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

Honors & Awards

2023-2024 **CEI Graduate Fellowship**, University of Washington, Clean Energy Institute

2020 **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

Presentations

Mar. 2024	**Liu, A.**; Hammes-Schiffer,S.; Li, X. Multicomponent Cholesky Decomposition: Application to Nuclear–Electronic Orbital Theory, ACS Spring 2024	*New Orleans, LA*
Sept. 2023	Chow, M.; **Liu, A.**; Lambros, E., Multiscale Nuclear-Electronic Orbital Quantum Dynamics in Complex Environments, EFRC-Hub-CMS-CCS PI Meeting	*Virtual*
Sept. 2023	Li, S; **Liu, A.**; Li, X.; Young, L., Radiolysis in Extreme Environments EFRC-Hub-CMS-CCS PI Meeting	*Virtual*
Aug. 2023	**Liu, A.**; Beck, R; Li, X.; A Computational Study of Potassium Potassium K-Edge XANES Spectra, IDREAM EFRC Meeting	*PNNL, WA*
Dec. 2022	**Liu, A.**; Li, X. Simultaneous Optimization of Nuclear–Electronic Orbitals, SciDac Summit, 2022	*LBNL, CA*
Sept. 2019	**Liu, A.**; Kuenze, G; Meiler, J; Structural Modeling and Validation of CNIH1 Protein, Vanderbilt Student Research Fair	*Nashville, TN*

Outreach Activities

Research Computing Club *University of Washington*

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