Aodong **Liu**

Chemistry Graduate Student · Research Assistant

Seattle, WA

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Computational Chemistry Ph.D Student

- **Driven and highly motivated** reseaaarcher with **5+ years** of modeling and computational experience.
- Expert in **developing optimized, scalable and high-performance methods/algorithms** for large chemical system simulations, with **4 first-author publications**.
- Proficient in **a variety of programming languages**, active developer for **Gaussian** (Fortran) and **ChronusQ** (C++) software.
- Eager to apply my skills and knowledge in a **team-oriented environment** to contribute to **AI driven materials discovery**.

Education

University of Washington — *Seattle, WA*

Ph.D. in Theoretical Chemistry — *Sept. 2020 - June 2025 (expected)*

Certificate in Quantum Information Science and Engineering,

Advisor: Prof. Xiaosong Li

GPA: 3.86

Vanderbilt University — *Nashville, TN*

B.A. in Physical Chemistry with Honors, Minor in Scientific Computing — *Aug. 2016 - May 2020*

Advisor: Prof. Jens Meiler

GPA: 3.81

Skills

Technical Communication	4 peer-reviewed publications, 6 conference presentations, 4 programming workshops.
Research and Problem Solving	Lead researcher on 4 projects, achieving first-author publications.
Programming	*Expert:* C++, Python, Fortran, CMake, Git, Latex, Markdown *Proficient:* C, Cuda, Java, Matlab.
DevOps	*Expert:* Linux administration. *Proficient:* CI/CD.

Publications

5. **Liu, A.***; Tang, D.*; Hammes-Schiffer,S.; Li, X., A Study of Electronic and Protonic Real-time Dynamics under the Influence of a Strong Uniform Magnetic field, *In Preparation*
   ***Co-First Authors**
4. **Liu, A.**; Lambros, E.; Kovtun, M.; Willams-Young, D.B; Hammes-Schiffer,S.; Li, X., GPU-Accelerated, Scalable and Efficient Nuclear–Electronic Orbital Real-Time Time Dependent Density Functional Theory with Cholesky Decomposed Integrals, *In Preparation*
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
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
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