Xinyang Li

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

Theoretical chemist with 8 years of experience in molecular dynamics and quantum dynamics, and 3 years of experience in Bayesian optimization and physics-informed neural networks for molecular systems. Highly skilled in technical communication and writing, and interdisciplinary collaboration.

Experience

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

Developed physics-informed deep neural networks for non-adiabatic molecular dynamics (NAMD).

- Developed and implemented the algorithms for excited-state predictions in the ***hippynn (https://github.com/lanl/hippynn)*** package based on *PyTorch*.
- Designed asynchronous parallel hyperparameter fine-tuning with *Ray* and *Ax*. The workflow has been adopted by ***hippynn*** users.
- Published the first paper in the field on designing a machine learning framework for exciton-polaritons.

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

- Contributed to the NAMD subroutines and improve their performances.
- Coordinated developing efforts among internal (within LANL) and external developers.
- Led the release of NEXMD 2.0 to the public.

Freelance Research Collaboration | Machine Learning Scientist **Mar 2024 – May 2024**

Collaborated on antibody design with a fellow researcher, focusing on optimizing antibody affinity and specificity using machine learning models.

- Developed sequence-based predictive models for protein properties.
- Filtered thousands of potential mutations, identifying two candidates with improved performance for experimental validation.
- Maintained strict confidentiality and discretion throughout the project.

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

Investigated chemical reactions controlled by nuclear quantum effects using ab-initio path-integral based molecular dynamics (MD) simulations combined with enhanced sampling techniques.

- Published the first *ab initio* ring polymer molecular dynamics rate calculation results.
- Obtained millions of CPU hours of experience in high-performance computing applications.
- Revealed how quantum mechanical tunnelling can dedicate chemical reaction mechanisms.

Developed reaction rate theories for ground-state chemical reactivities under light-matter interaction.

- Proposed the first theoretical explanations to the vibrational strong coupling reaction mechanism.
- 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

Thesis: Controlling Chemical Reactivities beyond Existing Paradigms Advisor: Prof. Pengfei Huo

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

Major: Chemistry

Selected 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
- 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
- **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
- For a complete list of my publications, please visit my Google Scholar profile at *https://scholar.google.com/citations?user=HqnNotUAAAAJ&hl=en*.

Selected Conferences

- “Predicting Excited-State Properties with Hierarchically Interacting Particle Neural Network” (talk), ACS Spring 2024, New Orleans, LA, March 2024
- “Machine Learning Framework for Modeling Exciton Polariton” (poster), Conference on Excited State Processes 2023, Santa Fe, NM, June 2023
- “Investigating Tunneling Controlled Reactions with Ring Polymer Molecular Dynamics” (talk), APS March Meeting 2019, Boston, MA, March 2019