for solving complex quantum chemistry problems. We are focused on numerical and AI strategies to mitigate the noise and errors in quantum measurement. These strategies aim to enhance the convergence of Variational Quantum Eigensolver (VQE) and diminish the required number of shots for simulations on quantum computers. Additionally, we are investigating the potential of using rare-earth and heavy-element based molecular magnets for realizing quantum sensors and information processing. This project is currently funded by the
  - NSF Principles and Practice of Scalable Systems supporting the development of quantum algorithm for quantum chemistry
  - DOE Quantum Information Sciences supporting studies of rare-earth and heavy-element complexes for potential use in quantum information sciences

## Publications (Google Scholar h-index 67; ~16,000 Publication Citations; ~69,000 Software Citations)

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- [304] S. M. Garner, S. Upadhyay, X. Li and S. Hammes-Schiffer, “Time-resolved Vibronic Spectra with Nuclear-Electronic Orbital Time-dependent Configuration Interaction”, *J. Chem. Phys.*, **2025**, *162*, 044108.
- [303] P. Kim, S. Roy, A. J. S. Valentine, X. Liu, S. Kromer, T. W. Kim, X. Li, F. N. Castellano and L. X. Chen, “Real-Time Capture of Nuclear Motions Influencing Photoinduced Electron Transfer”, *Chem. Sci.*, **2024**, *15*, 14766–14777.
- [302] D. Tang, S. Sun and X. Li, “Exact-Two-Component Complete Active Space Method with Variational Treatment of Magnetic Field and Spin–Orbit Coupling: Application to X-ray Magnetic Circular Dichroism Spectroscopy”, *J. Chem. Theory Comput.*, **2024**, *20*, 9917–9927.
- [301] S. Liang, L. Zhu, X. Liu, C. Yang and X. Li, “Artificial-Intelligence-Driven Shot Reduction in Quantum Measurement”, *Chem. Phys. Rev.*, **2024**, *5*, 041403.
- [300] H. Hu, S. Upadhyay, L. Lu, A. J. Jenkins, T. Zhang, A. Shayit, S. Knecht and X. Li, “Small Tensor Product Distributed Active Space (STP-DAS) Framework for Relativistic and Non-relativistic Multiconfiguration Calculations: Scaling from  $10^9$  on a Laptop to  $10^{12}$  Determinants on a Supercomputer”, *Chem. Phys. Rev.*, **2024**, *5*, 041404.
- [299] C. E. Hoyer, C. Liao, K. D. Shumilov, T. Zhang and X. Li, “State Interaction for Relativistic Four-Component Methods: Choose the Right Zeroth-Order Hamiltonian for Late-Row Elements”, *J. Chem. Theory Comput.*, **2024**, *20*, 7969–7978.
- [298] D. Dou, X. Zhou, T. Wang, Q. Yang, X. Tan, Z. Ling, M. Manz, X. Liu, G.-J. A. H. Wetzelaer, X. Li, M. Baumgarten, P. W. M. Blom and Y. Li, “Intramolecular Through-Space Charge-Transfer Effect for Achieving Room-Temperature Phosphorescence in Amorphous Film”, *Advanced Optical Materials*, **2024**, *12*, 2400976.
- [297] M. Kovtun, E. Lambros, A. Liu, D. Tang, D. B. Williams-Young and X. Li, “Accelerating Relativistic Exact-Two-Component Density Functional Theory Calculations with Graphical Processing Units”, *J. Chem. Theory Comput.*, **2024**, *20*, 7694–7699.
- [296] S. H. Yuwono, R. R. Li, T. Zhang, K. A. Surjuse, E. F. Valeev, X. Li and A. I. Eugene DePrince, “Relativistic Coupled Cluster with Completely Renormalized and Perturbative Triples Corrections”, *J. Phys. Chem. A*, **2024**, *128*, 6521–6539.
- [295] S. Sun, B. Gu, H. Hu, L. Lu, D. Tang, V. Y. Chernyak, X. Li and S. Mukamel, “Direct Probe of Conical Intersection Photochemistry by Time-Resolved X-ray Magnetic Circular Dichroism”, *J. Am. Chem. Soc.*, **2024**, *146*, 19863–19873.
- [294] H. Li, T. Wang, J. Han, Y. Xu, X. Kang, X. Li and M. Zhu, “Fluorescence Resonance Energy Transfer in Atomically Precise Metal Nanoclusters by Cocrystallization-Induced Spatial Confinement”, *Nat. Commun.*, **2024**, *15*, 5351.
- [293] S. M. Garner, S. Upadhyay, X. Li and S. Hammes-Schiffer, “Nuclear–Electronic Orbital Time-Dependent Configuration Interaction Method”, *J. Phys. Chem. Lett.*, **2024**, *15*, 6017–6023.
- [292] M. W. Mara, N. P. Weingartz, D. Leshchev, D. Hsu, A. Valentine, A. Mills, S. Roy, A. Chakraborty, P. Kim, E. Biasin, K. Haldrup, M. S. Kirschner, D. Rimmerman, M. Chollet, J. M. Glowina, T. B. vanDriel, F. N. Castellano, X. Li and L. X. Chen, “Deciphering Charge Transfer Processes in Transition Metal Complexes from the Perspective of Ultrafast Electronic and Nuclear Motions”, *J. Phys. Chem. Lett.*, **2024**, *15*, 5250–5258.
- [291] T. Zhang, S. Banerjee, L. N. Koulias, E. F. Valeev, A. E. I. DePrince and X. Li, “Dirac–Coulomb–Breit Molecular Mean-Field Exact-Two-Component Relativistic Equation-of-Motion Coupled-Cluster Theory”, *J. Phys. Chem. A*, **2024**, *128*, 3408–3418.
- [290] K. D. Shumilov, A. J. Jenkins, H. S. La Pierre, B. Vlasisavljevich and X. Li, “Overdestabilization vs Overstabilization in the Theoretical Analysis of f-Orbital Covalency”, *J. Am. Chem. Soc.*, **2024**, *146*, 12030–12039.
- [289] E. Lambros, J. H. Fetherolf, S. Hammes-Schiffer and X. Li, “A Many-Body Perspective of Nuclear Quantum Effects in Aqueous Clusters”, *J. Phys. Chem. Lett.*, **2024**, *15*, 4070–4075.



