Xiaosong **Li**

Larry R. Dalton Endowed Chair in Chemistry
Senior Associate Dean for Research , College of Arts & Sciences
Lab Fellow (Dual Appointment), Pacific Northwest National Laboratory
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Professional Experience

University of Washington — *Seattle, WA*

Senior Associate Dean for Research, College of Arts & Sciences	*2024 - present*
Larry R. Dalton Endowed Chair in Chemistry	*2022 - present*
Adjunct Professor of Physics	*2026 - present*
Adjunct Professor of Materials Science and Engineering	*2018 - present*
Professor of Chemistry	*2015 - present*
Associate Vice Provost for Research Cyberinfrastructure	*2022 - 2024*
Harry and Catherine Jaynne Boand Endowed Professor of Chemistry	*2017 - 2022*
Associate Chair of Graduate Program	*2018 - 2023*
Executive Director of Education and Outreach, Molecular Engineering Materials Center	*2020 - 2024*
Director, Master of Science in Applied Chemical Science and Technology	*2019 - 2022*
Associate Professor of Chemistry	*2012 - 2015*
Assistant Professor of Chemistry	*2005 - 2012*

Pacific Northwest National Laboratory

Lab Fellow (dual appointment)	*2020 - present*

American Institute of Physics

Editor-in-Chief, APL Computational Physics	*2025 - present*
Associate Editor, Chemical Physics Reviews	*2020 - 2024*

Honors & Awards

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
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 **Department of Chemistry Faculty Lectureship**, 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

Education

Yale University — *New Haven, CT*

Postdoctoral Research Associate; Advisor: Prof. John C. Tully	*Aug. 2003 - Jul. 2005*

Wayne State University — *Detroit, MI*

Ph. D., Theoretical Chemistry; Advisor: Prof. H. Bernhard Schlegel	*Aug. 1999 - Jul. 2003*

University of Science and Technology of China — *Hefei, China*

B.S., Chemical Physics; Advisor: Prof. QinQiang Guo	*Aug. 1994 - Jul. 1999*

Research (> 320 publications; Google scholar h-index 71; ∼19,000 publication citations; ∼36,000 software citations; > 220 invited presentations; graduated 25 Ph.D students; trained 35 Post-docs)

- **Relativistic Electronic Structure Theory:** We develop state-of-the-art relativistic quantum chemistry methods to accurately model molecules containing rare-earth and heavy elements. By treating the Dirac equation variationally with two- and four-component Dirac–Coulomb–Breit Hamiltonians, we achieve precise descriptions of scalar relativistic and spin–orbit effects. These capabilities enable reliable prediction of magnetic properties, spectroscopy, and spin-state dynamics in complex heavy-element systems, providing essential benchmarks for experiment and materials design.
- **Real-Time Many-Body Electron Dynamics:** We develop real-time electronic structure methods to simulate how electrons respond to ultrafast light fields, magnetic interactions, and spin dynamics. Extending these approaches to relativistic systems allows us to capture femtosecond charge transfer, spin manipulation, and excited-state evolution, advancing the understanding of light-driven processes in molecules and materials.
- **Nonadiabatic Dynamics & Nuclear–Electronic Orbital (NEO) Theory:** We develop quantum and mixed quantum–classical dynamics—such as *ab initio* Ehrenfest dynamics, surface hopping, and the NEO framework—to study photochemical reactions and spin-driven processes. Integrating these methods with relativistic electronic structure provides a powerful platform to predict reaction pathways, intersystem crossing, and spin conversion, helping design efficient photochemical and spintronic materials.
- **Computational Spectroscopies & Photochemistry:** We build highly accurate and efficient tools for spectroscopy simulation, from multi-reference and density functional theories to relativistic frameworks. Our methods predict X-ray, magneto-optical, and magnetic hysteresis spectra with quantitative accuracy, enabling direct interpretation of experiments and design of next-generation photoactive and magnetic materials.
- **Computational Molecular Sciences:** We design and model molecules and nanocrystals with tailored electronic, optical, and magnetic properties for use in photonics, spintronics, and photovoltaics. By understanding how defects and dopants induce new magnetic and photochemical behavior, we provide quantum-level insight and control strategies for advanced functional materials.
- **AI & Quantum Information Science:** We tackle noise and error challenges in quantum computing for chemistry. Using AI-driven measurement-error mitigation and shot-frugal strategies, we enhance the performance of variational quantum eigensolvers (VQE) on today's noisy quantum devices. We also explore rare-earth and heavy-element molecular magnets as candidates for quantum sensors and information processing, bridging quantum chemistry and quantum technology.

Synergistic Activities

- **Education and Mentorship.** As Executive Director of Education and Outreach at the NSF-funded *Molecular Engineering Materials Center* (MEM-C), I have expanded undergraduate research opportunities in materials science and lead the *Partnerships for Research and Education in Materials* (PREM) program with the University of Hawai'i at Mānoa and the University of Central Florida. My dedication to mentoring was recognized with the University of Washington's Distinguished Teaching Award in 2020.
- **Research Administration & Infrastructure Leadership.** As *Senior Associate Dean for Research* in the College of Arts & Sciences, I foster collaborative, cross-cutting research programs and strategic investments. As *Associate Vice Provost for Research Cyberinfrastructure*, I advance scalable high-performance computing, data management, and AI-driven analytics to empower interdisciplinary research.
- **Professional Service & Editorial Leadership.** I am currently *Editor-in-Chief of APL Computational Physics*, shaping the future of computational science publishing. I serve on the *Society Committee on Publications* of the American Chemical Society (ACS), the editorial board of *Chemical & Engineering News* (C&EN), and the *Journal of Physical Chemistry ABC* Advisory Board. I previously served on the *Journal of Physical Chemistry Letters* board and as *Associate Editor of Chemical Physics Reviews*.
- **Open-Source Software Development.** I lead the development of *Chronus Quantum (ChronusQ)*, an open-source quantum chemistry platform that integrates advanced relativistic methods and real-time electronic structure theories at scale. I actively support its community through workshops and hackathons, driving innovation in chemistry, materials science, and quantum information.

Publications (Google Scholar h-index 70; ∼16,000 Publication Citations; ∼69,000 Software Citations

[328] A. Shayit, C. Liao, S. Upadhyay, H. Hu, T. Zhang, A. E. DePrince III, C. Yang and X. Li, "Numerically Exact Configuration Interaction at Quadrillion-Determinant Scale", *Nat. Commun.*, **2025**, *16*, 11016.

[327] F. Khaliq, R. A. Beck, E. Svensson Grape, G. Navidi, M. Griffith, C. R. Marshall, X. Li and C. K. Brozek, "Size-Dependent Optical Band Gaps in Metal–Organic Framework Nanoparticles", *J. Am. Chem. Soc.*, **2025**, *147*, 45748–45762.

[326] C. W. Dalton, T. Wang, G. Morrison, H.-C. zurLoye, X. Li and D. A. Reed, "Magnetocaloric Effect in a Microporous Material Using a Rare-Earth-Free, Hybrid Perovskite", *J. Am. Chem. Soc.*, **2025**, *147*, 39401–39407.

[325] S. Liang, L. Zhu, X. Li and C. Yang, "QuGStep: Refining Step Size Selection in Gradient Estimation for Variational Quantum Algorithms", *APL Computational Physics*, **2025**, *1*, 026110.

[324] N. Bauman, L. A. Cunha, A. E. I. DePrince, J. Flick, J. J. I. Foley, N. Govind, G. Groenhof, N. Hoffmann, K. Kowalski, X. Li, M. Liebenthal, N. T. Maitra, R. Manderna, M. Matoušek, I. M. Mazin, D. Mejia-Rodriguez, A. Panyala, B. Peng, B. Peyton, L. Veis, N. Vu, J. D. Weidman, A. K. Wilson, R. A. Zarotiadis and Y. Zhang, "Perspective on Many-Body Methods for Molecular Polaritonic Systems", *J. Chem. Theory Comput.*, **2025**, *21*, 10035–10067.

[323] S. M. Garner, X. Li and S. Hammes-Schiffer, "Simulation of Vibronic Strong Coupling and Cavity-modified Hydrogen Tunneling Dynamics", *J. Chem. Phys.*, **2025**, *163*, 134113.

[322] Z. Zhang, X. Yang, L. Yan, S. Jung, W. You, T. Cao and X. Li, "Fusion Deep Learning for Predicting Conductivity in Electron-Doped Organic Polymers", *J. Am. Chem. Soc.*, **2025**, *147*, 36233–36243.

[321] Z. Tan, C.-H. Hsiung, J. Feng, Y. Zhang, Y. Wan, J. Chen, K. Sun, P. Lu, J. Zang, W. Yang, Y. Gao, J. Yin, T. Zhu, Y. Lu, Z. Pan, Y. Zou, C. Liao, X. Li, Y. Ye, Y. Liu9 and X. Zhang, "Time-resolved Fluorescent Proteins Expand Fluorescent Microscopy in Temporal and Spectral Domains", *Cell*, **2025**, *188*, 6987–7005.

[320] X. Li, "What is Computational Physics?", *APL Computational Physics*, **2025**, *1*, 010401.

[319] R. R. Li, S. H. Yuwono, M. D. Liebenthal, T. Zhang, X. Li and I. DePrinceA. Eugene, "Relativistic Two-component Double Ionization Potential Equation-of-Motion Coupled Cluster with the Dirac–Coulomb–Breit Hamiltonian", *J. Chem. Phys.*, **2025**, *163*, 104112.

[318] E. S. Ryland, X. Yang, D. Garratt, W. C. Henke, A. Kahraman, M. Taub, M. Sachs, E. Biasin, C. Y. Hampton, D. J. Hoffman, G. Coslovich, K. Kunnus, G. L. Dakovski, M. W. Mara, L. X. Chen, K. L. Mulfort, X. Li and A. A. Cordones, "Revealing Parallel Inter- and Intra-Ligand Charge Transfer Dynamics in $[Ru(L)_2(dppz)]^{2+}$ Molecular Lightswitch with N K-Edge X-Ray Absorption Spectroscopy", *Angew. Chem. Int. Ed.*, **2025**, *64*, e202509496.

[317] M. W. Mara, D. Leshchev, N. P. Weingartz, A. M. Chan, A. K. Nijhawan, A. J. S. Valentine, X. Liu, S. Kromer, D. Hsu, P. Kim, E. Biasin, T. B. vanDriel, F. N. Castellano, X. Li and L. X. Chen, "Characterizing Ultrafast Intersystem Crossing Pathways in Molecular Pt Dimers Using Time-Resolved Wide-Angle X-ray Scattering", *J. Phys. Chem. Lett.*, **2025**, *16*, 7120–7126.

[316] M. Yang, X. Yang, E. Lambros, S. Upadhyay, L. Yan, W. You and X. Li, "Unraveling Ground-State Electron Transfer in Photoredox n-Doping of Conjugated Polymers through Real-Time Quantum Dynamics", *J. Am. Chem. Soc.*, **2025**, *147*, 24095–24102.

[315] S. A. Roget, W. C. Henke, M. Taub, P. Kim, J. T. Yarranton, X. Li, K. L. Mulfort and L. X. Chen, "Tracking Photoinduced Charge Redistribution in a Cu(I) Diimine Donor–Bridge–Acceptor System with Time-Resolved Infrared Spectroscopy", *Photochem*, **2025**, *5*, 16.

[314] C. Liao, C. Rosenbaum, A. M. Glaudin, M. Taub, R. Banerjee Ghosh, S. Pristash, C. W. Schlenker and X. Li, "Spin–Vibronic Coupling Enhanced Intersystem Crossing beyond El-Sayed Restrictions", *J. Am. Chem. Soc.*, **2025**, *147*, 22176–22184.

[313] L. Yan, X. Yang, M. Yang, J. Neu, S. Kashani, R. Giridharagopal, Y. Olanrewaju, F. So, D. Ginger, H. Ade, X. Li and W. You, "Air-stable n-Type Dopant for Organic Semiconductors via a Single-Photon Catalytic Process", *Sci. Adv.*, **2025**, *11*, eadu8215.

[312] W. Chen, T. Wang, C.-C. Yu, Y. Jing, X. Li and W. Xiong, "Small Polaron-Induced Ultrafast Ferroelectric Restoration in $BiFeO_3$", *Phys. Rev. X*, **2025**, *15*, 021046.

[311] D. G. Truhlar and X. Li, "Introduction to Relativistic Electronic Structure Calculations", *J. Phys. Chem. A*, **2025**, *129*, 4301–4312.

[310] D. Tang, A. Liu, T. Culpitt, S. Hammes-Schiffer and X. Li, "Simulating Magnetic Field-Driven Real-Time Quantum Dynamics Using London Nuclear–Electronic Orbital Approach", *J. Chem. Theory Comput.*, **2025**, *21*, 4357–4364.

[309] D. Tang, C. Liao, M. Taub, G. C. Schatz, H. Guo and X. Li, "Photochemical Au(I)–Au(I) Bond Formation: A Battle between Intersystem Crossing and Internal Conversion", *J. Phys. Chem. Lett.*, **2025**, *16*, 3816–3821.

[308] T. E. Li, X. Li and S. Hammes-Schiffer, "Energy Conservation in Real-Time Nuclear–Electronic Orbital Ehrenfest Dynamics", *J. Chem. Phys.*, **2025**, *162*, 144106.

[307] S. H. Yuwono, R. R. Li, T. Zhang, X. Li and I. DePrinceA. Eugene, "Two-Component Relativistic Equation-of-Motion Coupled Cluster for Electron Ionization", *J. Chem. Phys.*, **2025**, *162*, 084110.

[306] H. Lim, X. Yang, C. B. Larsen, K. Ledbetter, M. R. Zoric, S. L. Raj, G. Kumar, N. Powers-Riggs, M. C. Hoffmann, M. Chollet, L. B. Gee, T. B. vanDriel, R. Alonso-Mori, V. Kabanova, A. Kahraman, P. J. M. Johnson, C. Cirelli, C. Bacellar, K. J. Gaffney, X. Li and A. A. Cordones, "Excited State Covalency, Dynamics, and Photochemistry of Square Planar Ni-Thiolate Complexes Revealed by Ultrafast X-ray Absorption", *J. Am. Chem. Soc.*, **2025**, *147*, 7496–7506.

[305] 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.

