Philip M. Nelson

github.com/philipmnel ◇ philip.nelson97@gmail.com

EDUCATION

Georgia Institute of Technology — Atlanta, GA
Ph.D., Computational Chemistry — August 2024
Thesis: *Efficient Quantum Chemistry for Applications in Anharmonic Vibrational Analysis and Molecular Crystals*

Colorado School of Mines — Golden, CO
B.S., Chemistry, *Magna cum laude* — May 2020
Minor in Computational and Applied Mathematics

RESEARCH

School of Chemistry and Biochemistry, GT — 2020 - 2024
Graduate Research, Advisor: Prof. C. David Sherrill

- Developed an open-source Python package for calculating anharmonic vibrational frequencies of molecules using quantum chemistry methods. Implemented a task-graph formulation to enable parallel deployment on hundreds of processors, significantly enhancing computational efficiency and scalability.
- Contributed to Psi4, an open-source quantum chemistry code, by implementing bug fixes, automating and expanding testing, enhancing documentation, and providing user support. Wrote C++ code for numerical computation of nuclear gradients.
- Investigated quantum chemistry methodologies for high-accuracy computation of many-body non-covalent interactions in molecular crystals.
- Collaborated with experimental biochemists to develop machine learning workflows to virtually screen potential ligands for G-protein coupled receptor targets.

Dept. of Chemical Engineering, CSM — 2019 - 2020
Undergraduate Research, Advisor: Prof. Diego Gómez-Gualdrón

- Applied density functional theory and grand canonical Monte Carlo methods to investigate the influence of ligand functionalization on gas adsorption and phase change behavior of flexible zeolitic-imidazolate frameworks

National Renewable Energy Laboratory — 2018
Undergraduate Research, Advisor: Prof. Thomas Gennett

- Characterized adsorbed chemical species in porous material samples using mass spectrometry

PUBLICATIONS

4. **P. M. Nelson** and C. D. Sherrill, "PYVPT2: Interoperable software for anharmonic vibrational frequency calculations", J. Chem. Phys. **162**, 032501 (2025).

3. **P. M. Nelson** and C. D. Sherrill, "Convergence of the many-body expansion in crystals of polar molecules: acetic acid, formamide, and imidazole", J. Chem. Phys. **161**, 214105 (2024).

2. Y. Zeng, A. Pavlova, **P. M. Nelson**, Z. L. Glick, L. Yang, Y. T. Pang, M. Spivak, G. Licari, E. Tajkhorshid, C. D. Sherrill, and J. C. Gumbart, "Broadening access to small-molecule parameterization with the force field toolkit", J. Chem. Phys. 160, 242501 (2024).

1. **P. M. Nelson**, Z. L. Glick, and C. D. Sherrill, "Approximating large-basis coupled-cluster theory vibrational frequencies using focal-point approximations", J. Chem. Phys. 159, 094104 (2023)

CODE CONTRIBUTIONS

- PYVPT2 (https://github.com/philipmnel/pyvpt2), author

- Psi4 (https://github.com/psi4/psi4), contributor

POSTERS AND PRESENTATIONS

7. Efficient Computation of Many-body Energies in Molecular Crystals, Poster, Southeastern Theoretical Chemistry Association, 2024

6. Interoperable Software for Accurate Anharmonic Frequency Calculations, Center for Computational Molecular Science and Technology Seminar, Georgia Tech, 2024

5. PYVPT2: An Open-source Package for Anharmonic Vibrational Analysis, Lightning Talk, Psi4 Developers' Conference, 2023

4. Accurate Anharmonic Vibrational Frequencies with Focal-Point Coupled-Cluster, Poster, Southeastern Theoretical Chemistry Association, 2023

3. Distributed Workflows for Anharmonic Frequency Calculations with Psi4 and QCFRAC-TAL, Lightning Talk, Psi4 Developers' Conference, 2022

2. Accurate Anharmonic Vibrational Frequencies with Focal-Point Coupled-Cluster, Poster, Southeastern Theoretical Chemistry Association, 2022

1. Anharmonic Frequencies with Vibrational Perturbation Theory (VPT2), Lightning Talk, Psi4 Developers' Conference, 2021

AWARDS

GT President's Fellowship, 2020-2024
CSM Chemistry Outstanding Graduating Senior, 2020
CSM Analytical Chemistry Award, 2020
CSM President's Scholarship, 2016 - 2020
CSM Dean's List, 2016-2019

SKILLS

Programming	Python, C++, OCaml, Bash, SQL
Tools	Git, Linux, NumPy, Pandas, scikit-learn, Matplotlib, OpenMP, CI/CD
Software	Psi4, rdkit, VMD
Languages	English (Native), Spanish (Fluent)