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- [287] H. Tateyama, A. C. Boggiano, C. Liao, K. S. Otte, X. Li and H. S. La Pierre, “Tetravalent Cerium Alkyl and Benzyl Complexes”, *J. Am. Chem. Soc.*, **2024**, *146*, 10268–10273.
- [286] C. Liao, C. E. Hoyer, R. Banerjee Ghosh, A. J. Jenkins, S. Knecht, M. J. Frisch and X. Li, “Comparison of Variational and Perturbative Spin–Orbit Coupling within Two-Component CASSCF”, *J. Phys. Chem. A*, **2024**, *128*, 2498–2506.
- [285] L. Zhu, S. Liang, C. Yang and X. Li, “Optimizing Shot Assignment in Variational Quantum Eigensolver Measurement”, *J. Chem. Theory Comput.*, **2024**, *20*, 2390–2403.
- [284] J. N. Ehrman, K. Shumilov, A. J. Jenkins, J. M. Kasper, T. Vitova, E. R. Batista, P. Yang and X. Li, “Unveiling Hidden Shake-Up Features in the Uranyl M4-Edge Spectrum”, *JACS Au*, **2024**, *4*, 1134–1141.
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- [282] E. S. Ryland, X. Liu, G. Kumar, S. L. Raj, Z.-L. Xie, A. K. Mengele, S. S. Fauth, K. Siewerth, B. Dietzek-Ivanšić, S. Rau, K. L. Mulfort, X. Li and A. A. Cordones, “Site-specific Electronic Structure of Covalently Linked Bimetallic Dyads from Nitrogen K-edge X-ray Absorption Spectroscopy”, *J. Chem. Phys.*, **2024**, *160*, 084307.
- [281] S. Li, L. Lu, S. Bhattacharyya, C. Pearce, K. Li, E. Nienhuis, G. Doumy, R. Schaller, S. Moeller, M.-F. Lin, G. Dakovski, D. Hoffman, D. Garratt, K. Larsen, J. Koralek, C. Hampton, D. DePonte, J. Cryan, A. Marinelli, X. Li, L. Inhester, R. Santra and L. Young, “Attosecond-Pump Attosecond-Probe X-ray Spectroscopy of Liquid Water”, *Science*, **2024**, *382*, 1118–1122.
- [280] S. F. Sandeno, K. J. Schnitzenbaumer, S. M. Krajewski, R. A. Beck, D. M. Ladd, K. R. Levine, D. Dayton, M. F. Toney, W. Kaminsky, X. Li and B. M. Cossairt, “Ligand Steric Profile Tunes the Reactivity of Indium Phosphide Clusters”, *J. Am. Chem. Soc.*, **2024**, *146*, 3102–3113.
- [279] C. Liao, E. Lambros, Q. Sun, K. G. Dyall and X. Li, “Exploring Locality in Molecular Dirac–Coulomb–Breit Calculations: A Perspective”, *J. Chem. Theory Comput.*, **2023**, *19*, 9009–9017.
- [278] E. Lambros, B. Link, M. Chow, F. Lipparini, S. Hammes-Schiffer and X. Li, “Assessing Implicit and Explicit Polarizable Solvation Models for Nuclear–Electronic Orbital Systems: Quantum Proton Polarization and Solvation Energetics”, *J. Phys. Chem. A*, **2023**, *127*, 9322–9333.
- [277] R. Di Felice, M. L. Mayes, R. M. Richard, D. B. Williams-Young, G. K.-L. Chan, W. A. deJong, N. Govind, M. Head-Gordon, M. R. Hermes, K. Kowalski, X. Li, H. Lischka, K. T. Mueller, E. Mutlu, A. M. N. Niklasson, M. R. Pederson, B. Peng, R. Shepard, E. F. Valeev, M. vanSchilfgaarde, B. Vlasisavljevich, T. L. Windus, S. S. Xantheas, X. Zhang and P. M. Zimmerman, “A Perspective on Sustainable Computational Chemistry Software Development and Integration”, *J. Chem. Theory Comput.*, **2023**, *19*, 7056–7076.
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- [273] J. Ehrman, E. Martinez-Baez, A. J. Jenkins and X. Li, “Improving One-Electron Exact-Two-Component Relativistic Methods with the Dirac–Coulomb–Breit-Parameterized Effective Spin–Orbit Coupling”, *J. Chem. Theory Comput.*, **2023**, *19*, 5785–5790.
- [272] S. H. Yuwono, B. C. Cooper, T. Zhang, X. Li and I. DePrinceA. Eugene, “Time-Dependent Equation-of-Motion Coupled-Cluster Simulations with a Defective Hamiltonian”, *J. Chem. Phys.*, **2023**, *159*, 044113.

- [271] M. Chow, E. Lambros, X. Li and S. Hammes-Schiffer, “Nuclear–Electronic Orbital QM/MM Approach: Geometry Optimizations and Molecular Dynamics”, *J. Chem. Theory Comput.*, **2023**, *19*, 3839–3848.
- [270] S. Sun, J. Ehrman, T. Zhang, Q. Sun, K. G. Dyall and X. Li, “Scalar Breit Interaction for Molecular Calculations”, *J. Chem. Phys.*, **2023**, *158*, 171101.
- [269] D. Leshchev, A. Valentine, P. Kim, A. Mills, a. chakraborty, E. Biasin, K. Haldrup, D. Hsu, M. Kirschner, D. Rimmerman, M. Chollet, J. Glowina, T. vanDriel, F. Castellano, X. Li and L. X. Chen, “Revealing Excited State Trajectories on Potential Energy Surfaces with Atomic Resolution in Real Time”, *Angew. Chem. Int. Ed.*, **2023**, *62*, e202304615.
- [268] N. Park, R. A. Beck, K. K. Hoang, D. M. Ladd, J. E. Abramson, R. A. Rivera-Maldonado, H. A. Nguyen, M. Monahan, G. T. Seidler, M. F. Toney, X. Li and B. M. Cossairt, “Colloidal, Room-Temperature Growth of Metal Oxide Shells on InP Quantum Dots”, *Inorg. Chem.*, **2023**, *62*, 6674–6687.
- [267] C. Liao, M. Zhu, D.-e. Jiang and X. Li, “Manifestation of the Interplay between Spin–Orbit and Jahn–Teller Effects in Au<sub>25</sub> Superatom UV-Vis Fingerprint Spectra”, *Chem. Sci.*, **2023**, *14*, 4666–4671.
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## Invited Presentations (Total 220 to date)

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### Talks at Conferences and Other Scientific Meetings

