Xinyang Li

Theoretical Division, Los Alamos National Laboratory | *lix@lanl.gov* | (585) 284-1928 | *https://github.com/tautomer*

Theoretical chemist with 8 years of experience in molecular dynamics and software development. 2 years of experience in developing neural networks for molecular systems. Looking for a research scientist role in computational chemistry.

Skills

Software development, scientific machine learning, shell scripting, molecular dynamics, quantum chemistry, high-performance computing, enhanced sampling methods.

Experience

Los Alamos National Laboratory | Postdoctoral Researcher **Jan 2022 – Present**

Developed physics-informed deep neural networks for excited-state non-adiabatic molecular dynamics.

- Designed workflows and prepared datasets from quantum mechanical calculations.
- Implemented the excited-state module in the ***hippynn*** package based on PyTorch.
- Conducted asynchronous parallel hyperparameter tuning with Ray and Ax.

Contributed to LANL open-source packages.

- ***hippynn (https://github.com/lanl/hippynn).*** Contributed to the codebase and documentation. Developed automated documentation builder and publisher with GitHub Actions.
- ***OpenMS (https://github.com/lanl/openms)***. Contributed to the molecular dynamics modules and interface to the ***hippynn*** package.

Organized monthly developer meetings for the ***NEXMD (https://github.com/lanl/nexmd)*** package.

- Coordinated developing efforts among internal (within LANL) and external developers, including a research group in Argentina.
- Promoted standard coding practices, such as pull requests, code reviews, and code formatting.
- Led the release of NEXMD 2.0 to the public.

University of Rochester | Graduate Research Assistant **Jan 2016 – Dec 2021**

Conducted research on chemical reactions controlled by nuclear quantum effects using ab-initio molecular dynamics simulations.

- Millions of CPU hours of experience in running high-performance computing applications.
- Skilled in calculating free energy, applying enhanced sampling methods, and using density-functional theory.

Developed reaction rate theories for ground-state chemical reactivities in polariton chemistry.

- Our *Nature Communications* paper is an ESI highly cited paper (top 1% of the field of chemistry).

Education

University of Rochester, Ph.D. **Sep 2015 – Dec 2021**

Major: Theoretical Chemistry

Wuhan University, B.S. **Sep 2010 – Jul 2014**

Major: Chemistry

Publications

- **Li, X.**; Lubbers, N.; Tretiak, S.; Barros, K.; Zhang, Y. Machine Learning Framework for Modeling Exciton-Polaritons in Molecular Materials. *J. Chem. Theory Comput.* **2024**, 20, 891-901
- **Li, X.**; Zhang, Y. First-principles molecular quantum electrodynamics theory at all coupling strengths, Submitted to *Nat. Commun. arXiv link available*
- Weight, B. M.; **Li**, **X.**; Zhang, Y. Theory and Modeling of Light-Matter Interactions in Chemistry: Current and Future. *Phys. Chem. Chem. Phys.* **2023**, 25, 31554-31577
- Freixas, V. M.; Malone, W.; **Li, X.**; Song, H.; Negrín-Yuvero, H.; Pérez-Castillo, R.; White, A.; Nelson, T.; Makhov, D. V.; Shalashilin, D. V.; Zhang, Y.; Fedik, N.; Kulichenko, M.; Messerly, R. A.; Mohanam, L. N.; Sharifzadeh, S.; Bastida, A.; Mukamel, S.; Fernandez-Alberti, S.; Tretiak, S. NEXMD V2.0 Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. *J. Chem. Theory and Comput.* **2023**, 19, 5356–5368
- Mandal, A.; Taylor, M. A. D.; Weight, B. M.; Koessler E. R.; **Li**, **X.**; Huo, P. Theoretical Advances in Polariton Chemistry and Molecular Cavity Quantum Electrodynamics. *Chem. Rev.* **2023**, 123, 9786–9879
- Mandal, A.; **Li**, **X.**; Huo, P. Theory of Vibrational Polariton Chemistry in the Collective Coupling Regime. *J. Chem. Phys.* **2022**, 156, 014101
- **Li, X.**; Mandal, A.; Huo, P. Theory of Mode-Selective Chemistry through Polaritonic Vibrational Strong Coupling. *J. Phys. Chem. Lett.* **2021**, 12, 6974–6982
- **Li, X.**; Huo, P. Investigating Tunneling-Controlled Chemical Reactions through Ab Initio Ring Polymer Molecular Dynamics. *J. Phys. Chem. Lett.* **2021**, 12, 6714–6721
- **Li, X.**; Mandal, A.; Huo, P. Cavity Frequency-Dependent Theory for Vibrational Polariton Chemistry. *Nat. Commun.* **2021**, 12, 1315

Conferences

- “Predicting Excited-State Properties with Hierarchically Interacting Particle Neural Network”, ACS Fall 2023, San Francisco, CA, August 2023
- “Machine Learning Framework for Modeling Exciton Polariton”, Conference on Excited State Processes 2023, Santa Fe, NM, June 2023
- “Modeling Excited-State Dynamics for Polariton Chemistry with Hierarchically Interacting Particle Neural Network”, APS March Meeting 2023, Las Vegas, NV, March 2023
- “Cavity Frequency-dependent Theory for Vibrational Polariton Chemistry”, ACS Fall 2022, Chicago, IL, August 2022
- “Cavity Frequency-dependent Theory for Vibrational Polariton Chemistry”, Gordon Research Conference (GRC) - Molecular Interactions and Dynamics, Easton, MA, July 2022
- “Investigating Tunneling Controlled Reactions with Ring Polymer Molecular Dynamics”, APS March Meeting 2019, Boston, MA, March 2019