Aodong **Liu**

Chemistry Graduate Student · Research Assistant

Seattle, WA

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Computational Chemistry Ph.D Student

- **Motivated researcher** with over **7+ years of 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 **5 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 — *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

Advisor: Prof. Jens Meiler — *Aug. 2016 - May 2020*

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

GPA: 3.81

Skills

Technical Communication	6 peer-reviewed publications, 7 conference presentations, 5 programming workshops.
Research and Problem Solving	Lead researcher on 5 projects, delivering first-author publications and scalable solutions.
Programming	*Expert:* C++, Python, Fortran, CMake, Git, Latex, Markdown *Proficient:* C, Cuda, Java, Matlab.
DevOps	*Expert:* Linux administration. *Proficient:* CI/CD automation.

Publications

6. **Liu, A.**; Lambros, E.; Hammes-Schiffer,S.; Li, X., Ultrafast Processes After Low-energy Electron Attachment in Water-Clusters: An *ab initio* Study by Real-Time Nuclear-Electronic Orbital Density Functional Theory, *In Preparation*

5. **Liu, A.***; Tang, D.*; Hammes-Schiffer,S.; Li, X., Simulating Vibrational Spectroscopy with Real-Time Nuclear-Electronic Orbital Density Functional Under 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

Oct. 2024 **Liu, A.**; Lambros, E.; Hammes-Schiffer,S.; Li, X., Ultrafast Processes After Low-energy Electron Attachment in Water-Clusters: An *ab initio* Study by Real-Time Nuclear-Electronic Orbital Density Functional Theory, IDREAM EFRC Meeting — *PNNL, WA*

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)

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.