144	Manipulating Molecular Electronic Properties by Vibrational Excitations: Novel Spectroscopies and Microscopies	<i>Bad Honnef, Germany</i>	Aug. 2025
143	Excited State Processes, Princeton Center for Theoretical Science	<i>Santa Fe, NM</i>	Jun. 2025
142	Nonadiabatic Dynamics, Electron-phonon Interactions, and Spin-phonon Couplings, Princeton Center for Theoretical Science	<i>Princeton, NJ</i>	Apr. 2025
141	Simulating Excited States, ACS National Meeting	<i>San Diego, CA</i>	Mar. 2025
140	Congress of the International Society for Theoretical Chemical Physics	<i>Qingdao, China</i>	Oct. 2024
139	International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics	<i>Groningen, Netherlands</i>	Oct. 2024
138	PHYS Awards, ACS National Meeting	<i>Denver, CO</i>	Aug. 2024
137	Symposium in Honor of the 80th Birthday of Prof. Donald G. Truhlar, ACS National Meeting	<i>Denver, CO</i>	Aug. 2024
136	Electron Donor-Acceptor Interactions, Gordon Research Conference	<i>Newport, RI</i>	Jul. 2024
135	American Conference on Theoretical Chemistry	<i>Chapel Hill, NC</i>	Jun. 2024
134	Materials Research by the LGBTQIA+ Community and a Vision for Inclusivity, MRS National Meeting	<i>Seattle, WA</i>	Apr. 2024
133	Informed Design of Quantum Dots and Quantum Dot Assemblies for Energy Applications, ACS National Meeting	<i>New Orleans, LA</i>	Mar. 2024
132	Recent Progress in Theoretical Methods for Coupled Quantum Systems, ACS National Meeting	<i>New Orleans, LA</i>	Mar. 2024
131	SIAM Conference on Parallel Processing for Scientific Computing	<i>Baltimore, MD</i>	Mar. 2024
130	Probing Structure and Dynamics with XUV and X-Ray Light: Ultrafast Studies of Photocatalysis and Water Radiolysis, APS National Meeting	<i>Minneapolis, MN</i>	Mar. 2024
129	The Path of Quantum Chemistry into the 21st Century	<i>Zürich, Switzerland</i>	Jan. 2024
128	AVS 69th International Symposium	<i>Portland, OR</i>	Nov. 2023
127	Summer Modeling 2023	<i>Castiglione della Pescaia, Italy</i>	Sep. 2023
126	Quantum International Frontiers	<i>Łódź, Poland</i>	Jun. 2023
125	Westlake Theory Symposium	<i>Hanzhou, China</i>	Apr. 2023
124	Award for Computers in Chemical & Pharmaceutical Research, ACS National Meeting	<i>Indianapolis, IN</i>	Mar. 2023
123	Science & Technology of Emerging Materials Symposium (STEMS)	<i>Orlando, FL</i>	Mar. 2023
122	2nd Theory Frontiers in Actinide Science (FACT)	<i>Santa Fe, NM</i>	Feb. 2023
121	13th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics	<i>Assisi, Italy</i>	Sep. 2022
120	Status and Perspectives of Computational Chemistry Toward 2030	<i>Ischia Island, Italy</i>	Sep. 2022
119	7th International Conference on Chemical Bonding	<i>Kauai, HI</i>	Sep. 2022

118	Computational Methods for Lanthanides and Actinides, ACS National Meeting	Chicago, IL	Aug. 2022
117	Open-source Software in Chemistry, ACS National Meeting	Chicago, IL	Aug. 2022
116	40 Years of Exploring Potential Energy Surfaces, ACS National Meeting	Chicago, IL	Aug. 2022
115	Quantum Chemistry: Current and Future Frontiers, ACS National Meeting	Chicago, IL	Aug. 2022
114	Electron Donor Acceptor Interactions, Gordon Research Conference	Newport, RI	Aug. 2022
113	Molecular Interactions and Dynamics, Gordon Research Conference	Easton, RI	Jul. 2022
112	Computational Science Applications in Nuclear & Radiochemistry, ACS National Meeting	San Diego, CA	Mar. 2022
111	Modeling Exciton and Charge Dynamics in Molecules and Clusters toward Optoelectronic Applications, Pacificchem	Honolulu, Hawaii	Dec. 2021
111	Quantum Coherence in Energy Transfer, Pacificchem	Honolulu, Hawaii	Dec. 2021
110	Heavy Element Chemistry: From Theoretical Development to Application, Pacificchem	Honolulu, Hawaii	Dec. 2021
109	Research Needs for Critical Minerals & Materials, ALS User Meeting	Virtual	Aug. 2021
108	Argonne National Lab Colloquium, Division of Chemical Sciences	Virtual	Apr. 2021
107	VISTA Symposium	Virtual	Mar. 2021
106	Molecular Quantum Dynamics	Virtual	Mar. 2021
105	Surface Science and Catalysis Studies by Advanced Techniques	Virtual	Jan. 2021
104	Theory and Simulation of Electronic and Optical Processes in Molecules and Materials	Virtual	Nov. 2020
103	Nuclear Chemistry and Technology, ACS National Meeting	Virtual	Jun. 2020
102	Low-scaling and Unconventional Electronic Structure Techniques	Virtual	Jun. 2020
101	Theory Frontiers in Actinide Sciences: Chemistry and Materials	Santa Fe, NM	Feb. 2020
100	Xiamen Workshop on Physical Chemistry	Xiamen, China	Dec. 2019
99	( <i>Frontier Lecture</i> ) Quantum International Frontiers	Shanghai, China	Nov. 2019
98	Next Generation Tohoku Synchrotron Facility Workshop Program	Seattle, WA	Oct. 2019
97	Mathematics of Quantum Physics, Math Frontiers Webinars, National Academies of Sciences, Engineering, and Medicine	Seattle, WA	Oct. 2019
96	Developments & Challenges in X-ray Spectroscopies and Ultrafast Dynamics: Experiment and Theory, SLAC National Accelerator Laboratory	Menlo Park, CA	Sep. 2019
95	Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry, ACS National Meeting	San Diego, CA	Aug. 2019
94	Computational Chemistry Workshop	Shenzhen, China	Aug. 2019
93	( <i>Keynote Speaker</i> ) 1st Symposium for Theoretical & Physical Chemistry Center, Southern University of Science and Technology	ShenZhen, China	Jul. 2019
92	Aspects of Heavy-Element Chemistry, 10th Congress of the International Society of Theoretical Chemical Physics (ISTCP-X)	Tromso, Norway	Jul. 2019
91	Theory Summit – IDREAM: Interfacial Dynamics in Radioactive Environments and Materials	Pullman, WA	Jun 2019
90	DOE Computational and Theoretical Chemistry Meeting	Gaithersburg, MD	May 2019

89	Modeling Dynamics in Dense Manifolds of Electronic States, ACS National Meeting	<i>Orlando, FL</i>	Mar. 2019
88	Sustainable Software for Computational Molecular Science, ACS National Meeting	<i>Orlando, FL</i>	Mar. 2019
87	Addressing Molecular Magnetic Qubits, APS National Meeting	<i>Boston, MA</i>	Mar. 2019
86	University of Washington – Tohoku University Academic Open Space Workshop	<i>Sendai, Japan</i>	Oct. 2018
85	From Potential Energy Surfaces to Dynamics & Kinetics, ACS National Meeting	<i>Boston, MA</i>	Aug. 2018
84	Computational Photocatalysis: Modeling of Photophysics & Photochemistry at Interfaces, ACS National Meeting	<i>Boston, MA</i>	Aug. 2018
83	Recent Advances in DFT & TDDFT: Theory & Simulations, ACS National Meeting	<i>Boston, MA</i>	Aug. 2018
82	Parallel Computing in Molecular Sciences	<i>Berkeley, CA</i>	Aug. 2018
81	Computational Chemistry, Gordon Research Conference	<i>Mount Snow, VT</i>	Jul. 2018
80	Developments in QM/MM and Embedding Models for Photochemical and Electron Transfer Processes	<i>Telluride, CO</i>	Jul. 2018
79	International Congress of Quantum Chemistry, Photoinduced Processes in Embedded Systems	<i>Pisa, Italy</i>	Jun 2018
78	Low-scaling and Unconventional Electronic Structure Techniques	<i>Telluride, CO</i>	Jun 2018
77	DOE Energy Frontier Center Meeting	<i>Gaithersburg, MD</i>	Apr. 2018
76	Zhang Dayu Young Investigator Lectureship, Dalian Institute of Chemical Physics	<i>Dalian, China</i>	Mar. 2018
75	Chirality from Molecules to Materials, ACS National Meeting	<i>New Orleans, LA</i>	Mar. 2018
74	University of Washington – Tohoku University Academic Open Space Workshop	<i>Seattle, WA</i>	Nov. 2017
73	DOE Condensed Phase and Interfacial Molecular Science Research Meeting	<i>Gaithersburg, MD</i>	Oct. 2017
72	World Association of Theoretical and Computational Chemists (WATOC)	<i>Munich, Germany</i>	Aug. 2017
71	DOE Energy Frontier Center Meeting	<i>Gaithersburg, MD</i>	Jul. 2017
70	Excited State Electronic Structure and Dynamics	<i>Telluride, CO</i>	Jul. 2017
69	(Plenary Lecture) Computational Software Workshop, National Science Foundation of China	<i>Dalian, China</i>	Jun. 2017
68	DOE Computational and Theoretical Chemistry Meeting	<i>Gaithersburg, MD</i>	May 2017
67	Strong Electron Correlation & Nonadiabatic Dynamics, ACS National Meeting	<i>San Francisco, CA</i>	Apr. 2017
66	In Silico Materials Chemistry, MRS National Meeting	<i>Boston, MA</i>	Nov. 2016
65	Workshop on Theoretical Chemistry	<i>Trujillo, Peru</i>	Sep. 2016
64	Molecular Electronic Structure Workshop	<i>Buenos Aires, Argentina</i>	Sep. 2016
63	Theory and Application of Computational Chemistry	<i>Seattle, WA</i>	Aug. 2016
62	Computational Chemistry Workshop	<i>Changchun, China</i>	Aug. 2016
61	Complex Systems Symposium, The 9th International Symposium of Theoretical Chemical Physics,	<i>Grand Forks, ND</i>	Jul. 2016
60	The 21st International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXI)	<i>Vancouver, Canada</i>	Jul. 2016
59	DOE Solar Photochemistry Meeting	<i>Gaithersburg, MD</i>	Jun. 2016

