# Hung **Pham**

Computational Quantum Chemist | Scientific Software Developer | AI for Scientific Discovery

*San Jose, CA*

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## Personal statement

My expertise spans programming, numerical modeling, convex optimization, and statistical algorithms (ML, DL, RL, LLM) for electronic structure computations, leveraging modern CPUs, GPUs, and emerging QPUs. I specialize in deriving new algorithms and developing high-performance scientific software for quantum chemistry to tackle industrial challenges. With expertise in algorithm design and application development, I create quantum-based data generators, produce high-fidelity data, and build models that enhance AI-driven chemical modeling for smarter predictions.

## Experience

**Research Scientist** – **ByteDance Research** *March 2022 - Current*

San Jose, CA | *Focus*: Scalable and High-Fidelity Quantum Chemical Computations on CPUs, GPUs, QPUs

**Postdoctoral Research Scientist** – **Columbia University** *June 2021 - March 2022*

*Advisor*: David Reichman | *Focus*: Quantum Monte Carlo for periodic solids

**Research Assistant** – **University of Minnesota, Twin Cities** *Jan 2017 - May 2021*

*Advisor*: Laura Gagliardi | *Focus*: Quantum embedding, Computational materials science, Photovoltaics

**Research Assistant** – **Center for Molecular and NanoArchitecture (MANAR) & Institute for Computational Science and Technology (ICST)** *Oct 2011 - Jul 2015*

*Advisor*: Nguyen-Nguyen Pham-Tran | *Focus*: Periodic DFT, Grand canonical Monte Carlo, Reticular chemistry

## Education and Training

**Ph.D. in Chemistry** – **University of Minnesota, Twin Cities** *Aug 2015 - May 2021*

Advisor: Laura Gagliardi

**B.Sc. in Chemistry** – **Vietnam National University Ho Chi Minh City - University of Science** *Sep 2007 - Sep 2011*

Honor program

## Coding experiences

I have led and contributed to multiple open-source production and research codes, developing scalable deterministic and stochastic algorithms for quantum chemistry and computational materials science while optimizing scientific computing on HPC and cloud platforms.

**Authored**: ByteQEmbed | cuRPA | pDMET | MCU | pyWannier90 - **Contributed:** | ByteQC | PySCF | iPie

**Programming:**: Python | C/C++ | Fortran90 | SQL | Git | Bash | Unix

**ML libraries**: Numpy | SciPy | Cupy | mpi4py | Pandas | cvxpy | PyTorch | Tensorflow | Jax | Keras | Scikit-learn | Matplotlib |Seaborn

**User**: VASP | Gaussian | CRYSTAL | ADF | Quantum Espresso | CP2K | Wannier90 | Forcite | CASTEP | Dmol3 | GROMACS | AMBER

## Projects and Skills

Full list of publications can be found in my **Google Scholar (clickable)** profile | **Note:** * Corresponding author | †Co-first author

**AI/ML for FinTech**: Learning AI and ML techniques for FinTech, focusing on portfolio optimization, risk management, and financial modeling. Conducting independent projects to apply and expand my knowledge in these domains.

**AI/ML for Materials Science**: Exploring ML techniques, including classical ML, deep learning, and large language models (LLMs), integrated with quantum calculations to enhance computational workflows for materials discovery. Leveraging expertise in computational materials science, high-performance computing, and statistical algorithms to advance this field.

**GPU-Accelerated Quantum Chemistry Simulations**: Developed optimized algorithms using GPU acceleration and MPI to enhance quantum chemistry simulations, achieving 10–100x speed-ups. Focused on tensor operation optimization for large-scale scientific simulations, integrating high-performance computing techniques to enable efficient data processing.

1. Z. Guo, Z. Huang, Q. Chen, J. Shao, G. Liu, **H. Q. Pham**, Y. Huang, C. Cao, J. Chen, D. Lv, **arXiv:2502.17963**, 2025, .
2. Y. Huang, Z. Guo, **H. Q. Pham**, D. Lv, **arXiv:2406.08314**, 2024, .

**Quantum Embedding for Simulations and Quantum Algorithms**: Developed quantum embedding algorithms for large-scale *ab initio* simulations and quantum algorithms on HPC and cloud platforms, scaling to over 20,000 orbitals. Advanced quantum chemistry beyond DFT limits, targeting 1 kcal/mol accuracy, and enabled foundations for *ab initio*-driven AI models.