[304] V. Blum, R. Asahi, J. Autschbach, C. Bannwarth, G. Bihlmayer, S. Blügel, L. A. Burns, T. D. Crawford, W. Dawson, W. A. deJong, C. Draxl, C. Filippi, L. Genovese, P. Giannozzi, N. Govind, S. Hammes-Schiffer, J. R. Hammond, B. Hourahine, A. Jain, Y. Kanai, P. R. C. Kent, A. H. Larsen, S. Lehtola, X. Li, R. Lindh, S. Maeda, N. Makri, J. Moussa, T. Nakajima, J. A. Nash, M. J. T. Oliveira, P. D. Patel, G. Pizzi, G. Pourtois, B. P. Pritchard, E. Rabani, M. Reiher, L. Reining, X. Ren, M. Rossi, H. B. Schlegel, N. Seriani, L. V. Slipchenko, A. Thom, E. F. Valeev, B. Van Troeye, L. Visscher, V. Vlček, H.-J. Werner, D. B. Williams-Young and T. L. Windus, "Roadmap on Methods and Software for Electronic Structure Based Simulations in Chemistry and Materials", *Electronic Structure*, **2024**, *6*, 042501.

[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. Glownia, 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. Vlaisavljevich 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.

[288] B. T. Phelan, Z.-L. Xie, X. Liu, X. Li, K. L. Mulfort and L. X. Chen, "Photodriven Electron-transfer Dynamics in a Series of Heteroleptic Cu(I)–Anthraquinone Dyads", *J. Chem. Phys.*, **2024**, *160*, 144905.

[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.

[283] S. F. Sandeno, S. M. Krajewski, R. A. Beck, W. Kaminsky, X. Li and B. M. Cossairt, "Synthesis and Single Crystal X-ray Diffraction Structure of an Indium Arsenide Nanocluster", *ACS Central Science*, **2024**, *10*, 744–751.

[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. Vlaisavljevich, 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.

[276] F. W. Eagle, S. Harvey, R. Beck, X. Li, D. R. Gamelin and B. M. Cossairt, "Enhanced Charge Transfer from Coinage Metal Doped InP Quantum Dots", *ACS Nanoscience Au*, **2023**, *3*, 451–461.

[275] S. Banerjee, T. Zhang, K. G. Dyall and X. Li, "Relativistic Resolution-of-the-Identity with Cholesky Integral Decomposition", *J. Chem. Phys.*, **2023**, *159*, 114119.

[274] A. Liu, T. Zhang, S. Hammes-Schiffer and X. Li, "Multicomponent Cholesky Decomposition: Application to Nuclear–Electronic Orbital Theory", *J. Chem. Theory Comput.*, **2023**, *19*, 6255–6262.

[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. Glownia, 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_{25} Superatom UV-Vis Fingerprint Spectra", *Chem. Sci.*, **2023**, *14*, 4666–4671.

[266] S. Kundu, H. Hu, X. Li, M. Schaible and T. M. Orlando, "Electron Scattering with Ethane Adsorbed on Rare Gas Multilayers: Hole Transfer, Coulomb Decay, and Ion Dissociation", *J. Chem. Phys.*, **2023**, *158*, 124309.

[265] E. Lambros, B. Link, M. Chow, S. Hammes-Schiffer and X. Li, "Solvent Induced Proton Polarization within the Nuclear–Electronic Orbital Framework", *J. Phys. Chem. Lett.*, **2023**, *14*, 2990–2995.

[264] X. Liu, D. Hayes, L. X. Chen and X. Li, "Bridge-Mediated Metal-to-Metal Electron and Hole Transfer in a Supermolecular Dinuclear Complex: A Computational Study Using Quantum Electron–Nuclear Dynamics", *J. Phys. Chem. A*, **2023**, *127*, 1831–1838.

[263] R. A. Beck, Y. Huang, A. Petrone, J. W. Abbott, P. J. Pauzauskie and X. Li, "Electronic Structures and Spectroscopic Signatures of Noble-Gas-Doped Nanodiamonds", *ACS Physical Chemistry Au*, **2023**, *3*, 299–310.

[262] C. Liao, J. M. Kasper, A. J. Jenkins, P. Yang, E. R. Batista, M. J. Frisch and X. Li, "State Interaction Linear Response Time-Dependent Density Functional Theory with Perturbative Spin–Orbit Coupling: Benchmark and Perspectives", *JACS Au*, **2023**, *3*, 358–367.

[261] H. Feng, Q. Zhao, B. Zhang, H. Hu, M. Liu, K. Wu, X. Li, X. Zhang, L. Zhang and Y. Liu, "Enabling Photo-Crosslinking and Photo-Sensitizing Properties for Synthetic Fluorescent Protein Chromophores", *Angew. Chem. Int. Ed.*, **2023**, *62*, e202215215.

[260] C. E. Hoyer, L. Lu, H. Hu, K. D. Shumilov, S. Sun, S. Knecht and X. Li, "Correlated Dirac–Coulomb–Breit Multiconfigurational Self-Consistent-Field Methods", *J. Chem. Phys.*, **2023**, *158*, 044101.

[259] F. Perrella, X. Li, A. Petrone and N. Rega, "Nature of the Ultrafast Interligands Electron Transfers in Dye-Sensitized Solar Cells", *JACS Au*, **2023**, *3*, 70–79.

[258] P. Kim, A. J. S. Valentine, S. Roy, A. Mills, F. N. Castellano, X. Li and L. X. Chen, "Ultrafast Branching in Intersystem Crossing Dynamics Revealed by Coherent Vibrational Wavepacket Motions in a Bimetallic Pt(II) Complex", *Faraday Discuss.*, **2022**, *237*, 259–273.

[257] R. A. Beck, S. Sun, X. Xu, D. R. Gamelin, T. Cao and X. Li, "Understanding External Pressure Effects and Interlayer Orbital Exchange Pathways in the Two-Dimensional Magnet–Chromium Triiodide", *J. Phys. Chem. C*, **2022**, *126*, 19327–19335.

[256] A. Liu, M. Chow, A. Wildman, M. J. Frisch, S. Hammes-Schiffer and X. Li, "Simultaneous Optimization of Nuclear–Electronic Orbitals", *J. Phys. Chem. A*, **2022**, *126*, 7033–7039.

[255] S. Sun, J. N. Ehrman, Q. Sun and X. Li, "Efficient Evaluation of the Breit Operator in the Pauli Spinor Basis", *J. Chem. Phys.*, **2022**, *157*, 064112.

[254] C. E. Hoyer, H. Hu, L. Lu, S. Knecht and X. Li, "Relativistic Kramers-Unrestricted Exact-Two-Component Density Matrix Renormalization Group", *J. Phys. Chem. A*, **2022**, *126*, 5011–5020.

[253] T. W. Kim, P. Kim, A. W. Mills, A. Chakraborty, S. Kromer, A. J. S. Valentine, F. N. Castellano, X. Li and L. X. Chen, "Ligand-Structure-Dependent Coherent Vibrational Wavepacket Dynamics in Pyrazolate-Bridged Pt(II) Dimers", *J. Phys. Chem. C*, **2022**, *126*, 11487–11497.

[252] M. C. Drummer, R. B. Weerasooriya, N. Gupta, E. J. Askins, X. Liu, A. J. S. Valentine, X. Li and K. D. Glusac, "Proton-Coupled Electron Transfer in a Ruthenium(II) Bipyrimidine Complex in Its Ground and Excited Electronic States", *J. Phys. Chem. A*, **2022**, *126*, 4349–4358.

[251] A. W. Mills, J. J. Goings, D. Beck, C. Yang and X. Li, "Exploring Potential Energy Surfaces Using Reinforcement Machine Learning", *J. Chem. Inf. Model*, **2022**, *62*, 3169–3179.

[250] L. Lu, H. Hu, A. J. Jenkins and X. Li, "Exact-Two-Component Relativistic Multireference Second-Order Perturbation Theory", *J. Chem. Theory Comput.*, **2022**, *18*, 2983–2992.

[249] A. Grofe and X. Li, "Relativistic Nonorthogonal Configuration Interaction: Application to $L_{2,3}$-edge X-ray Spectroscopy", *Phys. Chem. Chem. Phys.*, **2022**, *24*, 10745–10756.

[248] P. Sharma, A. J. Jenkins, G. Scalmani, M. J. Frisch, D. G. Truhlar, L. Gagliardi and X. Li, "Exact-Two-Component Multiconfiguration Pair-Density Functional Theory", *J. Chem. Theory Comput.*, **2022**, *18*, 2947–2954.

[247] A. J. S. Valentine and X. Li, "Intersystem Crossings in Late-Row Elements: A Perspective", *J. Phys. Chem. Lett.*, **2022**, *13*, 3039–3046.

[246] J. M. Kasper, X. Li, S. A. Kozimor, E. R. Batista and P. Yang, "Relativistic Effects in Modeling the Ligand K-Edge X-ray Absorption Near-Edge Structure of Uranium Complexes", *J. Chem. Theory Comput.*, **2022**, *18*, 2171–2179.

[245] A. Wildman, Z. Tao, L. Zhao, S. Hammes-Schiffer and X. Li, "Solvated Nuclear–Electronic Orbital Structure and Dynamics", *J. Chem. Theory Comput.*, **2022**, *18*, 1340–1346.

[244] M. C. Drummer, R. B. Weerasooriya, N. Gupta, B. T. Phelan, A. J. S. Valentine, A. A. Cordones, X. Li, L. X. Chen and K. D. Glusac, "Long-Lived Excited State in a Solubilized Graphene Nanoribbon", *J. Phys. Chem. C*, **2022**, *126*, 1946–1957.

[243] T. F. Stetina, A. Ciavarella, X. Li and N. Wiebe, "Simulating Effective QED on Quantum Computers", *Quantum*, **2022**, *6*, 622.

[242] M. W. Mara, B. T. Phelan, Z.-L. Xie, T. W. Kim, D. J. Hsu, X. Liu, A. J. S. Valentine, P. Kim, X. Li, S.-i. Adachi, T. Katayama, K. L. Mulfort and L. X. Chen, "Unveiling Ultrafast Dynamics in Bridged Bimetallic Complexes using Optical and X-ray Transient Absorption Spectroscopies", *Chem. Sci.*, **2022**, *13*, 1715–1724.

[241] A. J. Jenkins, H. Hu, L. Lu, M. J. Frisch and X. Li, "Two-Component Multireference Restricted Active Space Configuration Interaction for the Computation of L-Edge X-ray Absorption Spectra", *J. Chem. Theory Comput.*, **2022**, *18*, 141–150.

[240] Z.-L. Xie, X. Liu, A. J. S. Valentine, V. M. Lynch, D. M. Tiede, X. Li and K. L. Mulfort, "Bimetallic Copper/Ruthenium/Osmium Complexes: Observation of Conformational Differences Between the Solution Phase and Solid State by Atomic Pair Distribution Function Analysis", *Angew. Chem. Int. Ed.*, **2022**, *61*, e202111764.

[239] S. Lee, C. E. Hoyer, C. Liao, X. Li and V. C. Holmberg, "Phase-Controlled Synthesis and Quasi-Static Dielectric Resonances in Silver Iron Sulfide ($AgFeS_2$) Nanocrystals", *Small*, **2022**, *18*, 2104975.

[238] A. Lachowicz, E. H. Perez, N. S. Shuman, S. G. Ard, A. A. Viggiano, P. B. Armentrout, J. J. Goings, P. Sharma, X. Li and M. A. Johnson, "Determination of the SmO^+ Bond Energy by Threshold Photodissociation of the Cryogenically Cooled Ion", *J. Chem. Phys.*, **2021**, *155*, 174303.

[237] A. W. Mills, A. J. S. Valentine, K. Hoang, S. Roy, F. N. Castellano, L. X. Chen and X. Li, "General Design Rules for Bimetallic Platinum(II) Complexes", *J. Phys. Chem. A*, **2021**, *125*, 9438–9449.

[236] S. Sun, T. F. Stetina, T. Zhang and X. Li, In *Rare Earth Elements and Actinides: Progress in Computational Science Applications*; D. A. Penchoff, T. L. Windus and P. C. C. Ed.; American Chemical Society: 2021, Chapter 10 - On the Finite Nuclear Effect and Gaussian Basis Set for Four-Component Dirac Hartree-Fock Calculations., 207–218.

[235] T. Song, E. Anderson, M. W.-Y. Tu, K. Seyler, T. Taniguchi, K. Watanabe, M. A. McGuire, X. Li, T. Cao, D. Xiao, W. Yao and X. Xu, "Spin Photovoltaic Effect in Magnetic van der Waals Heterostructures", *Sci. Adv.*, **2021**, *7*, eabg8094.

[234] J. J. Goings, H. Hu, C. Yang and X. Li, "Reinforcement Learning Configuration Interaction", *J. Chem. Theory Comput.*, **2021**, *17*, 5482–5491.

[233] N. Park, F. W. Eagle, A. J. DeLarme, M. Monahan, T. LoCurto, R. Beck, X. Li and B. M. Cossairt, "Tuning the Interfacial Stoichiometry of InP Core and InP/ZnSe Core/Shell Quantum Dots", *J. Chem. Phys.*, **2021**, *155*, 084701.

[232] J. J. Araujo, C. K. Brozek, H. Liu, A. Merkulova, X. Li and D. R. Gamelin, "Tunable Band-Edge Potentials and Charge Storage in Colloidal Tin-Doped Indium Oxide (ITO) Nanocrystals", *ACS Nano*, **2021**, *15*, 14116–14124.

[231] P. Kim, A. J. S. Valentine, S. Roy, A. W. Mills, A. Chakraborty, F. N. Castellano, X. Li and L. X. Chen, "Ultrafast Excited-State Dynamics of Photoluminescent Pt(II) Dimers Probed by a Coherent Vibrational Wavepacket", *J. Phys. Chem. Lett.*, **2021**, *12*, 6794–6803.

[230] R. A. Beck, L. Lu, P. V. Sushko, X. Xu and X. Li, "Defect-Induced Magnetic Skyrmion in a Two-Dimensional Chromium Triiodide Monolayer", *JACS Au*, **2021**, *1*, 1362–1367.

[229] A. Grofe, J. Gao and X. Li, "Exact-Two-Component Block-Localized Wave Function: A Simple Scheme for the Automatic Computation of Relativistic $\triangle$SCF", *J. Chem. Phys.*, **2021**, *155*, 014103.

[228] B. C. Cooper, L. N. Koulias, D. R. Nascimento, X. Li and A. E. DePrince, "Short Iterative Lanczos Integration in Time-Dependent Equation-of-Motion Coupled-Cluster Theory", *J. Phys. Chem. A*, **2021**, *125*, 5438–5447.

[227] S. Sun, T. F. Stetina, T. Zhang, H. Hu, E. F. Valeev, Q. Sun and X. Li, "Efficient Four-Component Dirac–Coulomb–Gaunt Hartree–Fock in the Pauli Spinor Representation", *J. Chem. Theory Comput.*, **2021**, *17*, 3388–3402.

[226] T. Zhang, X. Liu, E. F. Valeev and X. Li, "Toward the Minimal Floating Operation Count Cholesky Decomposition of Electron Repulsion Integrals", *J. Phys. Chem. A*, **2021**, *125*, 4258–4265.