58	Low-scaling and Unconventional Electronic Structure Techniques	<i>Telluride, CO</i>	Jun. 2016
57	DOE Computational and Theoretical Chemistry Meeting	<i>Gaithersburg, MD</i>	May 2016
56	Time-Dependent Dynamics and Electronic Excited States, ACS National Meeting	<i>San Diego, CA</i>	Mar. 2016
55	Sanibel Symposium	<i>St. Simons Island, GA</i>	Feb. 2016
54	Mesilla Workshop	<i>Mesilla, NM</i>	Jan. 2016
53	Photocatalysis and Charge Transfer at Interfaces and Nanomaterials, Pacificchem	<i>Honolulu, HI</i>	Dec. 2015
52	Quantum Coherence in Energy Transfer, Pacificchem	<i>Honolulu, HI</i>	Dec. 2015
51	Computational Modeling of Magnetic Materials and Magnetic, Properties, Pacificchem	<i>Honolulu, HI</i>	Dec. 2015
50	Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Cluster, Pacificchem	<i>Honolulu, HI</i>	Dec. 2015
49	Open Quantum Systems Computational Methods	<i>Hong Kong, China</i>	Nov. 2015
48	Electronic Structure and Processes at Molecular-Based Interfaces VIII	<i>Tucson, AZ</i>	Oct. 2015
47	Non-equilibrium Phenomena	<i>Telluride, CO</i>	Jul. 2015
46	Excited State Electronic Structure Theory and Dynamics	<i>Telluride, CO</i>	Jul. 2015
45	Nanomaterials: Computation, Theory, and Experiment	<i>Telluride, CO</i>	Jun. 2015
44	Advances in Theoretical Spectroscopy	<i>Seattle, WA</i>	Jun. 2015
43	The 26th Annual Workshop on Recent Developments in Electronic Structure Theory	<i>Seattle, WA</i>	Jun. 2015
42	15th International Congress of Quantum Chemistry	<i>Beijing, China</i>	Jun. 2015
41	Charge Transfer Modeling in Chemistry: New Methods and Solutions for a Long-standing Problem	<i>Paris, France</i>	Apr. 2015
40	Electronic Structure Methods for Highly Polarizable Systems, 249th ACS National Meeting	<i>Denver, CO</i>	Mar. 2015
39	Modeling Excited States of Complex Systems, 249th ACS National Meeting	<i>Denver, CO</i>	Mar. 2015
38	Chemical Approaches to Spintronics Research, 249th ACS National Meeting	<i>Denver, CO</i>	Mar. 2015
37	Quantum Systems in Chemistry, Physics and Biology	<i>Taipei, Taiwan</i>	Nov. 2014
36	World Association of Theoretical and Computational Chemists (WATOC)	<i>Santiago, Chile</i>	Oct. 2014
35	Molecular Electronic Structure	<i>Amasya, Turkey</i>	Sep. 2014
34	International Conference on Chemical Bonding	<i>Kauai, HI</i>	Jul. 2014
33	Colloidal Semiconductor Nanocrystals, Gordon Research Conference	<i>Smithfield, RI,</i>	Jul. 2014
32	Excited State and Time-Dependent Electronic Structure Theory	<i>Telluride, CO</i>	Jul. 2014
31	12th Chinese National Meeting on Theoretical Chemistry	<i>Taiyuan, China</i>	Jun. 2014
30	Excited State Processes in Electronic and Nanomaterials	<i>Santa Fe, NM</i>	Jun. 2014
29	XXXVII Brazilian National Meeting of Condensed Matter Physicists	<i>Salvador, Brazil</i>	May 2014
28	Computational Photocatalysis, 246th ACS National Meeting	<i>Indianapolis, IN</i>	Sep. 2013
27	Nonequilibrium Phenomena, Nonadiabatic Dynamics	<i>Telluride, CO</i>	Jul. 2013
26	ACS Award Symposium, 245th ACS National Meeting	<i>New Orleans, LA</i>	Mar. 2013



