

LONG HOANG NGUYEN

📍 Seattle, WA | ✉ jackn11@uw.edu | [in LinkedIn](#) | [GitHub](#) | [Google Scholar](#) | [Portfolio](#)

RESEARCH INTERESTS

- Correlated and many-body electronic structure theory for condensed systems and excited state properties
- Post-Hartree-Fock methods: Ab-initio and Density Functional Theory
- Hydrogen bonding in condensed phases: solvation, polarization, and vibrational shifts
- Force field development for next-generation many-body models
- Machine Learning Interatomic Potentials and Atomistic Simulation
- High Performance Scientific Computing

EDUCATION

University of Washington

Jun. 2026 – Present

Doctor of Philosophy in Chemistry

Seattle, WA

- Focus: Theoretical and Computational Chemistry
- Advisor: Dr. Sotiris S. Xantheas

University of Washington

Sep. 2024 – Jun. 2026

Master of Science in Applied Chemical Science and Technology

Seattle, WA

- Focus: Theoretical and Computational Chemistry; GPA: 3.7
- Advisor: Dr. Sotiris S. Xantheas
- Thesis: *Electronic Structure and Vibrational Spectroscopy in Hydrogen Bonded Clusters: Application to Water*, University of Washington, 2026 — awarded the Lloyd E. and Florence M. West Prize for Best Thesis

Seattle Pacific University

Jan. 2022 – Dec. 2023

Bachelor of Science in Chemistry; Bachelor of Arts in Physics

Seattle, WA

- Advisor: Dr. Karisa Pierce; GPA: 3.4; Dean's List 2021–2022

Everett Community College

Sep. 2018 – Dec. 2021

Associate in Arts & Science in Chemistry

Everett, WA

- GPA: 3.2; High School Diploma completed concurrently

RESEARCH EXPERIENCE

University of Washington

Sep. 2024 – Present

Research Assistant, Xantheas Lab

Seattle, WA

- Applied many-body expansions to analyze Hartree-Fock and MP2/CCSD(T) correlation contributions to molecular interaction energies.
- Formulated reduced-cost geometric and excitation-space truncation schemes for high-level methods.
- Developed localized MP2 code using Laplace transform quadrature and localized orbital spaces to partition electron correlation by excitation character and molecular fragment.
- Developing a localized CCSD(T) framework that extends the excitation-space analysis to CCSD and perturbative triples (T) contributions.
- Built automated workflows for large-scale LMP2 and LCCSD(T) calculations, data extraction, many-body analysis, and benchmarking against canonical MP2 and CCSD(T) reference energies.
- Evaluated the environment dependence of the intramolecular vibrational frequencies of an embedded water molecule across first through third solvation shell networks at the MP2 and CCSD(T) levels.
- Developed Discrete Variable Representation treatments to compute anharmonic vibrational fundamentals.
- Benchmarked state-of-the-art water potentials (TTM, MB-pol, q-AQUA) against ab initio reference spectra.
- Developed ab initio environment-dependent, transferable one-body PES and DMS for water.
- Assessed multireference wavefunction methods (MCSCF, CASSCF, CASPT2) for hydrogen bonded clusters.
- Designed the implementations for distributed HPC workflows on NERSC Perlmutter and UW Hyak, enabling systematic calculations across large molecular cluster datasets.

Los Alamos National Laboratory

Jun. 2026

Selected Participant, Computational Condensed Matter Summer School (LACCMSS)

Los Alamos, NM

- Selected through competitive application for a two week DOE/NNSA program in T-4 Division.
- Ran Kohn–Sham DFT and computed optical absorption via the GW/Bethe–Salpeter equation formalism.
- Simulated XANES/EXAFS spectra using real-space Green’s-function theory in FEFF10.
- Applied quantum many-body Green’s function techniques and the dynamical cluster approximation (DCA++)
- Trained and validated SNAP machine-learned interatomic potentials with FitSNAP and performed molecular dynamics simulations using LAMMPS.

Seattle Pacific University

Sep. 2022 – Dec. 2022

Undergraduate Research Assistant, Pierce Lab

Seattle, WA

- Quantified arsenic in marine tissues using GFAAS and multipoint external-standard calibration.
- Developed, improved, and customized analytical methods (drying/ashing/acid extraction).