[225] V. W. D. Cruzeiro, A. Wildman, X. Li and F. Paesani, "Relationship between Hydrogen-Bonding Motifs and the $^1b_1$ Splitting in the X-ray Emission Spectrum of Liquid Water", *J. Phys. Chem. Lett.*, **2021**, *12*, 3996–4002.

[224] L. Zhao, A. Wildman, F. Pavošević, J. C. Tully, S. Hammes-Schiffer and X. Li, "Excited State Intramolecular Proton Transfer with Nuclear-Electronic Orbital Ehrenfest Dynamics", *J. Phys. Chem. Lett.*, **2021**, *12*, 3497–3502.

[223] M. L. Shelby, A. Wildman, D. Hayes, M. W. Mara, P. J. Lestrange, M. Cammarata, L. Balducci, M. Artamonov, H. T. Lemke, D. Zhu, T. Seideman, B. M. Hoffman, X. Li and L. X. Chen, "Interplays of Electron and Nuclear Motions along CO Dissociation Trajectory in Myoglobin Revealed by Ultrafast X-rays and Quantum Dynamics Calculations", *Proc. Natl. Acad. Sci. U.S.A.*, **2021**, *118*, e2018966118.

[222] S. Lee, S. Ghosh, C. E. Hoyer, H. Liu, X. Li and V. C. Holmberg, "Iron-Content-Dependent, Quasi-Static Dielectric Resonances and Oxidative Transitions in Bornite and Chalcopyrite Copper Iron Sulfide Nanocrystals", *Chem. Mater.*, **2021**, *33*, 1821–1831.

[221] W. Fu, T. Zhao, H. Liu, F. Lin, L. Zuo, X. Li and A. K.-Y. Jen, "High-Efficiency Quasi-2D Perovskite Solar Cells Incorporating 2,2′-Biimidazolium Cation", *Solar RRL*, **2021**, *5*, 2000700.

[220] L. Zhang, C. Kang, G. Zhang, Z. Pan, Z. Huang, S. Xu, H. Rao, H. Liu, S. Wu, X. Wu, X. Li, Z. Zhu, X. Zhong and A. K.-Y. Jen, "All-Inorganic $CsPbI_3$ Quantum Dot Solar Cells with Efficiency over 16% by Defect Control", *Adv. Func. Mater.*, **2021**, *31*, 2005930.

[219] A. Grofe, R. Zhao, A. Wildman, T. F. Stetina, X. Li, P. Bao and J. Gao, "Generalization of Block-Localized Wave Function for Constrained Optimization of Excited Determinants", *J. Chem. Theory Comput.*, **2021**, *17*, 277–289.

[218] L. Zhao, A. Wildman, Z. Tao, P. Schneider, S. Hammes-Schiffer and X. Li, "Nuclear–Electronic Orbital Ehrenfest Dynamics", *J. Chem. Phys.*, **2020**, *153*, 224111.

[217] J. M. Kasper, T. F. Stetina, A. J. Jenkins and X. Li, "Ab Initio Methods for L-edge X-ray Absorption Spectroscopy", *Chem. Phys. Rev.*, **2020**, *1*, 011304.

[216] L. Lu, A. Wildman, A. J. Jenkins, L. Young, A. E. Clark and X. Li, "The "Hole" Story in Ionized Water from the Perspective of Ehrenfest Dynamics", *J. Phys. Chem. Lett.*, **2020**, *11*, 9946–9951.

[215] B. M. Jones, H. Hu, A. Alexsandrov, W. Smith, A. E. Clark, X. Li and T. M. Orlando, "Efficient Intermolecular Energy Exchange and Soft Ionization of Water at Nanoplatelet Interfaces", *J. Phys. Chem. Lett.*, **2020**, *11*, 10088–10093.

[214] G. U. Kuda-Singappulige, A. Wildman, D. B. Lingerfelt, X. Li and C. M. Aikens, "Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene", *J. Phys. Chem. A*, **2020**, *124*, 9729–9737.

[213] V. Singh, N. Gupta, G. N. Hargenrader, E. J. Askins, A. J. S. Valentine, G. Kumar, M. W. Mara, N. Agarwal, X. Li, L. X. Chen, A. A. Cordones and K. D. Glusac, "Photophysics of Graphene Quantum Dot Assemblies with Axially Coordinated Cobaloxime Catalysts", *J. Chem. Phys.*, **2020**, *153*, 124903.

[212] C. Wolstenholme, H. Hu, S. Ye, B. Funk, D. Jain, C.-H. Hsiung, G. Ning, Y. Liu, X. Li and X. Zhang, "AggFluor: Fluorogenic Toolbox Enables Direct Visualization of the Multi-Step Protein Aggregation Process in Live Cells", *J. Am. Chem. Soc.*, **2020**, *142*, 17515–17523.

[211] C. E. Hoyer and X. Li, "Relativistic Two-Component Projection-Based Quantum Embedding for Open-Shell Systems", *J. Chem. Phys.*, **2020**, *153*, 094113.

[210] J. M. Kasper, A. J. Jenkins, S. Sun and X. Li, "Perspective on Kramers Symmetry Breaking and Restoration in Relativistic Electronic Structure Methods for Open-Shell Systems", *J. Chem. Phys.*, **2020**, *153*, 090903.

[209] T. Zhang, J. M. Kasper and X. Li, In *Annual Reports in Computational Chemistry*; D. A. Dixon Ed.; Elsevier: 2020, Chapter Two - Localized Relativistic Two-Component Methods for Ground and Excited State Calculations, 17–37.

[208] G. U. Kuda-Singappulige, D. B. Lingerfelt, X. Li and C. M. Aikens, "Ultrafast Nonlinear Plasmon Decay Processes in Silver Nanoclusters", *J. Phys. Chem. C*, **2020**, *124*, 20477–20487.

[207] O. A. Hull, D. B. Lingerfelt, X. Li and C. M. Aikens, "Electronic Structure and Nonadiabatic Dynamics of Atomic Silver Nanowire-N_2 Systems", *J. Phys. Chem. C*, **2020**, *124*, 20834–20845.

[206] R. A. Beck, L. Lu, A. Petrone, A. C. Ong, P. J. Pauzauskie and X. Li, "Spectroscopic Signatures of the B and H4 Polyatomic Nitrogen Aggregates in Nanodiamond", *J. Phys. Chem. C*, **2020**, *124*, 18275–18283.

[205] F. Pavošević, Z. Tao, T. Culpitt, L. Zhao, X. Li and S. Hammes-Schiffer, "Frequency and Time Domain Nuclear–Electronic Orbital Equation-of-Motion Coupled Cluster Methods: Combination Bands and Electronic–Protonic Double Excitations", *J. Phys. Chem. Lett.*, **2020**, *11*, 6435–6442.

[204] X. Li, N. Govind, C. Isborn, A. E. DePrince and K. Lopata, "Real-Time Time-Dependent Electronic Structure Theory", *Chem. Rev.*, **2020**, *120*, 9951–9993.

[203] T. Liu, J. Zhang, X. Wu, H. Liu, F. Li, X. Deng, F. Lin, X. Li, Z. Zhu and A. K.-Y. Jen, "Interfacial Modification through a Multifunctional Molecule for Inorganic Perovskite Solar Cells with over 18% Efficiency", *Solar RRL*, **2020**, *4*, 2000205.

[202] S. Sun and X. Li, "Relativistic Effects in Magnetic Circular Dichroism: Restricted Magnetic Balance and Temperature Dependence", *J. Chem. Theory Comput.*, **2020**, *16*, 4533–4542.

[201] H. Hu, A. J. Jenkins, H. Liu, J. M. Kasper, M. J. Frisch and X. Li, "Relativistic Two-Component Multireference Configuration Interaction Method with Tunable Correlation Space", *J. Chem. Theory Comput.*, **2020**, *16*, 2975–2984.

[200] L. Zhao, Z. Tao, F. Pavošević, A. Wildman, S. Hammes-Schiffer and X. Li, "Real-Time Time-Dependent Nuclear-Electronic Orbital Approach: Dynamics Beyond the Born-Oppenheimer Approximation", *J. Phys. Chem. Lett.*, **2020**, *11*, 4052–4058.

[199] J. M. Kasper and X. Li, "Natural Transition Orbitals for Complex Two-Component Excited State Calculations", *J. Comput. Chem.*, **2020**, *41*, 1557–1563.

[198] X. Zhang, C. A. Hoelzel, H. Hu, C. H. Wolstenholme, B. A. Karim, K. T. Munson, K. H. Jung, Y. Liu, H. P. Yennawar, J. B. Asbury and X. Li, "A General Strategy to Enhance Donor-Acceptor Molecules Using Solvent-Excluding Substituents", *Angew. Chem. Int. Ed.*, **2020**, *59*, 4785–4792.

[197] J. M. Kasper, D. R. Gamelin and X. Li, "Theoretical Investigation of Quantum Confinement on the Rashba Effect in ZnO Semiconductor Nanocrystals", *J. Chem. Phys.*, **2020**, *152*, 014308.

[196] V. Singh, M. R. Zoric, G. N. Hargenrader, A. J. S. Valentine, O. Zivojinovic, D. R. Milic, X. Li and K. D. Glusac, "Exciton Coherence Length and Dynamics in Graphene Quantum Dot Assemblies", *J. Phys. Chem. Lett.*, **2020**, *11*, 210–216.

[195] J. Wang, J. Zhang, Y. Zhou, H. Liu, Q. Xue, X. Li, C.-C. Chueh, H.-L. Yip, Z. Zhu and A. K. Y. Jen, "Highly Efficient All-Inorganic Perovskite Solar Cells with Suppressed Non-radiative Recombination by a Lewis Base", *Nat. Commun.*, **2020**, *11*, 177.

[194] D. B. Williams-Young, A. Petrone, S. Sun, T. F. Stetina, P. Lestrange, C. E. Hoyer, D. R. Nascimento, L. Koulias, A. Wildman, J. Kasper, J. J. Goings, F. Ding, A. E. DePrince III, E. F. Valeev and X. Li, "The Chronus Quantum (ChronusQ) Software Package", *WIREs Comput. Mol. Sci.*, **2020**, *10*, e1436.

[193] L. N. Koulias, D. B. Williams-Young, D. R. Nascimento, A. E. DePrince and X. Li, "Relativistic Time-Dependent Equation-of-Motion Coupled-Cluster", *J. Chem. Theory Comput.*, **2019**, *15*, 6617–6624.

[192] K. Xie, X. Li and T. Cao, "Theory and Ab Initio Calculation of Optically Excited States–Recent Advances in 2D Materials", *Adv. Mater.*, **2021**, *33*, 1904306.

[191] S. Sun, R. Beck, D. B. Williams-Young and X. Li, "Simulating Magnetic Circular Dichroism Spectra with Real-Time Time-Dependent Density Functional Theory in Gauge Including Atomic Orbitals", *J. Chem. Theory Comput.*, **2019**, *15*, 6824–6831.

[190] A. Clark, M. J. Servis, Z. Liu, E. Martinez-Baez, J. Su, E. R. Batista, P. Yang, A. Wildman, T. F. Stetina, X. Li, K. Newcomb, E. J. Maginn, J. Autschbach and D. A. Dixon, In *Ion Exchange and Solvent Extraction*; B. A. Moyer Ed.; CRC Press: 2019, .

[189] A. J. S. Valentine, J. J. Radler, F. N. Castellano, L. X. Chen and X. Li, "Resolving the Ultrafast Intersystem Crossing in a Bimetallic Platinum Complex", *J. Chem. Phys.*, **2019**, *151*, 114303.

[188] A. J. S. Valentine and X. Li, "Toward the Evaluation of Intersystem Crossing Rates with Variational Relativistic Methods", *J. Chem. Phys.*, **2019**, *151*, 084107.

[187] S. E. Creutz, H. Liu, M. E. Kaiser, X. Li and D. R. Gamelin, "Structural Diversity in Cesium-Bismuth-Halide Nanocrystals", *Chem. Mater.*, **2019**, *31*, 4685–4697.

[186] T. Stetina, S. Sun, D. B. Williams-Yong and X. Li, "Modeling Magneto-Photoabsorption Using Time-Dependent Complex Generalized Hartree-Fock", *ChemPhotoChem*, **2019**, *3*, 739–746.

[185] M. Crane, A. Petrone, R. A. Beck, M. Lim, X. Zhou, X. Li, R. M. Stroud and P. Pauzauskie, "High Pressure, High Temperature Molecular Doping of Nanodiamond", *Sci. Adv.*, **2019**, *5*, eaau6073.

[184] T. F. Stetina, J. M. Kasper and X. Li, "Modeling $L_{2,3}$-Edge X-ray Absorption Spectroscopy with Linear Response Exact Two-Component Relativistic Time-Dependent Density Functional Theory", *J. Chem. Phys.*, **2019**, *150*, 234103.

[183] R. D. Senanayake, D. B. Lingerfelt, G. U. Kuda-Singappulige, X. Li and C. M. Aikens, "Real-Time TDDFT Investigation of Optical Absorption in Gold Nanowires", *J. Phys. Chem. C*, **2019**, *123*, 14734–14745.

[182] T. F. Stetina, S. Sun, D. B. Lingerfelt, A. Clark and X. Li, "The Role of Excited-State Proton Relays in the Photochemical Dynamics of Water Nanodroplets", *J. Phys. Chem. Lett.*, **2019**, *10*, 3694–3698.

[181] A. J. Jenkins, H. Liu, J. M. Kasper, M. J. Frisch and X. Li, "Variational Relativistic Complete Active Space Self-Consistent Field Method", *J. Chem. Theory Comput.*, **2019**, *15*, 2974–2982.

[180] C. E. Hoyer, D. B. Williams-Young, C. Huang and X. Li, "Embedding Non-Collinear Two-Component Electronic Structure in a Collinear Quantum Environment", *J. Chem. Phys.*, **2019**, *150*, 174114.

[179] S. Sun, D. Williams-Young and X. Li, "An Ab Initio Linear Response Method for Computing Magnetic Circular Dichroism Spectra with Nonperturbative Treatment of Magnetic Field", *J. Chem. Theory Comput.*, **2019**, *15*, 3162–3169.

[178] J. D. Leger, M. R. Friedfeld, R. A. Beck, J. D. Gaynor, A. Petrone, X. Li, B. M. Cossairt and M. Khalil, "Carboxylate Anchors Act as Exciton Reporters in 1.3 nm Indium Phosphide Nanoclusters", *J. Phys. Chem. Lett.*, **2019**, *10*, 1833–1839.

[177] H. Liu, A. J. Jenkins, A. Wildman, M. J. Frisch, F. Lipparini, B. Mennucci and X. Li, "Time-Dependent Complete Active Space Embedded in a Polarizable Force Field", *J. Chem. Theory Comput.*, **2019**, *15*, 1633–1641.