25	Computational Methods for Complex Systems	<i>Hong Kong, China</i>	Dec. 2012
24	Connecticut Quantum Chemistry Meeting	<i>Wallingford, CT</i>	Oct. 2012
23	International Conference on Multiscale Materials Modeling	<i>Singapore</i>	Oct. 2012
22	Troy Electronic Structure Workshop	<i>Canakkale, Turkey</i>	Sep. 2012
21	Spintronics, SPIE	<i>San Diego, CA</i>	Aug. 2012
20	Geometry Optimization, 244th ACS National Meeting	<i>Philadelphia, PA</i>	Aug. 2012
19	Nanomaterials: Theory and Computation, Telluride Science Research Conference	<i>Telluride, CO</i>	Jul. 2012
18	Low-scaling and Unconventional Electronic Structure Techniques, Telluride Science Research Conference	<i>Telluride CO</i>	Jun. 2012
17	Applications of Computational Methods to Environmentally Sustainable Solutions, 243rd ACS National Meeting	<i>San Diego, CA</i>	Mar. 2012
16	Excited-State Dynamics: Theory and Experiment, 242nd ACS National Meeting	<i>Denver, CO</i>	Aug. 2011
15	Nonequilibrium Phenomena, Telluride Scientific Research Conference	<i>Telluride, CO</i>	Jul. 2011
14	Challenges for Density Functional Theory, 240th ACS National Meeting	<i>Boston, MA</i>	Aug. 2010
13	Physical Chemistry of Interfaces and Nanomaterials, SPIE National Conference	<i>San Diego, CA</i>	Aug. 2010
12	Applications and Development at Multiple Length and Time Scales, ACS NORM/RMRM Meeting	<i>Pullman, WA</i>	Jun. 2010
11	Physical Chemistry of Interfaces and Nanomaterials, SPIE National Conference	<i>San Diego, CA</i>	Aug. 2009
10	Nonequilibrium Phenomena, Telluride Scientific Research Conference	<i>Telluride, CO</i>	Jul. 2009
9	Excited State Processes	<i>Santa Fe, NM</i>	Jun. 2009
8	Conference on Nanotechnology	<i>Seattle, WA</i>	Jun. 2009
7	Advances in Electronic Structure Theory and First Principles Dynamics, 237th ACS National Meeting	<i>Salt Lake City, UT</i>	Mar. 2009
6	Convergence between Theory and Experiment in Surface Chemistry and Catalysis, 237th ACS National Meeting	<i>Salt Lake City, UT</i>	Mar. 2009
5	Transatlantic Frontiers in Chemistry Symposium	<i>Chester, UK</i>	Aug. 2008
4	Connecticut Quantum Chemistry Meeting	<i>Wallingford, CT</i>	Feb. 2008
3	Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride Scientific Research Conference	<i>Telluride, CO</i>	Jul. 2007
2	Workshop in High Performance Computing	<i>Beijing, China</i>	Apr. 2007
1	The Second International Conference on Theoretical Chemistry, Molecular Modeling and Life Sciences	<i>NanDaiHe, China</i>	Jul. 2006

## Seminars at Universities and Other Research Institutions

76	Haines-Morris Theoretical Chemistry and Chemical Physics Lecture, The University of Tennessee	<i>Knoxville, TN</i>	Mar. 2025
75	Department of Chemistry, Stony Brook University	<i>Stony Brook, NY</i>	Mar. 2025
74	Closs Lecture, University of Chicago	<i>Chicago, IL</i>	Mar. 2025
73	Harvard-MIT-BU Theory Meeting	<i>Boston, MA</i>	Nov. 2024
72	Institute for Molecular Physical Science, ETH Zürich	<i>Zürich, Switzerland</i>	Jan. 2024
71	Department of Physics, University of Texas, El Paso	<i>El Paso, TX</i>	Oct. 2023
70	Department of Chemistry, Boston College	<i>Boston, MA</i>	Feb. 2023
69	Department of Chemistry and Biochemistry, University of Oklahoma	<i>Norman, OK</i>	Jan. 2023
68	Department of Materials Science and Engineering, University of Washington	<i>Seattle, WA</i>	Jan. 2023
67	Department of Chemistry, Case Western Reserve University	<i>Cleveland, OH</i>	Oct. 2022
66	Colloquium, Department of Chemistry, University of California Riverside	<i>Riverside, CA</i>	May. 2022
65	Department of Chemistry, University of Michigan	<i>Ann Arbor, MI</i>	May. 2022
64	Department of Chemistry, Auburn University	<i>Auburn, AL</i>	Apr. 2022
63	Department of Chemistry, Whitman College	<i>Ann Arbor, MI</i>	Mar. 2022
62	Department of Chemistry, University of Wisconsin Madison	<i>Madison, WI</i>	Feb. 2022
61	Department of Chemistry, University of California Santa Barbara	<i>Santa Barbara, CA</i>	Jan. 2022
60	Department of Chemistry, University of North Dakota (Virtual)	<i>Grand Forks, ND</i>	Jan. 2021
59	Department of Chemistry, Wayne State University (Virtual)	<i>Detroit, MI</i>	Jan. 2021
58	Department of Chemistry, Wesleyan University (Virtual)	<i>Middletown, CT</i>	Nov. 2020
57	Department of Chemistry, Oakland University (Virtual)	<i>Rochester, MI</i>	Oct. 2020
56	Department of Chemistry, The Ohio State University	<i>Columbus, OH</i>	Feb. 2020
55	Department of Chemistry, Duke University	<i>Durham, NC</i>	Feb. 2020
54	Department of Chemistry, North Carolina State University	<i>Raleigh, NC</i>	Feb. 2020
53	Department of Chemistry, University of North Carolina	<i>Chapel Hill, NC</i>	Feb. 2020
52	College of Sciences, Southern University of Science and Technology	<i>Shenzhen, China</i>	Jul. 2019
51	Department of Chemistry, Shanghai Jiao Tong University	<i>Shanghai, China</i>	Jun. 2019
50	Department of Chemistry, University of Minnesota	<i>Minneapolis, MN</i>	May 2019
49	Department of Chemistry, University of Illinois – Chicago	<i>Chicago, IL</i>	May 2019
48	Argonne National Lab Colloquium	<i>Lemont, IL</i>	May 2019
47	Department of Chemistry, Washington State University	<i>Pullman, WA</i>	Apr. 2019
46	Department of Chemistry, California Institute of Technology	<i>Pasadena, CA</i>	Mar. 2019
45	Department of Chemistry, University of California – San Diego	<i>San Diego, CA</i>	Feb. 2019

44	( <i>Highlands in Chemistry Lecture</i> ) Virginia Tech	Blacksburg, VA	Feb. 2019
43	Dalian Institute of Chemical Physics, Chinese Academy of Science	Dalian, China	Mar. 2018
42	Department of Chemistry, University of Toronto	Toronto, Canada	Mar. 2018
41	Department of Chemistry, University of Kansas	Lawrence, KS	Feb. 2018
40	Department of Chemistry, Kansas State University	Manhattan, KS	Feb. 2018
39	Department of Chemistry, Florida State University	Tallahassee, FL	Feb. 2018
38	Department of Chemistry, University of Houston	Houston, TX	Feb. 2018
37	Annual Faculty Seminar, Department of Chemistry, University of Washington	Seattle, WA	Oct. 2017
38	Department of Materials Science and Engineering, University of Washington	Seattle, WA	May. 2017
35	Department of Chemistry Colloquium, University of Colorado – Denver	Denver, CO	Feb. 2016
34	Department of Chemistry Colloquium, LSU	Baton Rouge, LA	Feb. 2016
33	Department of Chemistry, Michigan State University,	Lansing, MI	Oct. 2015
32	Department of Chemistry, Northwestern University	Evanston, IL	Nov. 2014
31	( <i>Student Invited Colloquium</i> ) Department of Chemistry, University of Illinois	Urbana Champagne, IL	Nov. 2014
30	Department of Chemistry, University of Minnesota	Minneapolis, MN	Oct. 2014
29	Department of Chemistry, Beijing Normal University	Beijing, China	Aug. 2014
28	Department of Chemistry, University of Pisa	Pisa, Italy	Jun. 2014
27	Department of Chemistry, Jilin University	Changchun, China	Oct. 2013
26	Department of Chemistry, Washington State University	Pullman, WA	Sep. 2013
25	Department of Chemistry, Stanford University	Palo Alto, CA	May 2011
24	Department of Chemistry, University of Michigan	Ann Arbor, MI	Apr. 2011
23	Department of Chemistry, Wayne State University	Detroit, MI	Apr. 2011
22	Department of Chemistry, Indiana University	Bloomington, IN	Apr. 2011
21	Department of Chemistry, Purdue University	West Lafayette, IN	Apr. 2011
20	Department of Chemistry, The Ohio State University	Columbus, OH	Apr. 2011
19	Department of Chemistry, University of Oregon	Eugene, OR	Feb. 2011
18	Department of Chemistry, University of North Carolina	Chapel Hill, NC	Jan. 2011
17	Department of Chemistry, Duke University	Durham, NC	Jan. 2011
16	Department of Chemistry, University of California	Los Angeles, CA	Oct. 2011
15	Institute of Chemistry, Chinese Academy of Science	Beijing, China	Sep. 2011
14	Department of Chemistry, Nanjing University	Nanjing, China	Sep. 2011
13	Department of Chemistry, Yale University	New Haven, CT	Jun. 2010
12	Department of Chemistry, University of California at Berkeley	Berkeley, CA	May 2010
11	Department of Chemistry, California Institute of Technology	Pasadena, CA	Apr. 2010