1. **H. Q. Pham** *et al.*, **Nearly-exact Many-body Method for Ultra-large Metallic Surfaces (Manuscript in preparation)**, 2025, .
2. Z. Huang, Z. Guo, C. Cao, **H. Q. Pham**, X. Wen, G. H. Booth, J. Chen, D. Lv, **arXiv:2412.18553**, 2024, .
3. C. Cao, J. Sun, X. Yuan, H.-S. Hu, **H. Q. Pham**[*], D. Lv, **npj Comput. Mater**, 2023, 78.
4. A. Mitra[†], **H. Q. Pham**[†], R. Pandharkar, M. R. Hermes, L. Gagliardi, **J. Phys. Chem. Lett.** , 2021, 12, 48, 11688.
5. **H. Q. Pham**, M. R. Hermes, L. Gagliardi, **J. Chem. Theory Comput.**, 2020, 16, 130.
6. **H. Q. Pham**, V. Bernales, L. Gagliardi, **J. Chem. Theory Comput.**, 2018, 14, 1960.

**Quantum Monte Carlo Method Development**: Developed novel algorithms, numerical methods, and GPU acceleration, scaling AFQMC methods 10–100x faster than traditional approaches. Enabled efficient, accurate simulations of strongly correlated molecules and catalysis on metallic surfaces using embedding techniques.

1. J. Lee, **H. Q. Pham**, D. R. Reichman, **J. Chem. Theory Comput.**, 2022, 18, 12, 7024 **(Front Cover, ACS Editors' Choice)**.
2. **H. Q. Pham**[*], R. Ouyang, and D. Lv, **J. Chem. Theory Comput.**, 2024, 20, 9, 3524.

**Computational Design of Novel Materials**: Applied advanced techniques, including DFT, MC, MD, wave function methods, and tight-binding models, inventing new methods and analyses as needed, to simulate systems and drive the design of novel materials like organic topological insulators, MOFs, and COFs.

1. **H. Q. Pham**[*], N.-N. Pham-Tran, **Chem. Mater.**, 2021, 33, 4488.
2. **H. Q. Pham**, R. J. Holmes, E. S. Aydil, L. Gagliardi, **Nanoscale**, 2019, 11, 11173.
3. **H. Q. Pham**, T. Mai, N.-N. Pham-Tran, Y. Kawazoe, H. Mizuseki, D. Nguyen-Manh, **J. Phys. Chem. C**, 2014, 118 (9), 4567.

1. Q. Sun, ..., **H. Q. Pham**, ..., G. K.-L. Chan, **J. Chem. Phys**, 2020, 153.

## Honors & Awards

**Vietnam Education Foundation (VEF) Fellowship**, VEF (declined) *2015*
**Grant: VNU C2013-50-03**, Vietnam National University Ho Chi Minh City *2013*
**Visiting Student**, Omar Yaghi Lab, UCLA Department of Chemistry & Biochemistry *2011*
**Academic Excellent Scholarship**, Viet Nam National University Ho Chi Minh City - University of Science *2008-2011*
**Lawrence S. Ting Scholarship**, Lawrence S. Ting Memorial Fund *2008*
**3rd Place (Shared)**, Vietnam National Olympiad in Chemistry for High-School Students *2007*

## Invited talks

**MolSSI Workshop for Python Simulation Software** – Caltech, Pasadena, CA, USA *Jun 30,2018*
**Academy & Technology Collaboration Department** – Bytedance Inc., Beijing, China *July 8, 2021*

## Recent presentations

**256th ACS National Meeting** – Boston, MA, USA *Aug. 2018*
**APS March Meeting 2019** – Boston, MA, USA *Mar. 2019*
**Minnesota Supercomputing Research Exhibition 2017** – Minneapolis, MN, USA *Oct. 2017*
**Minnesota Workshop on ab initio Modeling in Solid State Chemistry with Crystal 2017** – Minneapolis, MN, USA *Jul. 2017*

## Service to The Community

**Reviewer for**: 1. Journal of Chemical Theory and Computation, ACS | 2. Journal of Chemical Physics, AIP | 3. Physical Chemistry Chemical Physics, RSC | 4. IEEE Transactions on Nanotechnology | 5. Solid State Communications, Elsevier | 6. New Journal of Chemistry, RSC | 7. Journal of Open Source Software. | 8. Future Drug Discovery, Taylor & Francis.

## Teaching

**University of Minnesota, Twin Cities** *Sep 2015 - Dec 2016*
Courses: General Chemistry Labs, Guest Lecture for Comp Chem (graduate level).

**Viet Nam National University Ho Chi Minh City - University of Science** *Oct 2011 - Jul 2015*
Courses: General Chemistry Labs, Physical chemistry labs, Computational chemistry labs.