[176] A. Wildman, G. Donati, F. Lipparini, B. Mennucci and X. Li, "Nonequilibrium Environment Dynamics in a Frequency-Dependent Polarizable Embedding Models", *J. Chem. Theory Comput.*, **2019**, *15*, 43–51.

[175] S. Sun, D. Williams-Young, T. F. Stetina and X. Li, "Generalized Hartree-Fock with Non-perturbative Treatment of Strong Magnetic Field: Application to Molecular Spin Phase Transition", *J. Chem. Theory Comput.*, **2019**, *15*, 348–356.

[174] T. Stetina, A. Clark and X. Li, "X-ray Absorption Signatures of Hydrogen-bond Structure in Water-Alcohol Solutions", *Int. J. Quant. Chem.*, **2019**, *119*, e25802.

[173] F. Bai, J. Zhang, Y. Yuan, H. Liu, X. Li, C.-C. Chueh, H. Yan, Z. Zhu and A. K.-Y. Jen, "A 0D/3D Heterostructured All-Inorganic Halide Perovskite Solar Cell with High Performance and Enhanced Phase Stability", *Adv. Mater.*, **2019**, *31*, 1904735.

[172] W. Fu, H. Liu, X. Shi, L. Zuo, X. Li and A. K.-Y. Jen, "Tailoring the Functionality of Organic Spacer Cations for Efficient and Stable Quasi-2D Perovskite Solar Cells", *Adv. Func. Mater.*, **2019**, *29*, 1900221.

[171] D. B. Williams-Young and X. Li, "On the Efficacy and High-Performance Implementation of Quaternion Matrix Multiplication", **2019**, *arXiv*, 1903.05575.

[170] J. D. Gaynor, A. Petrone, X. Li and M. Khalil, "Mapping Vibronic Couplings in Intramolecular Charge Transfer of a Solar Cell Dye with Polarization-Selective Two-Dimensional Electronic-Vibrational Spectroscopy", *J. Phys. Chem. Lett.*, **2018**, *9*, 6289–6295.

[169] A. Petrone, R. A. Beck, J. M. Kasper, M. J. Crane, P. J. Pauzauskie and X. Li, "Electronic Structures and Spectroscopic Signatures of Silicon-Vacancy Containing Nanodiamonds", *Phys. Rev. B*, **2018**, *98*, 205405.

[168] M. E. Ziffer, S. B. Jo, H. Zhong, L. Ye, H. Liu, F. Lin, J. Zhang, X. Li, H. W. Ade, A. K.-Y. Jen and D. S. Ginger, "Long-Lived, Non-Geminate, Radiative Recombination of Photogenerated Charges in a Polymer/Small-Molecule Acceptor Photovoltaic Blend", *J. Am. Chem. Soc.*, **2018**, *140*, 9996–100008.

[167] H. Hu, C. H. Wolstenholme, X. Zhang and X. Li, "Inverted Solvatochromic Stokes Shift in GFP-like Chromophores with Extended Conjugation", *Chinese J. Chem. Phys.*, **2018**, *31*, 599–607.

[166] C. Huang, X. Liao, K. Gao, L. Zuo, F. Lin, X. Shi, C.-Z. Li, H. Liu, X. Li, F. Liu, Y. Chen, H. Chen and A. K.-Y. Jen, "Highly Efficient Organic Solar Cells Based on S,N-Heteroacene Non-Fullerene Acceptors", *Chem. Mater.*, **2018**, *30*, 5429–5434.

[165] T. Zhao, H. Liu, M. E. Ziffer, A. Rajagopal, L. Zuo, D. S. Ginger, X. Li and A. K. Y. Jen, "Realization of a Highly Oriented $MAPbBr_3$ Perovskite Thin Film via Ion Exchange for Ultrahigh Color Purity Green Light Emission", *ACS Energy Lett.*, **2018**, *3*, 1662–1669.

[164] Y. Liu, C. H. Wolstenholme, G. C. Carter, H. Liu, H. Hu, L. S. Grainger, K. Miao, M. Fares, C. A. Hoelzel, H. P. Yennawar, G. Ning, M. Du, L. Bai, X. Li and X. Zhang, "Modulation of Fluorescent Protein Chromophores To Detect Protein Aggregation with Turn-On Fluorescence", *J. Am. Chem. Soc.*, **2018**, *140*, 7381–7384.

[163] A. Petrone, D. B. Williams-Young, S. Sun, T. F. Stetina and X. Li, "An Efficient Implementation of Two-Component Relativistic Density Functional Theory with Torque-Free Auxiliary Variables", *Euro. Phys. J. B*, **2018**, *91*, 169.

[162] S. T. Birkhold, J. T. Precht, H. Liu, R. Giridharagopal, G. E. Eperon, L. Schmidt-Mende, X. Li and D. S. Ginger, "Interplay of Mobile Ions and Injected Carriers Creates Recombination Centers in Metal Halide Perovskites under Bias", *ACS Energy Lett.*, **2018**, *3*, 1279–1286.

[161] F. Egidi, M. Fusè, A. Baiardi, J. Bloino, X. Li and V. Barone, "Computational Simulation of Vibrationally Resolved Spectra for Spin-Forbidden Transitions", *Chirality*, **2018**, *30*, 850–865.

[160] G. Donati, D. B. Lingerfelt, C. Aikens and X. Li, "Anisotropic Polarizability-Induced Plasmon Transfer", *J. Phys. Chem. C*, **2018**, *122*, 10621–10626.

[159] C. K. Brozek, D. Zhou, H. Liu, X. Li, K. R. Kittilstved and D. R. Gamelin, "Soluble Supercapacitors: Large and Reversible Charge Storage in Colloidal Iron-Doped ZnO Nanocrystals", *Nano Lett.*, **2018**, *18*, 3297–3302.

[158] A. Wildman, E. Martinez-Baez, J. Fulton, G. Schenter, C. Pearce, A. Clark and X. Li, "Anticorrelated Contributions to Pre-Edge Features of Aluminate Near-Edge X-ray Absorption Spectroscopy in Concentrated Electrolytes", *J. Phys. Chem. Lett.*, **2018**, *9*, 2444–2449.

[157] J. J. Radler, D. B. Lingerfelt, F. N. Castellano, L. X. Chen and X. Li, "Role of Vibrational Dynamics on Excited-State Electronic Coherence in a Binuclear Platinum Complex", *J. Phys. Chem. A*, **2018**, *122*, 5071–5077.

[156] R. Beck, A. Petrone, J. M. Kasper, M. J. Crane, P. J. Pauzauskie and X. Li, "Effect of Surface Passivation on Nanodiamond Crystallinity", *J. Phys. Chem. C*, **2018**, *122*, 8573–8580.

[155] J. M. Kasper, P. J. Lestrange, T. F. Stetina and X. Li, "Modeling $L_{2,3}$-Edge X-ray Absorption Spectroscopy with Real-Time Exact Two-Component Relativistic Time-Dependent Density Functional Theory", *J. Chem. Theory Comput.*, **2018**, *14*, 1998–2006.

[154] J. M. Kasper, D. B. Williams-Young, E. Vecharynski, C. Yang and X. Li, "A Well-Tempered Hybrid Method for Solving Challenging Time-Dependent Density Functional Theory (TDDFT) Systems", *J. Chem. Theory Comput.*, **2018**, *14*, 2034–2041.

[153] D. Nguyen, J. J. Goings, H. A. Nguyen, J. Lyding, X. Li and M. Gruebele, "Orientation-Dependent Imaging of Electronically Excited Quantum Dots", *J. Chem. Phys.*, **2018**, *148*, 064701.

[152] D. Ju, Y. Dang, Z. Zhu, H. Liu, C.-C. Chueh, X. Li, L. Wang, X. Hu, A. K.-Y. Jen and X. Tao, "Tunable Band Gap and Long Carrier Recombination Lifetime of Stable Mixed $CH_3NH_3Pb_xSn_{1-x}Br_3$ Single Crystals", *Chem. Mater.*, **2018**, *30*, 1556–1565.

[151] P. J. Lestrange, D. B. Williams-Young, A. Petrone, C. A. Jiménez-Hoyos and X. Li, "An Efficient Implementation of Variation After Projection Generalized Hartree-Fock", *J. Chem. Theory Comput.*, **2018**, *14*, 588–596.

[150] J. J. Goings, P. J. Lestrange and X. Li, "Real-Time Time-Dependent Electronic Structure Theory", *WIREs Comput. Mol. Sci.*, **2018**, *8*, e1341.

[149] J. J. Goings, F. Egidi and X. Li, "Current Development of Non-collinear Electronic Structure Theory", *Int. J. Quant. Chem.*, **2018**, *118*, e25398.

[148] P. J. Lestrange, M. R. Hoffmann and X. Li, "Time-Dependent Configuration Interaction using the Graphical Unitary Group Approach: Nonlinear Electric Properties", *Adv. Quantum Chem.*, **2018**, *76*, 295–313.

[147] K. Gao, B. Xu, C. Hong, X. Shi, H. Liu, X. Li, L. Xie and A. K.-Y. Jen, "Di-Spiro-Based Hole-Transporting Materials for Highly Efficient Perovskite Solar Cells", *Adv. Energy Mater.*, **2018**, *8*, 1800809.

[146] H. Liu, C. K. Brozek, S. Sun, D. B. Lingerfelt, D. R. Gamelin and X. Li, "A Hybrid Quantum-Classical Model of Electrostatics in Multiply Charged Quantum Dots", *J. Phys. Chem. C*, **2017**, *121*, 26086–26095.

[145] G. Donati, A. Wildman, S. Caprasecca, D. B. Lingerfelt, F. Lipparini, B. Mennucci and X. Li, "Coupling Real-Time Time-Dependent Density Functional Theory with Polarizable Force Field", *J. Phys. Chem. Lett.*, **2017**, *8*, 5283–5289.

[144] R. Van Beeumen, D. B. Williams-Young, J. M. Kasper, C. Yang, E. G. Ng and X. Li, "Model Order Reduction Algorithm for Estimating the Absorption Spectrum", *J. Chem. Theory Comput.*, **2017**, *13*, 4950–4961.

[143] B. Xu, Z. Zhu, J. Zhang, H. Liu, C.-C. Chueh, X. Li and A. K.-Y. Jen, "4-Tert-Butylpyridine Free Organic Hole Transporting Materials for Stable and Efficient Planar Perovskite Solar Cells", *Adv. Energy Mater.*, **2017**, *7*, 1700683.

[142] J. L. Stein, M. I. Steimle, M. W. Terban, A. Petrone, S. J. L. Billinge, X. Li and B. M. Cossairt, "Cation Exchange Induced Transformation of InP Magic-Sized Clusters", *Chem. Mater.*, **2017**, *29*, 7984–7992.

[141] G. Donati, D. B. Lingerfelt, C. M. Aikens and X. Li, "Molecular Vibration Induced Plasmon Decay", *J. Phys. Chem. C*, **2017**, *121*, 15368–15374.

[140] F. Egidi, S. Sun, J. J. Goings, G. Scalmani, M. J. Frisch and X. Li, "Two-Component Non-Collinear Time-Dependent Spin Density Functional Theory for Excited State Calculations", *J. Chem. Theory Comput.*, **2017**, *13*, 2591–2603.

[139] F. Egidi, D. B. Williams-Young, A. Baiardi, J. Bloino, G. Scalmani, M. J. Frisch, X. Li and V. Barone, "Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: the VPT2-TDDFT Route", *J. Chem. Theory Comput.*, **2017**, *13*, 2789–2803.

[138] A. Petrone, D. B. Williams-Young, D. B. Lingerfelt and X. Li, "Ab Initio Excited State Transient Raman Analysis", *J. Phys. Chem. A*, **2017**, *121*, 3958–3965.

[137] H. D. Nelson, S. O. M. Hinterding, R. Fainblat, S. E. Creutz, X. Li and D. R. Gamelin, "Mid-Gap States and Normal vs Inverted Bonding in Luminescent Cu^+- and Ag^+-Doped CdSe Nanocrystals", *J. Am. Chem. Soc.*, **2017**, *139*, 6411–6421.

[136] Y. Liu, K. Miao, N. P. Dunham, H. Liu, M. Fares, A. K. Boal, X. Li and X. Zhang, "The Cation-π Interaction Enables a Halo-Tag Fluorogenic Probe for Fast No-Wash Live Cell Imaging and Gel-Free Protein Quantification", *Biochem.*, **2017**, *56*, 1585–1595.

[135] D. B. Lingerfelt, P. J. Lestrange, J. J. Radler, S. E. Brown-Xu, P. Kim, F. N. Castellano, L. X. Chen and X. Li, "Can Excited State Electronic Coherence Be Tuned via Molecular Structural Modification? A First-Principles Quantum Electronic Dynamics Study of Pyrazolate-Bridged Pt(II) Dimers", *J. Phys. Chem. A*, **2017**, *121*, 1932–1939.

[134] C.-C. Chueh, C.-Z. Li, F. Ding, Z. Li, N. Cernetic, X. Li and A. K.-Y. Jen, "Doping Versatile n-Type Organic Semiconductors via Room-Temperature Solution-Processable Anionic Dopants", *ACS Appl. Mater. Interfaces*, **2017**, *9*, 1136–1144.

[133] D. C. Gary, A. Petrone, X. Li and B. M. Cossairt, "Investigating the Role of Amine in InP Nanocrystal Syntheses: Destabilizing Cluster Intermediates by Z-Type Ligand Displacement", *Chem. Commun.*, **2017**, *53*, 161–164.

[132] Z. Zhu, J.-Q. Xu, C.-C. Chueh, H. Liu, Z. Li, X. Li, H. Chen and A. K.-Y. Jen, "A Low-Temperature, Solution-Processable Organic Electron-Transporting Layer Based on Planar Coronene for High-performance Conventional Perovskite Solar Cells", *Adv. Mater.*, **2016**, *28*, 10786–10793.

[131] J. J. Goings, D. B. Lingerfelt and X. Li, "Can Quantized Vibrational Effects Be Obtained from Ehrenfest Mixed Quantum-Classical Dynamics?", *J. Phys. Chem. Lett.*, **2016**, *7*, 5193–5197.

[130] A. Petrone, D. B. Lingerfelt, D. B. Williams-Young and X. Li, "Ab Initio Transient Vibrational Spectral Analysis", *J. Phys. Chem. Lett.*, **2016**, *7*, 4501–4508.

[129] D. Williams-Young, J. J. Goings and X. Li, "Accelerating Real-Time Time-Dependent Density Functional Theory with a Non-Recursive Chebyshev Expansion of the Quantum Propagator", *J. Chem. Theory Comput.*, **2016**, *12*, 5333–5338.

[128] D. Williams-Young, F. Egidi and X. Li, "Relativistic Two-Component Particle-Particle Tamm-Dancoff Approximation", *J. Chem. Theory Comput.*, **2016**, *12*, 5379–5384.