10	Department of Chemistry, Beijing Normal University	<i>Beijing, China</i>	Sep. 2009
9	Department of Chemistry, Tsinghua University	<i>Beijing, China</i>	Sep. 2009
8	Department of Chemistry, Fudan University	<i>Shanghai, China</i>	Sep. 2009
7	Department of Chemistry, Northwestern University	<i>Evanston, IL</i>	Apr. 2009
6	Department of Chemistry, University of Wisconsin	<i>Madison, WI</i>	Apr. 2009
5	Department of Chemistry, University of New Mexico	<i>Albuquerque, NM</i>	Apr. 2009
4	Department of Physics, University of Washington	<i>Seattle, WA</i>	Jan. 2009
3	Keynote Lecture, Department of Chemistry, Wayne State University	<i>Detroit, MI</i>	Oct. 2008
2	Department of Applied Mathematics, University of Washington	<i>Seattle, WA</i>	Feb. 2008
1	Korean Advanced Institute of Science and Technology (KAIST)	<i>Daejeon, South Korea</i>	Feb. 2008

# University & Professional Service

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## University Service

2024-present	Co-Chair, AI Oversight Committee
2024	Co-Chair, Infrastructure Working Group on the AI Task Force
2023	Leadership Search Committee Chair for Associate Vice President of Research Computing
2023	Leadership Search Committee for Associate Vice President and Chief Information Security Officer
2023	Chair Search Committee, Department of Materials Science & Engineering
2022-2024	President's Designee, Faculty Council on Information Technology & Cybersecurity
2020-2024	Executive Director of Education and Outreach, Molecular Engineering Materials Center
2020-2022	Graduate School Council
2020-2022	UWC2 Advisory Council
2014-2017	University of Washington Post-doc Advisory Committee
2013-2017	Royalty Research Fund Review Committee
2005-present	Graduate School Representative (GSR) on student exams

## Department Service

2018-2023	Associate Chair of the Graduate Program
2019-2022	Director, Master of Science in Applied Chemical Science & Technology
2014-2022	Undergraduate Education Committee
2015-2018	Faculty Award Committee
2012-2014	Physical Chemistry Faculty Search Committee
2007-present	Graduate Admissions & Good Standing Committee
2004-present	Graduate Exam Committees
2008-present	Management of Department of Chemistry Computer Cluster
2005-2011	Graduate Recruiting Committee

## Conference Organization

July 2024	Organizer, Relativistic Electronic Structure Theory of Heavy-Element Chemistry, 11th Triennial Congress of the International Society for Theoretical Chemical Physics, Qingdao, China
July 2022	Discussion Leader, Molecular Interactions and Dynamics Gordon Research Conference, Easton, MA
March 2022	Organizer, Symposium on Opportunities and Challenges in Ultrafast X-ray Science in Chemistry: Theory and Experiment, ACS National Meeting, San Diego, CA
October 2019	Organizer, NSF Workshop on the Future Directions of the CSSI Program, Austin, TX
July 2017	Organizer, Excited State Electronic Structure Theory and Dynamics, Telluride, CO
August 2016	Organizer, Theory and Application of Computational Chemistry, Seattle, WA
July 2015	Organizer, Excited State Electronic Structure Theory and Dynamics, Telluride, CO
July 2014	Organizer, Excited State and Time-Dependent Electronic Structure Theory, Telluride, CO
August 2012	Organizer, Symposium on Exploring Potential Energy Surfaces in Quantum Chemistry, Computational Chemistry Division, 244th ACS National Meeting, Philadelphia, PA
July 2012	Organizer, Nanomaterials: Theory and Computation, Telluride Scientific Research Conference, Telluride, CO
March 2012	Organizer, Symposium on Nonadiabatic Dynamics and 40 Years of Surface Hopping, Physical Chemistry Division, 243rd ACS National Meeting, San Diego, CA
July 2011	Session Chair: Nonequilibrium Phenomena, Telluride Scientific Research Conference, Telluride, CO
August 2010	Organizer, Symposium on Challenges for Density Functional Theory, Physical Chemistry Division, 240th ACS National Meeting, Boston, MA
August 2009	Session Chair: Physical Chemistry of Interfaces and Nanomaterials, SPIE National Conference, San Diego, CA
July 2009	Session Chair: Nonequilibrium Phenomena, Telluride Scientific Research Conference, Telluride, CO

## Journal Editor

2025-present	Editor-in-Chief, APL Computational Physics, American Institute of Physics
2020-2024	Associate Editor, Chemical Physics Reviews, American Institute of Physics
2024-present	Editorial Advisory Board, Chemical Reviews
2023-present	Editorial Advisory Board, Chemical Science
2022-present	Editorial Advisory Board, Journal of Physical Chemistry ABC
2020-present	Associate Editor, Chemical Physics Reviews, American Institute of Physics
2018-2021	Editorial Advisory Board, Journal of Physical Chemistry Letters
2016-2021	Editorial Advisory Board, Journal of Physical Chemistry ABC
2013-2014	Editorial Advisory Board, Journal of Chemical Physics
2012	Guest Editor, Special Issue on Nonadiabatic Dynamics, Journal of Chemical Physics
2012	Guest Editor, Special Issue on Exploring Potential Energy Surface, Journal of Chemical Theory and Computation

## Community Service

2023	ACS Electrochemistry Search Committee
2022-present	C&EN Editorial Board, American Chemical Society
2016-present	Society Committee on Publications, American Chemical Society

## Current Postdoctoral Research Associates and Scientists

Dr. Tianyuan Zhang	06/2019
Dr. Ryan Beck	09/2021
Dr. Linghua Zhu	09/2021
Dr. Tian Wang	02/2022
Dr. Xinzheng Yang	02/2022
Dr. Eleftherios Lambros	06/2022
Dr. Samraghi Banerjee	10/2022
Dr. Diandong Tang	05/2023
Dr. Xuechen Zheng	06/2023
Dr. Shiv Upadhyay	07/2023
Dr. Mengqi Yang	01/2024
Dr. Rajat Majumder	11/2024

