Aodong Liu

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Summary of Qualifications

- **Motivated researcher** with over **8+ years of deep and extensive experience** in modeling, algorithm development, and large-scale simulations of complex chemical systems.
- **Active developer** for the widely-used quantum chemistry software **Gaussian** (Fortran) and **ChronusQ** (C++), with proficiency in diverse programming languages.
- Proven expertise in developing **scalable, high-performance algorithms** and cutting-edge **quantum dynamics** methods, supported by **first-author publications** demonstrating leadership and innovation in research.
- **Strong team player**, eager to apply expertise in **cross-disciplinary, data-driven environments** on collaborate on innovative solutions to complex problems.

Education

University of Washington *Sept. 2020 - Jun. 2026 (expected)*

Ph.D. in Theoretical Chemistry (Advisor: Xiaosong Li) *Seattle, WA*

Certificate in Quantum Information Science and Engineering

Vanderbilt University *Aug. 2016 - May 2020*

B.A. in Physical Chemistry with Honors (Advisor: Jens Meiler), Minor in Scientific Computing *Nashville, TN*

Thesis: *de novo* Modeling of CNIH1 Protein and Its Docking Mechanism with AMPA Receptor

Computational Proficiency

Programming Languagues	*Expert:* C++, Python, Fortran, Bash/Shell. *Proficient:* C, Cuda, Java, Matlab.
Software Devlopment	Gaussian (Fortran), ChronusQ (C++).
High-Performance Computing	Parallel programming with MPI/OpenMP; scalable distributed-memory code design.
DevOps	*Expert:* CMake, Git, Linux administration. *Proficient:* CI/CD automation.

Experience

Research Assistant @ University of Washington *Sept. 2021- Present*

Seattle, Washington

- Developed efficient, high-perfomance methods/algorithms to enable large-scale quantum chemsitry calculations
- Developed non-adiabatic, non-Born-Oppenheimer quantum dynamics methods to accurately model chemically interesting systems

Software Developer @ Gaussian *Feb. 2023; Apr., Sept. 2024*

Wallingford, CT

- Lead developer for Nuclear-Electronic Orbital (NEO) module in Gaussian 25
- Collaborated with industry experts to develop advanced quantum chemistry methodologies, resulting in multiple high-impact publications

Teaching Assistant @ University of Washington *Winter 2022, Winter 2023*

Seattle, Washington

- Chem 465: Computational Chemistry (Graduate-level), which introduces electronic structure methods
- Guided and mentored graduate students in utilizing quantum chemistry softwares, including Gaussian to solve chemical problems

Publications

1. **Liu, A.**; Chow, M.; Wildman, A.; Frisch, M.J.; Hammes-Schiffer,S.; Li, X., Simultaneous Optimization of Nuclear–Electronic Orbitals, *The Journal of Physical Chemistry A*, 2022, 26, 39, 7033-7039, DOI: 10.1021/acs.jpca.2c05172

2. **Liu, A.**; Zhang, T.; Hammes-Schiffer,S.; Li, X., Multicomponent Cholesky Decomposition: Application to Nuclear–Electronic Orbital Theory, *Journal of Chemical Theory and Computation*, 2023, 19, 18, 6255–6262, DOI: 10.1021/acs.jctc.3c00686

3. Kovtun, M.; Lambros, E.; **Liu, A.**; Tang, D.; Williams-Young, D. B.; Li, X. Accelerating Relativistic Exact-Two-Component Density Functional Theory Calculations with Graphical Processing Units, *Journal of Chemical Theory and Computation*, 2024, 20, 18, 7694–7699, DOI: 10.1021/acs.jctc.4c00843

4. Tang, D.*; **Liu, A.***; Hammes-Schiffer,S.; Li, X., Simulating Magnetic Field-Driven Real-Time Quantum Dynamics Using London Nuclear–Electronic Orbital Approach, *Journal of Chemical Theory and Computation*, 2025, 21, 9, 4357–4364, DOI: 10.1021/acs.jctc.5c00273 ***Co-First Authors**