[127] N. Li, Z. Zhu, C.-C. Chueh, H. Liu, B. Peng, A. Petrone, X. Li, L. Wang and A. K.-Y. Jen, "Mixed Cation $FA_xPEA_{1-x}PbI_3$ with Enhanced Phase and Ambient Stability toward High-Performance Perovskite Solar Cells", *Adv. Energy Mater.*, **2016**, *7*, 1601307.

[126] A. Petrone, J. J. Goings and X. Li, "Quantum Confinement Effects on Optical Transitions in Nanodiamonds Containing Nitrogen Vacancies", *Phys. Rev. B*, **2016**, *94*, 165402.

[125] L. X. Chen, M. L. Shelby, P. J. Lestrange, N. E. Jackson, K. Haldrup, M. W. Mara, A. B. Stickrath, D. Zhu, H. Lemke, M. Chollet, B. M. Hoffman and X. Li, "Imaging Ultrafast Excited State Pathways in Transition Metal Complexes by X-Ray Transient Absorption and Scattering Using X-Ray Free Electron Laser Source", *Faraday Discuss.*, **2016**, *194*, 639–658.

[124] G. Donati, D. B. Lingerfelt, A. Petrone, N. Rega and X. Li, ""Watching" Polaron Pair Formation from First-Principles Electron-Nuclear Dynamics", *J. Phys. Chem. A*, **2016**, *120*, 7255–7261.

[123] J. J. Goings, J. M. Kasper, F. Egidi, S. Sun and X. Li, "Real Time Propagation of the Exact Two Component Time-Dependent Density Functional Theory", *J. Chem. Phys.*, **2016**, *145*, 104107.

[122] E. Q. Chong, D. B. Lingerfelt, A. Petrone and X. Li, "Classical or Quantum? A Computational Study of Small Ion Diffusion in II-VI Semiconductor Quantum Dots", *J. Phys. Chem. C*, **2016**, *120*, 19434–19441.

[121] C. E. Weller, A. Dhall, F. Ding, E. Linares, S. D. Whedon, N. A. Senger, E. L. Tyson, J. D. Bagert, X. Li, O. Augusto and C. Chatterjee, "Aromatic Thiol-Mediated Cleavage of N-O Bond Enables Chemical Ubiquitylation of Folded Proteins", *Nat. Commun.*, **2016**, *7*, 12979.

[120] R. Pepin, A. Petrone, K. J. Laszlo, M. F. Bush, X. Li and F. Tureček, "Does Thermal Breathing Affect Collision Cross Sections of Gas-Phase Peptide Ions? An Ab Initio Molecular Dynamics Study", *J. Phys. Chem. Lett.*, **2016**, *7*, 2765–2771.

[119] F. Egidi, J. J. Goings, M. J. Frisch and X. Li, "Direct Atomic-Orbital-Based Relativistic Two-Component Linear Response Method for Calculating Excited-State Fine Structures", *J. Chem. Theory Comput.*, **2016**, *12*, 3711–3718.

[118] J. J. Goings and X. Li, "An Atomic Orbital Based Real-Time Time-Dependent Density Functional Theory for Computing Electronic Circular Dichroism Band Spectra", *J. Chem. Phys.*, **2016**, *144*, 234102.

[117] M. L. Shelby, P. J. Lestrange, N. E. Jackson, K. Haldrup, M. W. Mara, A. B. Stickrath, D. Zhu, H. T. Lemke, M. Chollet, B. M. Hoffman, X. Li and L. X. Chen, "Ultrafast Excited State Relaxation of a Metalloporphyrin Revealed by Femtosecond X-ray Absorption Spectroscopy", *J. Am. Chem. Soc.*, **2016**, *138*, 8752–8764.

[116] Z. Li, R. Toivola, F. Ding, J. Yang, P.-N. Lai, T. Howie, G. Georgeson, S.-H. Jang, X. Li, B. D. Flinn and A. K.-Y. Jen, "Highly Sensitive Built-In Strain Sensors for Polymer Composites: Fluorescence Turn-On Response through Mechanochemical Activation", *Adv. Mater.*, **2016**, *28*, 6592–6597.

[115] H. D. Nelson, X. Li and D. R. Gamelin, "Computational Studies of the Electronic Structures of Copper-Doped CdSe Nanocrystals: Oxidation States, Jahn–Teller Distortions, Vibronic Bandshapes, and Singlet–Triplet Splittings", *J. Phys. Chem. C*, **2016**, *120*, 5714–5723.

[114] D. C. Gary, S. E. Flowers, W. Kaminsky, A. Petrone, X. Li and B. M. Cossairt, "Single-Crystal and Electronic Structure of a 1.3 nm Indium Phosphide Nanocluster", *J. Am. Chem. Soc.*, **2016**, *138*, 1510–1513.

[113] D. B. Lingerfelt, D. B. Williams-Young, A. Petrone and X. Li, "Direct Ab Initio (Meta-)Surface-Hopping Dynamics", *J. Chem. Theory Comput.*, **2016**, *12*, 935–945.

[112] P. J. Lestrange, F. Egidi and X. Li, "The Consequences of Improperly Describing Oscillator Strengths Beyond the Electric Dipole Approximation", *J. Chem. Phys.*, **2015**, *143*, 234103.

[111] L. Nienhaus, J. J. Goings, D. Nguyen, S. Wieghold, J. Lyding, X. Li and M. Gruebele, "Imaging Excited Orbitals of Quantum Dots: Experiment and Electronic Structure Theory", *J. Am. Chem. Soc.*, **2015**, *137*, 14743–14750.

[110] J. J. Goings, F. Ding, E. R. Davidson and X. Li, "Approximate Singly Excited States from a Two-Component Hartree Fock Reference", *J. Chem. Phys.*, **2015**, *143*, 144106.

[109] F. Ding, J. J. Goings, H. Liu, D. B. Lingerfelt and X. Li, "Ab Initio Two-Component Ehrenfest Dynamics", *J. Chem. Phys.*, **2015**, *143*, 114105.

[108] B. Peng, P. J. Lestrange, J. J. Goings, M. Caricato and X. Li, "Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to K-Edge X-Ray Absorption Spectroscopy", *J. Chem. Theory Comput.*, **2015**, *11*, 4146–4153.

[107] J. J. Intemann, K. Yao, F. Ding, Y. Xu, X. Xin, X. Li and A. K.-Y. Jen, "Enhanced Performance of Organic Solar Cells with Increased End Group Dipole Moment in Indacenodithieno[3,2-b]thiophene-Based Molecules", *Adv. Func. Mater.*, *12*, 4889–4897.

[106] P. J. Lestrange, P. D. Nguyen and X. Li, "Calibration of Energy-Specific TDDFT for Modeling K-Edge XAS Spectra of Light Elements", *J. Chem. Theory Comput.*, **2015**, *11*, 2994–2999.

[105] C.-Z. Li, P.-W. Liang, D. B. Sulas, P. D. Nguyen, X. Li, D. S. Ginger, C. W. Schlenker and A. K.-Y. Jen, "Modulation of Hybrid Organic-Perovskite Photovoltaic Performance by Controlling the Excited Dynamics of Fullerenes", *Mater. Horiz.*, **2015**, *2*, 414–419.

[104] J. J. Goings, F. Ding, M. J. Frisch and X. Li, "Stability of the Complex Generalized Hartree-Fock Equations", *J. Chem. Phys.*, **2015**, *142*, 154109.

[103] B. Peng, D. B. Lingerfelt, F. Ding, C. M. Aikens and X. Li, "Real-Time TDDFT Studies of Exciton Decay and Transfer in Silver Nanowire Arrays", *J. Phys. Chem. C*, **2015**, *119*, 6421–6427.

[102] B. Zhao, C.-Z. Li, S.-Q. Liu, J. J. Richards, C.-C. Chueh, F. Ding, L. D. Pozzo, X. Li and A. K.-Y. Jen, "A Conductive Liquid Crystal via Facile Doping of an n-type Benzodifurandione Derivative", *J. Mater. Chem. A*, **2015**, *3*, 6929–6934.

[101] F. Ding, D. B. Lingerfelt, B. Mennucci and X. Li, "Time-Dependent Non-Equilibrium Dielectric Response in QM/Continuum Approaches", *J. Chem. Phys.*, **2015**, *142*, 034120.

[100] F. Ding, J. J. Goings, M. J. Frisch and X. Li, "Ab Initio Non-Relativistic Spin Dynamics", *J. Chem. Phys.*, **2014**, *141*, 214111.

[99] J. J. Goings, A. M. Schimpf, J. W. May, R. W. Johns, D. R. Gamelin and X. Li, "Theoretical Characterization of Conduction-Band Electrons in Photodoped and Aluminum-Doped Zinc Oxide (AZO) Quantum Dots", *J. Phys. Chem. C*, **2014**, *118*, 26584–26590.

[98] J. J. Goings, M. Caricato, M. J. Frisch and X. Li, "Assessment of Low-Scaling Approximations to the Equation of Motion Coupled-Cluster Singles and Doubles Equations", *J. Chem. Phys.*, **2014**, *141*, 164116.

[97] A. Petrone, D. B. Lingerfelt, N. Rega and X. Li, "From Charge-Transfer to a Charge-Separated State: A Perspective from the Real-Time TDDFT Excitonic Dynamics", *Phys. Chem. Chem. Phys.*, **2014**, *16*, 24457–24465.

[96] S. A. Fischer, D. B. Lingerfelt, J. W. May and X. Li, "Non-Adiabatic Molecular Dynamics Investigation of Photoionization State Formation and Lifetime in Mn^{2+}-Doped ZnO Quantum Dots", *Phys. Chem. Chem. Phys.*, **2014**, *16*, 17507–17514.

[95] F. Ding, E. B. Guidez, C. M. Aikens and X. Li, "Quantum Coherent Plasmon in Silver Nanowires: A Real-Time TDDFT Study", *J. Chem. Phys.*, **2014**, *140*, 244705.

[94] J. W. May, J. Ma, E. Badaeva and X. Li, "Effect of Excited-State Structural Relaxation on Midgap Excitations in Co^{2+}-Doped ZnO Quantum Dots", *J. Phys. Chem. C*, **2014**, *118*, 13152–13156.

[93] P. J. Lestrange, B. Peng, F. Ding, G. W. Trucks, M. J. Frisch and X. Li, "Density of States Guided Möller-Plesset Perturbation Theory", *J. Chem. Theory Comput.*, **2014**, *10*, 1910–1914.

[92] B. Peng, J. W. May, D. R. Gamelin and X. Li, "Effects of Crystallographic and Shape Anisotropies on Dopant-Carrier Exchange Interactions in Magnetic Semiconductor Quantum Dots", *J. Phys. Chem. C*, **2014**, *118*, 7630–7636.

[91] L. R. Bradshaw, J. W. May, J. L. Dempsey, X. Li and D. R. Gamelin, "Ferromagnetic Excited-State Mn^{2+} Dimers in $Zn_{1-x}Mn_xSe$ Quantum Dots Observed by Time-Resolved Magnetophotoluminescence", *Phys. Rev. B*, **2014**, *89*, 115312.

[90] M. Gliboff, D. Sulas, D. Nordlund, D. W. deQuilettes, P. D. Nguyen, G. T. Seidler, X. Li and D. S. Ginger, "Direct Measurement of Acceptor Group Localization on Donor-Acceptor Polymers Using Resonant Auger Spectroscopy", *J. Phys. Chem. C*, **2014**, *118*, 5570–5578.

[89] D. B. Lingerfelt, S. A. Fischer, J. W. May and X. Li, "Dynamical Investigations of Inhomogenous Vibrational Broadening in Diluted Magnetic Semiconductor Nanocrystals", *J. Phys. Chem. C*, **2014**, *118*, 3266–3273.

[88] J. J. Goings, F. Ding and X. Li, "Self-Consistent Field Using Direct Inversion in Iterative Subspace Method and Quasi-Newton Vectors", *Adv. Quantum Chem.*, **2014**, *68*, 77–86.

[87] B. Peng, B. E. Van Kuiken, F. Ding and X. Li, "A Guided Self-Consistent-Field Method for Excited State Wave Function Optimization: Applications to Ligand Field Transitions in Transition Metal Complexes", *J. Chem. Theory Comput.*, **2013**, *9*, 3933–3938.

[86] C.-Z. Li, C.-C. Chueh, F. Ding, H.-L. Yip, P.-W. Liang, X. Li and A. K.-Y. Jen, "Doping of Fullerenes via Anion-Induced Electron Transfer and Its Implication for Surfactant Facilitated High Performance Polymer Solar Cells", *Adv. Mater.*, **2013**, *25*, 4425–4430.

[85] C. T. Chapman, W. Liang and X. Li, "Solvent Effects on Intramolecular Charge Transfer Dynamics in a Fullerene Derivative", *J. Phys. Chem. A*, **2013**, *117*, 2687–2691.

[84] C.-Z. Li, C.-C. Chueh, H.-L. Yip, F. Ding, X. Li and A. K.-Y. Jen, "Solution-Processable Highly Conducting Fullerenes", *Adv. Mater.*, **2013**, *25*, 2457–2461.

[83] F. Ding, B. E. Van Kuiken, B. E. Eichinger and X. Li, "An Efficient Method for Calculating Dynamical Hyperpolarizabilities Using Real-Time Time-Dependent Density Functional Theory", *J. Chem. Phys.*, **2013**, *138*, 064104.

[82] H. P. Hratchian and X. Li, "Thirty Years of Geometry Optimization in Quantum Chemistry and Beyond: A Tribute to Berny Schlegel", *J. Chem. Theory Comput.*, **2012**, *8*, 4853–4855.

[81] Y.-X. Xu, C.-C. Chueh, H.-L. Yip, F.-Z. Ding, Y.-X. Li, C.-Z. Li, X. Li, W.-C. Chen and A. K.-Y. Jen, "Improved Charge Transport and Absorption Coefficient in Indacenodithieno[3,2-b]thiophene-Based Ladder-Type Polymer Leading to Highly Efficient Polymer Solar Cells", *Adv. Mater.*, **2012**, *24*, 6356–6361.

[80] C. W. Schlenker, K.-S. Chen, H.-L. Yip, C.-Z. Li, L. R. Bradshaw, S. T. Ochsenbein, F. Ding, X. Li, D. R. Gamelin, A. K.-Y. Jen and D. S. Ginger, "Polymer Triplet Energy Levels Need Not Limit Photocurrent Collection in Organic Solar Cells", *J. Am. Chem. Soc.*, **2012**, *134*, 19661–19668.

[79] P. Nguyen, F. Ding, S. A. Fischer, W. Liang and X. Li, "Solvated First-Principles Excited State Charge Transfer Dynamics with Time-Dependent Polarizable Continuum Model and Solvent Dielectric Relaxation", *J. Phys. Chem. Lett.*, **2012**, *3*, 2898–2904.