## Current Ph.D. Students

Mr. Can Liao	01/2021
Mr. Aoding Liu	01/2021
Mr. Ziyu Zhang	06/2022
Mr. Maxwell Taub	01/2023
Mr. Mikael Kovtun	07/2023
Mr. Alexandros Peltekis	01/2024
Mr. Agam Shayit	01/2024
Mr. Jonathan Bersson	01/2024
Mr. Chenrui Shao	01/2025

## Current Visiting Scholars

Professor Yue Huang, Department of Materials Science and Engineering, University of Washington	06/2017
Dr. Kedy Edme, Department of Chemistry, University of North Carolina at Chapel Hill	06/2020

## Ph.D. Dissertations Supervised

Mr. Xiaolin Liu, Postdoctoral Researcher, Vanderbilt University	June 2024
Dr. Lauren Koulias, Postdoctoral Researcher, Florida State University	August 2023
Dr. Hang Hu, Software Engineer, Meta	June 2023
Dr. Lixin Lu, Postdoctoral Researcher, Stanford University	June 2023
Dr. Alexis Mills, Data Scientists, Microsoft	August 2022
Dr. Ryan Beck, Postdoctoral Researcher, University of Washington	June 2021
Dr. Andrew Wildman, Research Scientist, IQbit	June 2021
Dr. Torin Stetina, Research Scientist, IonQ	June 2021
Dr. Joseph Kasper, Staff Scientist, Los Alamos National Laboratory	June 2020
Dr. Shichao Sun, Postdoctoral Researcher, University of Californian, Irvine	June 2020
Dr. Hongbin Liu, Senior Software Engineer, Microsoft	June 2019
Dr. David Williams-Young, Senior Software Engineer, Microsoft	June 2018
Dr. David Lingerfelt, Staff Scientist, Oakridge National Laboratory	June 2017
Dr. Joshua Goings, Software Engineer, IonQ	June 2017
Dr. Patrick Lestrangle, Data Scientist, Boeing	June 2017
Dr. Erica Chong, Professor, Highline College	May 2016
Dr. Phu Nguyen, Software Engineer, Amazon	May 2016
Dr. Bo Peng, Staff Scientist, Pacific Northwest National Laboratory	May 2016



Dr. Feizhi Ding, Senior Software Engineer, Entos	May 2015
Dr. Joseph May, High School Science Teacher, Las Vegas	May 2014
Dr. Sean Fischer, Regulatory Review Scientist, U.S. Food and Drug Administration	March 2013
Dr. Wenkel Liang, Senior Data Scientist, DRINKS	April 2011
Dr. Ekaterina Badaeva, Research Scientist, Boeing	April 2010
Dr. Christine Isborn, Associate Professor, University of California, Merced	May 2009

### Former Postdoctoral Research Associates

Dr. Chad Hoyer, Assistant Professor, University of Texas, El Paso	01/2018-06/2024
Dr. Andrew Jenkins, Software Engineer, Microsoft	01/2017-06/2023
Dr. Ernesto Martinez	06/2020-06/2023
Dr. Andrew Valentine, Data Scientist, Ansatz AI	09/2018-01/2022
Dr. Adam Grofe, Software Engineer, Microsoft	06/2020-04/2022
Dr. Prachi Sharma, Software Engineer, Intel	12/2020-01/2022
Dr. Andrew Wildman, Software Engineer, 1Qbit	07/2021-01/2022
Dr. Torin Stetina, Research Scientist, IonQ	07/2021-09/2021
Dr. Luning Zhao, Research Scientist, IonQ	08/2019-04/2021
Dr. Hongbin Liu, Software Engineer, Microsoft	07/2019-04/2020
Dr. Alessio Petrone, Assistant Professor, University of Naples	06/2014-09/2018
Dr. Greta Donati, Research Scientist, University of Naples	06/2016-02/2018
Dr. David Lingerfelt, Staff Scientist, Oakridge National Laboratory	06/2017-06/2018
Dr. Patrick Lestrangle, Data Scientist, Boeing	06/2017-01/2018
Dr. Joshua Goings, Research Scientist, IonQ	06/2020-07/2021
Dr. Franco Egidi, Software Engineer, ADF	01/2015-09/2016
Dr. Sean Fischer, Regulatory Review Scientist, U.S. Food and Drug Administration	03/2013-12/2013
Dr. Ekaterina Badaeva, Research Scientist, Boeing	04/2011-07/2011
Dr. Bo Peng, Staff Science, Pacific Northwest National Laboratory	09/2010-09/2011
Dr. Craig Chapman, Assistant Professor, University of New Hampshire	04/2010-04/2013
Dr. Yong Feng, Software Engineer, Microsoft	08/2007-07/2010
Dr. Christine Isborn, Associate Professor, University of California, Merced	06/2009-08/2009

### Former Visitors and Other Researchers

Ms. Layal Mahfoud, Master Graduate Student	01/2023-10/2023
Mr. Kirill Shumilov, Master Graduate Student	01/2022-10/2023
Mr. Jordan Ehrman, Master Graduate Student	01/2021-10/2023
Mr. Ben Link, Master Graduate Student	01/2021-06/2023
Mr. Kollin Trujillo, Master Graduate Student	04/2021-06/2022
Mr. Asher DeLarmer, Master Graduate Student	09/2020-08/2021
Professor Xinzhen Yang, Institute of Chemistry, Chinese Academy of Sciences, China	02/2017-07/2020
Mr. Laurence Giodano, Master Graduate Student	01/2020-06/2020
Professor Yutaka Oya, Visiting Scholar, Tohoku University	03/2018-03/2019
Mr. Yosef Bedaso, Master Graduate Student	01/2019-01/2020
Ms. Kara Gallo, Master Graduate Student	01/2019-09/2019
Professor Chenwei Jiang, Visiting Scholar, XiAn Jiaotong University, China	08/2016-08/2017
Mr. Joseph Radler, Master Graduate Student	09/2015-09/2018
Mr. Sajan Silwal, Master Graduate Student	09/2015-06/2014
Mr. Yonghao Gu, Visiting Graduate Student, Fudan University	06/2014-09/2014
Mr. Shichao Sun, Visiting Undergraduate Student, Fudan University	06/2014-09/2014
Ms. Greta Donati, Visiting Graduate Student, University of Napoli	06/2015-09/2015
Mr. Alessio Petrone, Visiting Graduate Student, University of Napoli	09/2013-01/2014
Mr. Winston Wright, Summer Researcher, Interlake High School	06/2013-08/2013

Mr. Jeremy Lehner, Master Graduate Student	09/2011-09/2013
Ms. Alicia Key, Master Graduate Student	09/2008-07/2009
Dr. Christopher Moss, Master Graduate Student	07/2007-06/2010