5. Aieta, C.; Garner, S.M.; **Liu, A.**; Li, X.; Hammes-Schiffer,S., Nuclear-Electronic Orbital Quasiclassical Trajectory Method for Vibrational Spectroscopy, *Submitted*, 2025

6. **Liu, A.**; Zhang, T.; Lambros, E.; Hammes-Schiffer,S.; Li, X., Nuclear–Electronic Orbital Method at Scale: A Two-Stage Distributed Cholesky Decomposition Approach, *Submitted*, 2025

7. Yang, M.; Upadhyay, S.; **Liu, A.**; Li, X., Spin-Orbit-Resolved Strong-Field Ionization from Real-Time Relativistic Dynamics, *Submitted*, 2025

8. Zheng, J.; **Liu, A.**; Li, X.; Frisch, M.J., A tutorial for Nuclear-Electronic Orbital (NEO) method in the Gaussian program. *In preparation*, 2026

9. Lambros, E.*; **Liu, A.***; Beck, R.; Hammes-Schiffer,S.; Li, X., Forming the Bound Electron: Non-Equilibrium Electronic Ionization Dynamics of Water Clusters, *In preparation*, 2026 ***Co-First Authors**

Honors & Awards

2024 **Clean Energy Institute Graduate Fellowship,** University of Washington, Clean Energy Institute
2021 **Excellence in Chemistry Graduate Fellowship Award,** University of Washington
2020 **Thomas W. Martin Award,** Vanderbilt University
2019 **Dr.Sidney & Becca Fleischer Award,** Vanderbilt University
2018 **Vanderbilt Undergraduate Summer Research Program Fellowship,** Vanderbilt University

Conferences/Presentations

Mar. 2026 **ACS Spring 2026**, Oral Presentation: Large-scale Real-Time NEO–TDDFT Simulations of Ultrafast Solvated Electron Dynamics — *Atlanta, GA*

Oct. 2025 **IDREAM EFRC All Hands Meeting**, — *PNNL, WA*

Oct. 2024 **IDREAM EFRC Meeting**, Oral Presentation: Ultrafast Processes After Low-energy Electron Attachment in Water-Clusters: An *ab initio* Study by Real-Time Nuclear-Electronic Orbital Density Functional Theory. — *PNNL, WA*

Mar. 2024 **ACS Spring 2024**, Oral Presentation: Multicomponent Cholesky Decomposition: Application to Nuclear–Electronic Orbital Theory. — *New Orleans, LA*

Sept. 2023 **EFRC-Hub-CMS-CCS PI Meeting**, Poster: Multiscale Nuclear-Electronic Orbital Quantum Dynamics in Complex Environments. — *Virtual*

Sept. 2023 **EFRC-Hub-CMS-CCS PI Meeting**, Poster: Radiolysis in Extreme Environments. — *Virtual*

Aug. 2023 **IDREAM EFRC Meeting**, Oral Presentation: A Computational Study of Potassium Potassium K-Edge XANES Spectra. — *PNNL, WA*

Dec. 2022 **SciDac Summit**, Oral Presentation: Simultaneous Optimization of Nuclear–Electronic Orbitals, SciDac Summit, 2022 — *LBNL, CA*

Sept. 2019 **Vanderbilt Student Research Fair**, Oral Presentation: Structural Modeling and Validation of CNIH1 Protein. — *Nashville, TN*

Outreach and Community Services

Research Computing Club

University of Washington

- Hyak Governance Board (since 2023)
- RCC Officer (since 2023)
- RCC mentorship program [Mentor] (since 2022)

Engineering Discovery Days

University of Washington

- Volunteered for MEM-C exhibit titled ”A Magnetic Moment with MEM-C,” demonstrating quantum levitation and MAGLEV technology to K-12 students.
- Engaged with visitors, providing hands-on guidance and explaining the principles of superconductivity and quantum levitation.