[78] J. W. May, J. D. Lehner, M. J. Frisch and X. Li, "Transition State Search Using a Guided Direct Inversion in the Iterative Subspace Method", *J. Chem. Theory Comput.*, **2012**, *8*, 5175–5179.

[77] F. Ding, C. T. Chapman, W. Liang and X. Li, "Mechanisms of Bridge-Mediated Electron Transfer: A TDDFT Electronic Dynamics Study", *J. Chem. Phys.*, **2012**, *137*, 22A512.

[76] J. W. May, R. J. McMorris and X. Li, "Ferromagnetism in p-Type Manganese-Doped Zinc Oxide Quantum Dots", *J. Phys. Chem. Lett.*, **2012**, *3*, 1374–1380.

[75] B. Peng, W. Liang, M. A. White, D. R. Gamelin and X. Li, "Theoretical Evaluation of Spin-Dependent Auger De-Excitation in Mn^{2+}-Doped Semiconductor Nanocrystals", *J. Phys. Chem. C*, **2012**, *116*, 11223–11231.

[74] W. Liang, C. T. Chapman, F. Ding and X. Li, "Modeling Ultrafast Solvated Electronic Dynamics Using Time-Dependent Density Functional Theory and Polarizable Continuum Model", *J. Phys. Chem. A*, **2012**, *116*, 1884–1890.

[73] C. Moss, W. Liang, X. Li and F. Tureček, "The Early Life of a Peptide Cation-Radical. Ground and Excited-State Trajectories of Electron-Based Peptide Dissociations During the First 330 Femtoseconds", *J. Am. Soc. Mass Spectrom.*, **2012**, *23*, 446–459.

[72] R. Beaulac, Y. Feng, J. W. May, E. Badaeva, D. R. Gamelin and X. Li, "Orbital Pathways for Mn^{2+}-Carrier sp–d Exchange in Diluted Magnetic Semiconductor Quantum Dots", *Phys. Rev. B*, **2011**, *84*, 195324.

[71] F. Ding, W. Liang, C. T. Chapman, C. M. Isborn and X. Li, "On the Gauge Invariance of Nonperturbative Electronic Dynamics Using the Time-Dependent Hartree-Fock and Time-Dependent Kohn-Sham", *J. Chem. Phys.*, **2011**, *135*, 164101.

[70] S. A. Fischer, C. T. Chapman and X. Li, "Surface Hopping with Ehrenfest Excited Potential", *J. Chem. Phys.*, **2011**, *135*, 144102.

[69] W. Liang, S. A. Fischer, M. J. Frisch and X. Li, "Energy-Specific Linear Response TDHF/TDDFT for Calculating High-Energy Excited States", *J. Chem. Theory Comput.*, **2011**, *7*, 3540–3547.

[68] E. Badaeva, J. W. May, J. Ma, D. R. Gamelin and X. Li, "Characterization of Excited-State Magnetic Exchange in Mn^{2+}-Doped ZnO Quantum Dots Using Time-Dependent Density Functional Theory", *J. Phys. Chem. C*, **2011**, *115*, 20986–20991.

[67] W. Liang, X. Li, L. R. Dalton, B. H. Robinson and B. E. Eichinger, "Solvents Level Dipole Moments", *J. Phys. Chem. B*, **2011**, *115*, 12566–12570.

[66] W. Liang, C. T. Chapman and X. Li, "Efficient First-Principles Electronic Dynamics", *J. Chem. Phys.*, **2011**, *134*, 184102.

[65] C. T. Chapman, W. Liang and X. Li, "Ultrafast Coherent Electron-Hole Separation Dynamics in a Fullerene Derivative", *J. Phys. Chem. Lett.*, **2011**, *2*, 1189–1192.

[64] D. H. Bale, B. E. Eichinger, W. Liang, X. Li, L. R. Dalton, B. H. Robinson and P. J. Reid, "Dielectric Dependence of the First Molecular Hyperpolarizability for Electro-Optic Chromophores", *J. Phys. Chem. B*, **2011**, *115*, 3505–3513.

[63] C. T. Chapman, W. Liang and X. Li, "Open-System Electronic Dynamics and Thermalized Electronic Structure", *J. Chem. Phys.*, **2011**, *134*, 024118.

[62] W. Liang, C. T. Chapman, M. J. Frisch and X. Li, "Geometry Optimization with Multilayer Methods Using Least-Squares Minimization", *J. Chem. Theory Comput.*, **2010**, *6*, 3352–3357.

[61] J. Hung, W. Liang, J. Luo, Z. Shi, A. K.-Y. Jen and X. Li, "Rational Design Using Dewar's Rules for Enhancing the First Hyperpolarizability of Nonlinear Optical Chromophores", *J. Phys. Chem. C*, **2010**, *114*, 22284–22288.

[60] W. Liang, H. Wang, J. Hung, X. Li and M. J. Frisch, "Eigenspace Update for Molecular Geometry Optimization in Nonredundant Internal Coordinate", *J. Chem. Theory Comput.*, **2010**, *6*, 2034–2039.

[59] Z. Shi, W. Liang, J. Luo, S. Huang, B. M. Polishak, X. Li, T. R. Younkin, B. A. Block and A. K.-Y. Jen, "Tuning the Kinetics and Energetics of Diels-Alder Cycloaddition Reactions to Improve Poling Efficiency and Thermal Stability of High-Temperature Cross-Linked Electro-Optic Polymers", *Chem. Mater.*, **2010**, *22*, 5601–5608.

[58] W. Liang, C. M. Isborn, A. Lindsay, X. Li, S. M. Smith and R. J. Levis, "Time-Dependent Density Functional Theory Calculations of Ehrenfest Dynamics of Laser Controlled Dissociation of NO^+: Pulse Length and Sequential Multiple Single-Photon Processes", *J. Phys. Chem. A*, **2010**, *114*, 6201–6206.

[57] Y. Feng, E. Badaeva, D. R. Gamelin and X. Li, "Excited-State Double Exchange in Manganese-Doped ZnO Quantum Dots: A Time-Dependent Density-Functional Study", *J. Phys. Chem. Lett.*, **2010**, *1*, 1927–1931.

[56] S. M. Smith, D. A. Romanov, X. Li, J. A. Sonk, H. B. Schlegel and R. J. Levis, "Numerical Bound State Electron Dynamics of Carbon Dioxide in the Strong-Field Regime", *J. Phys. Chem. A*, **2010**, *114*, 2576–2587.

[55] W. Liang, C. M. Isborn and X. Li, "Obtaining Hartree-Fock and Density Functional Theory Doubly Excited States with Car-Parrinello Density Matrix Search", *J. Chem. Phys.*, **2009**, *131*, 204101.

[54] S. T. Ochsenbein, Y. Feng, K. M. Whitaker, E. Badaeva, W. K. Liu, X. Li and D. R. Gamelin, "Charge-Controlled Magnetism in Colloidal Doped Semiconductor Nanocrystals", *Nat. Nano.*, **2009**, *4*, 681–687.

[53] C. M. Isborn and X. Li, "Singlet-Triplet Transitions in Real-Time Time-Dependent Hartree-Fock/Density Functional Theory", *J. Chem. Theory Comput.*, **2009**, *5*, 2415–2419.

[52] C. L. Moss, C. M. Isborn and X. Li, "Ehrenfest Dynamics with a Time-Dependent Density-Functional-Theory Calculation of Lifetimes and Resonant Widths of Charge-Transfer States of Li^+ Near an Aluminum Cluster Surface", *Phys. Rev. A*, **2009**, *80*, 024503.

[51] X. Li, C. L. Moss, W. Liang and Y. Feng, "Car-Parrinello Density Matrix Search with a First Principles Fictitious Electron Mass Method for Electronic Wave Function Optimization", *J. Chem. Phys.*, **2009**, *130*, 234115.

[50] W. Liang, C. M. Isborn and X. Li, "Laser-Controlled Dissociation of $C_2H_2^{2+}$: Ehrenfest Dynamics Using Time-Dependent Density Functional Theory", *J. Phys. Chem. A*, **2009**, *113*, 3463–3469.

[49] E. Badaeva, C. M. Isborn, Y. Feng, S. T. Ochsenbein, D. R. Gamelin and X. Li, "Theoretical Characterization of Electronic Transitions in Co^{2+}- and Mn^{2+}-Doped ZnO Nanocrystals", *J. Phys. Chem. C*, **2009**, *113*, 8710–8717.

[48] C. M. Isborn and X. Li, "Modeling the Doubly Excited State with Time-Dependent Hartree–Fock and Density Functional Theories", *J. Chem. Phys.*, **2008**, *129*, 204107.

[47] C. M. Isborn, S. V. Kilina, X. Li and O. V. Prezhdo, “Generation of Multiple Excitons in PbSe and CdSe Quantum Dots by Direct Photoexcitation: First-Principles Calculations on Small PbSe and CdSe Clusters”, *J. Phys. Chem. C*, **2008**, *112*, 18291–18294.

[46] C. L. Moss and X. Li, “First Order Simultaneous Optimization of Molecular Geometry and Electronic Wave Function”, *J. Chem. Phys.*, **2008**, *129*, 114102.

[45] J. A. Davies, A. Elangovan, P. A. Sullivan, B. C. Olbricht, D. H. Bale, T. R. Ewy, C. M. Isborn, B. E. Eichinger, B. H. Robinson, P. J. Reid, X. Li and L. R. Dalton, “Rational Enhancement of Second-Order Nonlinearity: Bis-(4-methoxyphenyl)hetero-aryl-amino Donor-Based Chromophores: Design, Synthesis, and Electrooptic Activity”, *J. Am. Chem. Soc.*, **2008**, *130*, 10565–10575.

[44] E. Badaeva, Y. Feng, D. R. Gamelin and X. Li, “Investigation of Pure and Co^{2+}-Doped ZnO Quantum Dot Electronic Structures Using the Density Functional Theory: Choosing the Right Functional”, *New J. Phys.*, **2008**, *10*, 055013.

[43] K. L. Wustholz, E. D. Bott, C. M. Isborn, X. Li, B. Kahr and P. J. Reid, “Dispersive Kinetics from Single Molecules Oriented in Single Crystals of Potassium Acid Phthalate”, *J. Phys. Chem. C*, **2007**, *111*, 9146–9156.

[42] C. M. Isborn, X. Li and J. C. Tully, “TDDFT Ehrenfest Dynamics: Collisions between Atomic Oxygen and Graphite Clusters”, *J. Chem. Phys.*, **2007**, *126*, 134307.

[41] X. Li and J. C. Tully, “Ab Initio Time-Resolved Density Functional Theory for Lifetimes of Excited Adsorbate States at Metal Surfaces”, *Chem. Phys. Lett.*, **2007**, *439*, 199–203.

[40] S. M. Smith, X. Li, A. Markevitch, D. Romanov, R. J. Levis and H. B. Schlegel, “Numerical Simulation of Nonadiabatic Electron Excitation in the Strong-Field Regime. 3. Polyacene Neutrals and Cations”, *J. Phys. Chem. A*, **2007**, *111*, 6920–6932.

[39] H. B. Schlegel, S. M. Smith and X. Li, “Electronic Optical Response of Molecules in Intense Fields: Comparison of TD-HF, TD-CIS, and TD-CIS(D) Approaches”, *J. Chem. Phys.*, **2007**, *126*, 244110.

[38] X. Li and M. J. Frisch, “Energy-Represented Direct Inversion in the Iterative Subspace within a Hybrid Geometry Optimization Method”, *J. Chem. Theory Comput.*, **2006**, *2*, 835–839.

[37] S. M. Smith, X. Li, A. N. Markevitch, D. A. Romanov, R. J. Levis and H. B. Schlegel, “Numerical Simulation of Nonadiabatic Electron Excitation in the Strong Field Regime. 2. Linear Polyene Cations”, *J. Phys. Chem. A*, **2005**, *109*, 10527–10534.

[36] X. Li, J. C. Tully, H. B. Schlegel and M. J. Frisch, “Ab Initio Ehrenfest Dynamics”, *J. Chem. Phys.*, **2005**, *123*, 084106.

[35] X. Li, S. M. Smith, A. N. Markevitch, D. A. Romanov, R. J. Levis and H. B. Schlegel, “A Time-Dependent Hartree-Fock Approach for Studying the Electronic Optical Response of Molecules in Intense Fields”, *Phys. Chem. Chem. Phys.*, **2005**, *7*, 233–239.

[34] S. M. Smith, X. Li, A. N. Markevitch, D. A. Romanov, R. J. Levis and H. B. Schlegel, “A Numerical Simulation of Nonadiabatic Electron Excitation in the Strong Field Regime: Linear Polyenes”, *J. Phys. Chem. A*, **2005**, *109*, 5176–5185.

[33] J. Li, X. Li, S. Shaik and H. B. Schlegel, “Single Transition State Serves Two Mechanisms. Ab Initio Classical Trajectory Calculations of the Substitution-Electron Transfer Branching Ratio in $CH_2O^{\bullet-}$+CH_3Cl”, *J. Phys. Chem. A*, **2004**, *108*, 8526–8532.

[32] X. Li and H. B. Schlegel, “Ab Initio Classical Trajectory Calculations of Acetylene Dication Dissociation”, *J. Phys. Chem. A*, **2004**, *108*, 468–472.

[31] Y. Feng, L. Liu, J.-T. Wang, X.-S. Li and Q.-X. Guo, “Blue-Shifted Lithium Bonds”, *Chem. Commun.*, **2004**, *1*, 88–89.

[30] Y. Feng, S.-W. Zhao, L. Liu, J.-T. Wang, X.-S. Li and Q.-X. Guo, “Blue-Shifted Dihydrogen Bonds”, *J. Phys. Org. Chem.*, **2004**, *17*, 1099–1106.

[29] S. M. Smith, A. N. Markevitch, D. A. Romanov, X. Li, R. J. Levis and H. B. Schlegel, "Static and Dynamic Polarizabilities of Conjugated Molecules and Their Cations", *J. Phys. Chem. A*, **2004**, *108*, 11063–11072.

[28] J.-X. Wang, Y. Feng, L. Liu, X.-S. Li and Q.-X. Guo, "On the Correlation between the Blue Shif of Hydrogen Bonding and the Proton Donor-Proton Acceptor Distance", *Chinese J. Chem.*, **2004**, *22*, 642–648.

[27] X. Li, J. M. Millam, G. E. Scuseria, M. J. Frisch and H. B. Schlegel, "Density Matrix Search Using Direct Inversion in the Iterative Subspace as a Linear Scaling Alternative to Diagonalization in Electronic Structure Calculations", *J. Chem. Phys.*, **2003**, *119*, 7651.