PUBLICATIONS

- 1) **L. H. Nguyen** and S. S. Xantheas, “Many-Body Expansion of the MP2 Correlation Contribution to the Binding Energies of Water Clusters: A Localized Excitation Analysis”, *J. Chem. Theory Comput.*, (2026). DOI: 10.1021/acs.jctc.6c01287
- 2) **L. H. Nguyen**, G. D. Santis, and S. S. Xantheas, “Environmental effects in the vibrational shifts of water: from the monomer to models of the bulk”, *J. Chem. Phys.*, Accepted (2026). DOI 10.1063/5.0340361
- 3) **L. H. Nguyen**, T. H. Dunning, Jr., and S. S. Xantheas, “A Cautionary Tale: Failure of the Valence CASSCF to Describe the Hallmark of Hydrogen Bonding”, *J. Chem. Theory Comput.* 2026, 22 (13), 6283-6289. DOI: 10.1021/acs.jctc.6c00606
- 4) **L. H. Nguyen**, “Electronic Structure and Vibrational Spectroscopy in Hydrogen Bonded Clusters: Application to Water.” M.S. thesis, University of Washington, 2026. ProQuest Dissertations & Theses Global.
- 5) **L. H. Nguyen** and S. S. Xantheas, “Many-Body Expansion of the CCSD and (T) Correlation Contribution to the Binding Energies of Water Clusters”, *J. Chem. Theory Comput.*, Under revision (2026).
- 6) **L. H. Nguyen** and S. S. Xantheas, “Prediction of complete basis set MP2 and CCSD(T) binding energies of water clusters of arbitrary size and geometry from their Hartree–Fock energies and pre-computed monomer and dimer correlation grids”, *J. Chem. Theory Comput.* submitted (2026).

TECHNICAL SKILLS

Programming: Python, Fortran, MATLAB, R, Bash

Machine Learning & Atomistic Simulation: TensorFlow/Keras, FitSNAP, SNAP, LAMMPS

Quantum Software: PySCF, NWChem, Gaussian 16, ORCA, Q-Chem, GAMESS, MOLPRO, OpenMOLCAS, Quantum Espresso, BerkeleyGW, FEFF10, DCA++

Methods: Hartree–Fock, DFT, MP2, CCSD(T), MCSCF/CASSCF, CASPT2, GW/BSE

High Performance Computing: Linux, Slurm, NERSC Perlmutter, LANL Chicoma, UW Hyak

Visualization & Documentation: VMD, Avogadro, Jmol, GaussView, ChemCraft, MacMolPlt, $\LaTeX$

AWARDS

- Excellence in Chemistry Graduate Award for Incoming Ph.D. Student, University of Washington, 2026–2027
- Lloyd E. and Florence M. West Prize for Best Thesis (one per year), M.S. program in Applied Chemical Science & Technology, Department of Chemistry, University of Washington, 2025–2026 — [announcement](#)
- Travel Scholarship, Los Alamos Computational Condensed Matter Summer School, Los Alamos National Laboratory, June 2026 — competitive two-week research program in condensed matter physics
- Honorable Mention, Lloyd E. and Florence M. West Prize for Excellence in Research, M.S. program in Applied Chemical Science & Technology, Department of Chemistry, University of Washington, 2024–2025
- Wes Lingren Award for Excellence in Analytical Chemistry, Seattle Pacific University, June 2023
- Excellence in Physical Chemistry Award, Seattle Pacific University, June 2023
- Wellspring Undergraduate Scholarship, Wellspring Education, Jan. 2022 – Dec. 2023

TEACHING EXPERIENCE

Huntington Learning Center

Jan. 2024 – Jul. 2026

Science Tutor

Bellevue, WA

- Tutor chemistry, physics, mathematics, and test prep ISEE, SSAT, ACT, SAT for K–12 and undergraduate.
- Design individualized visual and verbal strategies for neurodivergent and physical disabilities students.
- Build confidence and independence by progressing from guided practice to self-directed problem solving.

Seattle Pacific University

Sep. 2022 – Jun. 2023

Chemistry Tutor

Seattle, WA

- Led general and physical chemistry tutoring sessions for groups of up to 10 students.

MENTOR/VOLUNTEER EXPERIENCE

University of Washington

Sep. 2026 – Present

Mentor

Seattle, WA

- Supervise a student's independent project on *ab initio* methods for hydrogen bonded clusters, from project design through analysis

University of Washington

Sep. 2025 – Jun. 2026

Master's student mentor

Seattle, WA

- Volunteered for the chemistry's master program to guide and provide resources for new master students.

Everett Community College

Jan. 2019 – Jun. 2019

International Student Ambassador

Everett, WA

- Volunteered for the international student service for on boarding new students – Outstanding Ambassador