### Former Undergraduate Students

Mr. Jirui Yang, University of Hawai'i	06/2024-08/2024
Mr. Rahoul Banerjee Ghosh, University of Washington	04/2022-06/2023
Mr. Kevin Hoang, University of Washington	07/2020-06/2023
Mr. Gerardo Salgado, University of Washington	07/2022-06/2023
Ms. Amanda Bunken, Rochester Institute of Technology	06/2023-09/2023
Ms. Winnie Lau, University of Hawai'i	06/2023-09/2023
Ms. Nils Melbourne, University of Hawai'i	06/2023-09/2023
Ms. Shelby Mitchell, University of Hawai'i	06/2022-09/2022
Ms. Laura Reed, University of Washington	06/2021-09/2021
Ms. Isabel Chapa, University of Texas, Austin	06/2021-09/2021
Mr. Ethan Vo, Columbia University	01/2019-06/2020
Ms. Molly Slann, University of College London	09/2018-06/2019
Mr. Joseph Abbott, University of Bristol	09/2018-06/2019
Ms. Amanda Ong, University of Washington	07/2018-09/2018
Ms. Red Dimaculangan, Highline Community College	07/2018-09/2018
Mr. Xudong Yang, Shanghai Jiaotong University	07/2018-12/2018
Mr. Anthony Botello, University of Washington	01/2018-07/2018
Mr. Nan Cheng, University of Chinese Academy of Sciences	06/2018-09/2018
Mr. Malte Lange, University of Washington	06/2014-06/2016
Mr. Ryan McMorris, University of Washington	06/2011-06/2013
Ms. Katherine Lacy, Willamette University	06/2013-08/2013
Ms. Sara Tweedy, Harvey Mudd College	06/2012-08/2012
Ms. Jane Hung, University of Washington	07/2008-07/2012
Ms. Jiao Ma, University of Washington	11/2009-06/2011
Mr. Christopher Poon, University of Washington	07/2009-06/2011
Mr. Sean Ryan, University of Washington	10/2010-06/2011
Mr. Alex Lindsay, University of Washington	06/2009-08/2010
Ms. Patricia Tsai, University of Washington	06/2008-08/2009
Ms. Ariana Hernandez, University of Washington	06/2008-08/2009
Mr. Nuttavikhom Phanthuwongpakdee, University of Washington	06/2008-08/2009
Mr. Robert Snoeberger III, University of Washington	09/2005-07/2006

## STUDENT AWARDS AND RECOGNITIONS

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### Graduate Students

Maxwell Taub	Clean Energy Institute Graduate Fellowship (2024)
Can Liao	Clean Energy Institute Graduate Fellowship (2023)
Lauren Koulias	Chemistry Outstanding TA Award (2023)
Ben Link	Clean Energy Institute Graduate Fellowship (2022)
Xiaolin Liu	Clean Energy Institute Graduate Fellowship (2022)
Lixin Lu	ACS Chemical Computing Group Excellence Award (2022); Rabinovitch, Benton Seymour Endowed Fellowship (2018); Clean Energy Institute Graduate Fellowship (2020)
Hang Hu	Clean Energy Institute Graduate Fellowship (2019)
Alexis Mills	NSF NRT Fellowship (2019); NSF Graduate Research Fellowship Honorable Mention (2019); UW Gudiksen, Paul H. and Karen S. Endowed Fellowship (2018); Excellence in Chemistry Graduate Fellowship Award (2018)
Shichao Sun	Graduate Merit Fellowship (2020); Alma Mater Travel Award (2019); Clean Energy Institute Travel Award (2019); Excellence in Chemistry Graduate Fellowship (2015) Gudiksen, Paul H. and Karen S. Merit Fellowship (2019); Best Poster Award, Northwest Theoretical and Computational Chemistry Conference (2019); NSF Graduate Research Fellowship Honorable Mention (2018); Clean Energy Institute Graduate Fellowship (2017); NSF NRT Fellowship (2017); PNNL Graduate Fellowship (2017)
Andrew Wildman	Graduate Merit Fellowship (2020); NSF NRT Fellowship (2018); Excellence in Chemistry Graduate Fellowship (2016)
Ryan Beck	NSF MoSSI Software Fellowship (2020); Clean Energy Institute Graduate Fellowship (2018); NSF NRT Fellowship (2017)
Torin Stetina	NWTCC Best Poster Award (2017)
Joseph Radler	NSF NRT Fellowship (2020); NSF MoSSI Software Fellowship (2019); Benton Seymour Rabinovitch Endowed Fellowship (2018)
Lauren Koulias	Data Science Accelerator Award (2018); Alma Mater Travel Award (2017); NSF NRT Fellowship (2016); UW Clean Energy Institute Fellowship (2016); UW Chemistry Merit Award (2016)
Hongbin Liu	Scott, Amy and Stephen C. Alley Endowed Graduate Student Fellowship (2019); Alma Mater Travel Award (2019); Honorable Mention in NSF Graduate Fellowship (2017); NSF NRT Fellowship (2016); PNNL Graduate Fellowship (2016); Howard J. Ringold Endowed Fellowship (2016)
Joseph Kasper	UW Chemistry Merit Award (2016); NSF MoSSI Fellowship (2017); ACS Computational Chemistry Award (2017)
David Williams-Young	Linus Pauling Distinguished Postdoctoral Fellowship (2016); ACS Computational Chemistry Award (2015)
Bo Peng	ACS Computational Chemistry Award (2017); National Science Foundation Graduate Fellowship Honorary Mention (2012, 2103); Clean Energy Institute Fellowship (2015); UW Chemistry Merit Award (2014); UW Travel Award (2015)
Patrick Lestrangle	Clean Energy Institute Fellowship (2015); UW Chemistry Merit Award (2014); UW Travel Award (2015)
David Lingerfelt	ACS Computational Chemistry Award (2016); National Science Foundation Graduate Fellowship Award (2013); UW Chemistry Merit Award (2014) UW Travel Award (2015)
Joshua Goings	

Feizhi Ding	Department of Chemistry Travel Award (2013); HHMI University of Washington Nominee (2013)
Joseph May	ACS Computational Chemistry Award (2013); Intel Fellowship University of Washington Nominee (2013); Graduate Medal Finalist (2013)
Sean Fischer	ACS Computational Chemistry Award (2012)
Wenkel Liang	ACS Computational Chemistry Award (2011); Graduate Medal Finalist (2011)
Ekaterina Badaeva	IBM-Zerner Graduate Student Fellowship Award (2009), Center for Nanotechnology UIF Fellowship (2009, 2010)
Christine Isborn	ACS Women Chemists Committee Travel Award (2006), Alvin L. Kwiram/Council for Chemical Research Graduate Student Fellowship (2006), UIF Fellowship through the UW Center for Nanotechnology (2007), IBM-Zerner Graduate Student Fellowship Award (2008)

## Undergraduate Students

Rahoul Banerjee Ghosh	Mary Gates Scholarship (2023); Julia Ann Rutherford Memorial Scholarship, Puget Sound Section of the American Chemical Society (2023)
Ethan Vo	Distinguished Research in Chemistry Award (2020); Earl W. Davie Endowed Scholarship in Chemistry (2019); Student Service Award (2018); General Chemistry Achievement Award (2018)
Malte Large	Mary Gates Scholarship (2015); Washington State Research Award (2015)
Jane Hung	NASA Fellowship (2007, 2008), Mary Gates Scholarship (2008, 2009), Washington State Research Foundation Fellowship (2010), Goldwater Fellowship (2011), College of Arts and Sciences Dean's Dean's Medal (2012), President Medal (2012)
Ryan McMorris	Mary Gates Scholarship (2012)
Jiao Ma	PC Cross Award (2011)
Patricia Tsai	Merck Award (2010)