[26] J.-T. Wang, Y. Feng, L. Liu, X.-S. Li and Q.-X. Guo, "Blue-Shifted Hydrogen Bonds with Proton-Donors Incapable of Rehybridization", *Chem. Lett.*, **2003**, *32*, 746–747.

[25] X. Li, S. Anand, J. M. Millam and H. B. Schlegel, "An Ab Initio Direct Classical Trajectory Study of S-tetrazine Photodissociation", *Phys. Chem. Chem. Phys.*, **2002**, *4*, 2554–2559.

[24] X. Li, L. Liu and H. B. Schlegel, "On the Physical Origin of Blue-Shifted Hydrogen Bonds", *J. Am. Chem. Soc.*, **2002**, *124*, 9639–9647.

[23] H. B. Schlegel, S. S. Iyengar, X. Li, J. M. Millam, G. A. Voth, G. E. Scuseria and M. J. Frisch, "Ab Initio Molecular Dynamics: Propagating the Density Matrix with Gaussian Orbitals. III. Comparison with Born-Oppenheimer Dynamics", *J. Chem. Phys.*, **2002**, *117*, 8694.

[22] R. Chen, Y.-H. Cheng, L. Liu, X.-S. Li and Q.-X. Guo, "π-Type and Σ-Type Cation-π Complexes of Atomic Cations", *Res. Chem. Intermediat.*, **2002**, *28*, 41–48.

[21] Y.-H. Cheng, L. Liu, Y. Fu, R. Chen, X.-S. Li and Q.-X. Guo, "Counterion Effects on the Cation-π Interaction between Alkaline Earth Cations and Benzene", *J. Phys. Chem. A*, **2002**, *106*, 11215–11220.

[20] J.-M. Fan, K.-C. Zhang, L. Liu, X.-S. Li and Q.-X. Guo, "Substituent Effects on the Blue-Shifting Hydrogen Bonds between X–C≡C–CF_2–H and Water", *Chinese J. Chem.*, **2002**, *20*, 247–251.

[19] Y. Fang, J.-M. Fan, L. Liu, X.-S. Li and Q.-X. Guo, "Steric Effect Is an Additional Possible Cause of Blue-Shifting Hydrogen Bonds", *Chem. Lett.*, **31**, *2002*, 116–117.

[18] Y. Fang, L. Liu, Y. Feng, X.-S. Li and Q.-X. Guo, "Effects of Hydrogen Bonding to Amines on the Phenol/Phenoxyl Radical Oxidation", *J. Phys. Chem. A*, **2002**, *106*, 4669–4678.

[17] K.-S. Song, Y.-H. Cheng, Y. Fu, L. Liu, X.-S. Li and Q.-X. Guo, "Radical Stabilization Energies of Substituted XNH· Radicals", *J. Phys. Chem. A*, **2002**, *106*, 6651–6658.

[16] R. Chen, K.-C. Zhang, L. Liu, X.-S. Li and Q.-X. Guo, "Substituent Effects in X–C≡C–H···NH_3 (Or OH_2, FH) Hydrogen Bonding", *Chem. Phys. Lett.*, **2001**, *338*, 61–66.

[15] X. Li, J. M. Millam and H. B. Schlegel, "Glyoxal Photodissociation. An Ab Initio Direct Classical Trajectory Study of $C_2H_2O_2 \rightarrow H_2$ + 2CO", *J. Chem. Phys.*, **2001**, *114*, 8897–8904.

[14] X. Li, J. M. Millam and H. B. Schlegel, "Glyoxal Photodissociation. II. An Ab Initio Direct Classical Trajectory Study of $C_2H_2O_2 \rightarrow$CO + H_2CO", *J. Chem. Phys.*, **2001**, *115*, 6907–6912.

[13] X. Li and H. B. Schlegel, "Photodissociation of Glyoxal: Resolution of a Paradox", *J. Chem. Phys.*, **2001**, *114*, 8–10.

[12] L. Liu, K.-S. Song, X.-S. Li and Q.-X. Guo, "Charge-Transfer Interaction: A Driving Force for Cyclodextrin Inclusion Complexation", *J. Incl. Phenom. Macro.*, **2001**, *40*, 35–39.

[11] T.-W. Mu, L. Liu, X.-S. Li and Q.-X. Guo, "A Theoretical Study on the Inclusion Complexation of Cyclodextrins with Radical Cations and Anions", *J. Phys. Org. Chem.*, **2001**, *14*, 559–565.

[10] K.-S. Song, C.-R. Hou, L. Liu, X.-S. Li and Q.-X. Guo, "A Quantum-Chemical Study on the Molecular Recognition of β-Cyclodextrin with Ground and Excited Xanthones", *J. Photochem. Photobiol.*, **2001**, *139*, 105–109.

[9] X.-S. Li, L. Liu, T.-W. Mu and Q.-X. Guo, "A Systematic Quantum Chemistry Study on Cyclodextrins", *Monatsh. Chem.*, **2000**, *131*, 849–855.

[8] X.-S. Li, L. Liu, T.-W. Mu, Q.-X. Guo and Y.-C. Liu, "A Theoretical Study on the Structure and Properties of Phenothiazine Derivatives and Their Radical Cations", *Res. Chem. Intermediat.*, **2000**, *26*, 375–384.

[7] X. Li, J. M. Millam and H. B. Schlegel, "Ab Initio Molecular Dynamics Studies of the Photodissociation of Formaldehyde, $H_2CO \rightarrow H_2$ + CO: Direct Classical Trajectory Calculations by MP2 and Density Functional Theory", *J. Chem. Phys.*, **2000**, *113*, 10062–10067.

[6] L. Liu, X.-S. Li and Q.-X. Guo, "Orientation Conversion in the Complexation of A-Cyclodextrin with 4-Fluorophenol: A PM3 Quantum Chemical Study", *J. Mol. Struct.*, **2000**, *530*, 31–37.

[5] L. Liu, X.-S. Li, T.-W. Mu, Q.-X. Guo and Y.-C. Liu, "Interplay between Molecular Recognition and Redox Properties: A Theoretical Study of the Inclusion Complexation of B-Cyclodextrin with Phenothiazine and Its Radical Cation", *J. Incl. Phenom. Macro.*, **2000**, *38*, 199–206.

[4] L. Liu, X.-S. Li, K.-S. Song and Q.-X. Guo, "PM3 Studies on the Complexation of A-cyclodextrin with Benzaldehyde and Acetophenone", *J. Mol. Struct.*, **2000**, *531*, 127–134.

[3] K.-S. Song, L. Liu, C.-R. Hou, X.-S. Li and Q.-X. Guo, "Molecular Orbital and DFT Studies of the Alimemazine Radical Cation", *Res. Chem. Intermediat.*, **2000**, *26*, 739–745.

[2] X.-S. Li, L. Liu, Q.-X. Guo, S.-D. Chu and Y.-C. Liu, "PM3 Molecular Orbital Calculations on the Complexation of A-Cyclodextrin with Acetophenone", *Chem. Phys. Lett.*, **1999**, *307*, 117–120.

[1] L. Liu, X.-S. Li, Q.-X. Guo and Y.-C. Liu, "Hartree-Fock and Density Functional Theory Studies on the Molecular Recognition of the Cyclodextrin", *Chinese Chem. Lett.*, **1999**, *10*, 1053–1056.

Invited Presentations (Total 240 to date)

Talks at Conferences and Other Scientific Meetings

160	New Directions and Implications of the Chirality Induced Spin Selectivity Effect	*Bad-Honnef, Germany*	Nov. 2026
159	15th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics	*Okazaki, Japan*	Oct. 2026
158	Empowering Actinide Science and Talent, ACS National Meeting	*Chicago, IL*	Aug. 2026
157	Summer School: Frontiers in Ab Initio Quantum Molecular Dynamics (CECAM Flagship School)	*Beijing, China*	Jul. 2026
156	46th International Conference on Coordination Chemistry	*Odense, Denmark*	Jul. 2026
155	Solid State to Biophysics XII	*Dubrovnik, Croatia*	Jun. 2026
154	CECAM Workshop: Conceptual DFT and Interpretative Methods for Excited, Protonic, Muonic, and Positronic States	*Paris, France*	Jun. 2026
153	Advances in Electronic Structure Theory and Dynamics	*Merced, CA*	Jun. 2026
152	Chemical Dynamics, Chinese Chemical Society National Meeting	*ChongQing, China*	Apr. 2026
151	Pittsburg Quantum Institute	*Pittsburgh, PA*	Apr. 2026
150	Symposium in Honor of the 65th Birthday of Dr. Weitao Yang: DFT and Beyond, ACS National Meeting	*Atlanta, GA*	Mar. 2026
149	Electronic Structure Methods For Time-Dependent, Frequency-Dependent and Spectroscopic Properties, ACS National Meeting	*Atlanta, GA*	Mar. 2026
148	Frontiers in Actinide Chemistry: From Fundamental Systems to Practical Applications, Pacifichem	*Honolulu, HI*	Dec. 2025
147	NSF Workshop on Ultrafast Spectroscopy	*Alexandria, VA*	Oct. 2025
146	Manipulating Molecular Electronic Properties by Vibrational Excitations: Novel Spectroscopies and Microscopies	*Bad Honnef, Germany*	Aug. 2025
145	Excited State Processes	*Santa Fe, NM*	Jun. 2025
144	Chirality-Induced Spin Selectivity Workshop	*Golden, CO*	May 2025
143	Nonadiabatic Dynamics, Electron-phonon Interactions, and Spin-phonon Couplings, Princeton Center for Theoretical Science	*Princeton, NJ*	Apr. 2025
142	Simulating Excited States, ACS National Meeting	*San Diego, CA*	Mar. 2025
141	Congress of the International Society for Theoretical Chemical Physics	*Qingdao, China*	Oct. 2024
140	International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics	*Groningen, Netherlands*	Oct. 2024
139	PHYS Awards, ACS National Meeting	*Denver, CO*	Aug. 2024
138	Symposium in Honor of the 80th Birthday of Prof. Donald G. Truhlar, ACS National Meeting	*Denver, CO*	Aug. 2024
137	NeXUS User Workshop	*Columbus, OH*	Jul. 2024
136	Electron Donor-Acceptor Interactions, Gordon Research Conference	*Newport, RI*	Jul. 2024
135	American Conference on Theoretical Chemistry	*Chapel Hill, NC*	Jun. 2024

134	Materials Research by the LGBTQIA+ Community and a Vision for Inclusivity, MRS National Meeting	*Seattle, WA*	Apr. 2024
133	Informed Design of Quantum Dots and Quantum Dot Assemblies for Energy Applications, ACS National Meeting	*New Orleans, LA*	Mar. 2024
132	Recent Progress in Theoretical Methods for Coupled Quantum Systems, ACS National Meeting	*New Orleans, LA*	Mar. 2024
131	SIAM Conference on Parallel Processing for Scientific Computing	*Baltimore, MD*	Mar. 2024
130	Probing Structure and Dynamics with XUV and X-Ray Light: Ultrafast Studies of Photocatalysis and Water Radiolysis, APS National Meeting	*Minneapolis, MN*	Mar. 2024
129	The Path of Quantum Chemistry into the 21st Century	*Zürich, Switzerland*	Jan. 2024
128	AVS 69th International Symposium	*Portland, OR*	Nov. 2023
127	Summer Modeling 2023	*Castiglione della Pescaia, Italy*	Sep. 2023
126	Quantum International Frontiers	*Łódź, Poland*	Jun. 2023
125	Westlake Theory Symposium	*Hanzhou, China*	Apr. 2023
124	Award for Computers in Chemical & Pharmaceutical Research, ACS National Meeting	*Indianapolis, IN*	Mar. 2023
123	Science & Technology of Emerging Materials Symposium (STEMS)	*Orlando, FL*	Mar. 2023
122	2nd Theory Frontiers in Actinide Science (FACT)	*Santa Fe, NM*	Feb. 2023
121	13th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics	*Assisi, Italy*	Sep. 2022
120	Status and Perspectives of Computational Chemistry Toward 2030	*Ischia Island, Italy*	Sep. 2022
119	7th International Conference on Chemical Bonding	*Kauai, HI*	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, Pacifichem	*Honolulu, Hawaii*	Dec. 2021
111	Quantum Coherence in Energy Transfer, Pacifichem	*Honolulu, Hawaii*	Dec. 2021
110	Heavy Element Chemistry: From Theoretical Development to Application, Pacifichem	*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	(*Frontier Lecture*) 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	(*Keynote Speaker*) 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	*Orlando, FL*	Mar. 2019
88	Sustainable Software for Computational Molecular Science, ACS National Meeting	*Orlando, FL*	Mar. 2019
87	Addressing Molecular Magnetic Qubits, APS National Meeting	*Boston, MA*	Mar. 2019
86	University of Washington – Tohoku University Academic Open Space Workshop	*Sendai, Japan*	Oct. 2018
85	From Potential Energy Surfaces to Dynamics & Kinetics, ACS National Meeting	*Boston, MA*	Aug. 2018
84	Computational Photocatalysis: Modeling of Photophysics & Photochemistry at Interfaces, ACS National Meeting	*Boston, MA*	Aug. 2018
83	Recent Advances in DFT & TDDFT: Theory & Simulations, ACS National Meeting	*Boston, MA*	Aug. 2018
82	Parallel Computing in Molecular Sciences	*Berkeley, CA*	Aug. 2018
81	Computational Chemistry, Gordon Research Conference	*Mount Snow, VT*	Jul. 2018
80	Developments in QM/MM and Embedding Models for Photochemical and Electron Transfer Processes	*Telluride, CO*	Jul. 2018
79	International Congress of Quantum Chemistry, Photoinduced Processes in Embedded Systems	*Pisa, Italy*	Jun 2018
78	Low-scaling and Unconventional Electronic Structure Techniques	*Telluride, CO*	Jun 2018
77	DOE Energy Frontier Center Meeting	*Gaithersburg, MD*	Apr. 2018

76	Zhang Dayu Young Investigator Lectureship, Dalian Institute of Chemical Physics	*Dalian, China*	Mar. 2018
75	Chirality from Molecules to Materials, ACS National Meeting	*New Orleans, LA*	Mar. 2018
74	University of Washington – Tohoku University Academic Open Space Workshop	*Seattle, WA*	Nov. 2017
73	DOE Condensed Phase and Interfacial Molecular Science Research Meeting	*Gaithersburg, MD*	Oct. 2017
72	World Association of Theoretical and Computational Chemists (WATOC)	*Munich, Germany*	Aug. 2017
71	DOE Energy Frontier Center Meeting	*Gaithersburg, MD*	Jul. 2017
70	Excited State Electronic Structure and Dynamics	*Telluride, CO*	Jul. 2017
69	(*Plenary Lecture*) Computational Software Workshop, National Science Foundation of China	*Dalian, China*	Jun. 2017
68	DOE Computational and Theoretical Chemistry Meeting	*Gaithersburg, MD*	May 2017
67	Strong Electron Correlation & Nonadiabatic Dynamics, ACS National Meeting	*San Francisco, CA*	Apr. 2017
66	In Silico Materials Chemistry, MRS National Meeting	*Boston, MA*	Nov. 2016
65	Workshop on Theoretical Chemistry	*Trujillo, Peru*	Sep. 2016
64	Molecular Electronic Structure Workshop	*Buenos Aires, Argentina*	Sep. 2016
63	Theory and Application of Computational Chemistry	*Seattle, WA*	Aug. 2016
62	Computational Chemistry Workshop	*Changchun, China*	Aug. 2016
61	Complex Systems Symposium, The 9th International Symposium of Theoretical Chemical Physics,	*Grand Forks, ND*	Jul. 2016
60	The 21st International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXI)	*Vancouver, Canada*	Jul. 2016
59	DOE Solar Photochemistry Meeting	*Gaithersburg, MD*	Jun. 2016
58	Low-scaling and Unconventional Electronic Structure Techniques	*Telluride, CO*	Jun. 2016
57	DOE Computational and Theoretical Chemistry Meeting	*Gaithersburg, MD*	May 2016
56	Time-Dependent Dynamics and Electronic Excited States, ACS National Meeting	*San Diego, CA*	Mar. 2016
55	Sanibel Symposium	*St. Simons Island, GA*	Feb. 2016
54	Mesilla Workshop	*Mesilla, NM*	Jan. 2016
53	Photocatalysis and Charge Transfer at Interfaces and Nanomaterials, Pacifichem	*Honolulu, HI*	Dec. 2015
52	Quantum Coherence in Energy Transfer, Pacifichem	*Honolulu, HI*	Dec. 2015
51	Computational Modeling of Magnetic Materials and Magnetic, Properties, Pacifichem	*Honolulu, HI*	Dec. 2015
50	Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Cluster, Pacifichem	*Honolulu, HI*	Dec. 2015
49	Open Quantum Systems Computational Methods	*Hong Kong, China*	Nov. 2015
48	Electronic Structure and Processes at Molecular-Based Interfaces VIII	*Tuscon, AZ*	Oct. 2015
47	Non-equilibrium Phenomena	*Telluride, CO*	Jul. 2015
46	Excited State Electronic Structure Theory and Dynamics	*Telluride, CO*	Jul. 2015
45	Nanomaterials: Computation, Theory, and Experiment	*Telluride, CO*	Jun. 2015
44	Advances in Theoretical Spectroscopy	*Seattle, WA*	Jun. 2015

43	The 26th Annual Workshop on Recent Developments in Electronic Structure Theory	*Seattle, WA*	Jun. 2015
42	15th International Congress of Quantum Chemistry	*Beijing, China*	Jun. 2015
41	Charge Transfer Modeling in Chemistry: New Methods and Solutions for a Long-standing Problem	*Paris, France*	Apr. 2015
40	Electronic Structure Methods for Highly Polarizable Systems, 249th ACS National Meeting	*Denver, CO*	Mar. 2015
39	Modeling Excited States of Complex Systems, 249th ACS National Meeting	*Denver, CO*	Mar. 2015
38	Chemical Approaches to Spintronics Research, 249th ACS National Meeting	*Denver, CO*	Mar. 2015
37	Quantum Systems in Chemistry, Physics and Biology	*Taipei, Taiwan*	Nov. 2014
36	World Association of Theoretical and Computational Chemists (WATOC)	*Santiago, Chile*	Oct. 2014
35	Molecular Electronic Structure	*Amasya, Turkey*	Sep. 2014
34	International Conference on Chemical Bonding	*Kauai, HI*	Jul. 2014
33	Colloidal Semiconductor Nanocrystals, Gordon Research Conference	*Smithfield, RI,*	Jul. 2014
32	Excited State and Time-Dependent Electronic Structure Theory	*Telluride, CO*	Jul. 2014
31	12th Chinese National Meeting on Theoretical Chemistry	*Taiyuan, China*	Jun. 2014
30	Excited State Processes in Electronic and Nanomaterials	*Santa Fe, NM*	Jun. 2014
29	XXXVII Brazilian National Meeting of Condensed Matter Physicists	*Salvador, Brazil*	May 2014
28	Computational Photocatalysis, 246th ACS National Meeting	*Indianapolis, IN*	Sep. 2013
27	Nonequilibrium Phenomena, Nonadiabatic Dynamics	*Telluride, CO*	Jul. 2013
26	ACS Award Symposium, 245th ACS National Meeting	*New Orleans, LA*	Mar. 2013
25	Computational Methods for Complex Systems	*Hong Kong, China*	Dec. 2012
24	Connecticut Quantum Chemistry Meeting	*Wallingford, CT*	Oct. 2012
23	International Conference on Multiscale Materials Modeling	*Singapore*	Oct. 2012
22	Troy Electronic Structure Workshop	*Canakkale, Turkey*	Sep. 2012
21	Spintronics, SPIE	*San Diego, CA*	Aug. 2012
20	Geometry Optimization, 244th ACS National Meeting	*Philadelphia, PA*	Aug. 2012
19	Nanomaterials: Theory and Computation, Telluride Science Research Conference	*Telluride, CO*	Jul. 2012
18	Low-scaling and Unconventional Electronic Structure Techniques, Telluride Science Research Conference	*Telluride CO*	Jun. 2012
17	Applications of Computational Methods to Environmentally Sustainable Solutions, 243rd ACS National Meeting	*San Diego, CA*	Mar. 2012
16	Excited-State Dynamics: Theory and Experiment, 242nd ACS National Meeting	*Denver, CO*	Aug. 2011
15	Nonequilibrium Phenomena, Telluride Scientific Research Conference	*Telluride, CO*	Jul. 2011
14	Challenges for Density Functional Theory, 240th ACS National Meeting	*Boston, MA*	Aug. 2010
13	Physical Chemistry of Interfaces and Nanomaterials, SPIE National Conference	*San Diego, CA*	Aug. 2010
12	Applications and Development at Multiple Length and Time Scales, ACS NORM/RMRM Meeting	*Pullman, WA*	Jun. 2010

11	Physical Chemistry of Interfaces and Nanomaterials, SPIE National Conference	*San Diego, CA*	Aug. 2009
10	Nonequilibrium Phenomena, Telluride Scientific Research Conference	*Telluride, CO*	Jul. 2009
9	Excited State Processes	*Santa Fe, NM*	Jun. 2009
8	Conference on Nanotechnology	*Seattle, WA*	Jun. 2009
7	Advances in Electronic Structure Theory and First Principles Dynamics, 237th ACS National Meeting	*Salt Lake City, UT*	Mar. 2009
6	Convergence between Theory and Experiment in Surface Chemistry and Catalysis, 237th ACS National Meeting	*Salt Lake City, UT*	Mar. 2009
5	Transatlantic Frontiers in Chemistry Symposium	*Chester, UK*	Aug. 2008
4	Connecticut Quantum Chemistry Meeting	*Wallingford, CT*	Feb. 2008
3	Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride Scientific Research Conference	*Telluride, CO*	Jul. 2007
2	Workshop in High Performance Computing	*Beijing, China*	Apr. 2007
1	The Second International Conference on Theoretical Chemistry, Molecular Modeling and Life Sciences	*NanDaiHe, China*	Jul. 2006

Seminars at Universities and Other Research Institutions

80	Department of Chemistry, University of California, Santa Cruz	*Santa Cruz, CA*	May 2026
79	Abbott Lecture, Department of Chemistry, University of North Dakota	*Grand Forks, ND*	Apr. 2026
78	Department of Chemistry, Wake Forest University	*Winston-Salem, NC*	Mar. 2026
77	Department of Chemistry, Oregon State University	*Corvallis, OR*	Feb. 2026
76	Haines-Morris Theoretical Chemistry and Chemical Physics Lecture, The University of Tennessee	*Knoxville, TN*	Mar. 2025
75	Department of Chemistry, Stony Brook University	*Stony Brook, NY*	Mar. 2025
74	Closs Lecture, University of Chicago	*Chicago, IL*	Mar. 2025
73	Harvard-MIT-BU Theory Meeting	*Boston, MA*	Nov. 2024
72	Institute for Molecular Physical Science, ETH Zürich	*Zürich, Switzerland*	Jan. 2024
71	Department of Physics, University of Texas, El Paso	*El Paso, TX*	Oct. 2023
70	Department of Chemistry, Boston College	*Boston, MA*	Feb. 2023
69	Karcher Lecture, University of Oklahoma	*Norman, OK*	Jan. 2023
68	Department of Materials Science and Engineering, University of Washington	*Seattle, WA*	Jan. 2023
67	Department of Chemistry, Case Western Reserve University	*Cleveland, OH*	Oct. 2022
66	Colloquium, Department of Chemistry, University of California Riverside	*Riverside, CA*	May. 2022
65	Department of Chemistry, University of Michigan	*Ann Arbor, MI*	May. 2022
64	Department of Chemistry, Auburn University	*Auburn, AL*	Apr. 2022
63	Department of Chemistry, Whitman College	*Ann Arbor, MI*	Mar. 2022

62	Department of Chemistry, University of Wisconsin Madison	*Madison, WI*	Feb. 2022
61	Department of Chemistry, University of California Santa Barbara	*Santa Barbara, CA*	Jan. 2022
60	Department of Chemistry, University of North Dakota (Virtual)	*Grand Forks, ND*	Jan. 2021
59	Department of Chemistry, Wayne State University (Virtual)	*Detroit, MI*	Jan. 2021
58	Department of Chemistry, Wesleyan University (Virtual)	*Middletown, CT*	Nov. 2020
57	Department of Chemistry, Oakland University (Virtual)	*Rochester, MI*	Oct. 2020
56	Department of Chemistry, The Ohio State University	*Columbus, OH*	Feb. 2020
55	Department of Chemistry, Duke University	*Durham, NC*	Feb. 2020
54	Department of Chemistry, North Carolina State University	*Raleigh, NC*	Feb. 2020
53	Department of Chemistry, University of North Carolina	*Chapel Hill, NC*	Feb. 2020
52	College of Sciences, Southern University of Science and Technology	*Shenzhen, China*	Jul. 2019
51	Department of Chemistry, Shanghai Jiao Tong University	*Shanghai, China*	Jun. 2019
50	Department of Chemistry, University of Minnesota	*Minneapolis, MN*	May 2019
49	Department of Chemistry, University of Illinois – Chicago	*Chicago, IL*	May 2019
48	Argonne National Lab Colloquium	*Lemont, IL*	May 2019
47	Department of Chemistry, Washington State University	*Pullman, WA*	Apr. 2019
46	Department of Chemistry, California Institute of Technology	*Pasadena, CA*	Mar. 2019
45	Department of Chemistry, University of California – San Diego	*San Diego, CA*	Feb. 2019
44	(*Highlands in Chemistry Lecture*) 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	(*Student Invited Colloquium)* 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	*Beijing, China*	Sep. 2009
9	Department of Chemistry, Tsinghua University	*Beijing, China*	Sep. 2009
8	Department of Chemistry, Fudan University	*Shanghai, China*	Sep. 2009
7	Department of Chemistry, Northwestern University	*Evanston, IL*	Apr. 2009
6	Department of Chemistry, University of Wisconsin	*Madison, WI*	Apr. 2009
5	Department of Chemistry, University of New Mexico	*Albuquerque, NM*	Apr. 2009
4	Department of Physics, University of Washington	*Seattle, WA*	Jan. 2009
3	Keynote Lecture, Department of Chemistry, Wayne State University	*Detroit, MI*	Oct. 2008
2	Department of Applied Mathematics, University of Washington	*Seattle, WA*	Feb. 2008
1	Korean Advanced Institute of Science and Technology (KAIST)	*Daejoon, South Korea*	Feb. 2008

University & Professional Service

University Service

2025-present	Co-Chair, Research Resilience and Transformation Faculty Advisory 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

October 2025	Organizer, NSF Workshop on Ultrafast Spectroscopy, Alexandria, VA
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

Mentoring

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. Diandong Tang	05/2023
Dr. Shiv Upadhyay	07/2023
Dr. Rajat Majumder	11/2024
Dr. Tanner Culpitt	09/2025

Current Ph.D. Students

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. Jonathan Bersson	01/2024
Ms. Nova Zhang	01/2026
Ms. Qiwei Ying	01/2026
Mr. Martijn Oele	03/2026

Ph.D. Dissertations Supervised

Dr. Agam Shayit, Software Engineer, Microsoft	January 2025
Dr. Can Liao, Postdoctoral Researcher, ETC	June 2025
Dr. 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, 1Qbit	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 Lestrange, 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. Mengqi Yang	12/2023-12/2025
Dr. Xuechen Zheng, China Petrochemical Corporation	06/2023-06/2025
Dr. Eleftherios Lambros, Assistant Professor, California State University, Fullerton	06/2022-06/2025
Dr. Samragni Banerjee	10/2022-03/2025
Dr. Chad Hoyer, Assistant Professor, University of Texas, El Paso	01/2018-06/2024
Dr. Andrew Jenkins, Software Engineer, PsiQuantum	01/2017-06/2023
Dr. Ernesto Martinez, Data Scientist, Microsoft	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 Lestrange, 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 Xinzheng 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

Graduate Students

Jonathan Bersson	LANL Seaborg Fellowship (2025); NSF AQET Fellowship (2024)
Maxwell Taub	Clean Energy Institute Graduate Fellowship (2024);LANL Seaborg Fellowship (2026)
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)
Andrew Wildman	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)
Ryan Beck	Graduate Merit Fellowship (2020); NSF NRT Fellowship (2018); Excellence in Chemistry Graduate Fellowship (2016)
Torin Stetina	NSF MolSSI Software Fellowship (2020); Clean Energy Institute Graduate Fellowship (2018); NSF NRT Fellowship (2017)
Joseph Radler	NWTCC Best Poster Award (2017)
Lauren Koulias	NSF NRT Fellowship (2020); NSF MolSSI Software Fellowship (2019); Benton Seymour Rabinovitch Endowed Fellowship (2018)
Hongbin Liu	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)
Joseph Kasper	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)
David Williams-Young	UW Chemistry Merit Award (2016); NSF MolSSI Fellowship (2017); ACS Computational Chemistry Award (2017)
Bo Peng	Linus Pauling Distinguished Postdoctoral Fellowship (2016); ACS Computational Chemistry Award (2015)
Patrick Lestrange	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)
David Lingerfelt	Clean Energy Institute Fellowship (2015); UW Chemistry Merit Award (2014); UW Travel Award (2015)
Joshua Goings	ACS Computational Chemistry Award (2016); National Science Foundation Graduate Fellowship Award (2013); UW Chemistry Merit Award (2014) UW Travel Award (2015)

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)