Hung **Pham**

Quantum Chemistry | High-performance computing | Quantum algorithms

San Jose, CA

pqh3.14@gmail.com | hungqpham.com | hungpham2017 | hung-pham-4b46598b

Research statement

I specialize in developing advanced and scalable quantum chemical algorithms rooted in electronic structure theory for *ab initio* simulations on both high-performance classical and quantum computers. My experience in both creating and utilizing quantum chemical software allows me to translate theoretical concepts into powerful tools that deliver simulations with enhanced precision and efficiency. With deep expertise in electronic structure for chemistry and materials science, and extensive experience applying computational chemistry across key industries—such as quantum technology, energy, pharmaceuticals, chemical sciences, and materials—I bring a unique perspective on how quantum chemistry can enhance fundamental understanding, deliver high-quality data for AI4Science, and drive transformative innovations across industrial sectors.

Education

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

Advisor: Laura Gagliardi

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

Honor program

Research Experience

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

San Jose, CA | *Focus*: Scalable Quantum Chemical Solutions for Industry

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

Advisor: David Reichman | *Focus*: Quantum Monte Carlo for quantum chemistry

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

Research Impact

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

Scalable Quantum Embedding and Quantum Algorithms for Material Simulations: I have developed novel quantum embedding algorithms (DMET, PET, ASET, etc) designed for accurate and efficient *ab initio* simulations of materials on classical and quantum computer. My work has broadened quantum chemistry's industrial impact across various sectors, including surface chemistry, homogeneous catalysis, superconducting materials, and defective systems as qubits.

1. Changsu Cao, Jinzhao Sun, Xiao Yuan, Han-Shi Hu, **H. Q. Pham***, Dingshun Lv, **npj Comput. Mater**, 2023, 78.
2. A. Mitra†, **H. Q. Pham**†, R. Pandharkar, M. R. Hermes, L. Gagliardi, **J. Phys. Chem. Lett.** , 2021, 12, 48, 11688.
3. **H. Q. Pham**, M. R. Hermes, L. Gagliardi, **J. Chem. Theory Comput.**, 2020, 16, 130.
4. **H. Q. Pham**, V. Bernales, L. Gagliardi, **J. Chem. Theory Comput.**, 2018, 14, 1960.

Precise Quantum Monte Carlo for Quantum Chemistry: Leveraging locality and modern GPUs, I have developed advanced algorithms and applied AFQMC methods to scale quantum chemistry for large-scale, real-world applications while maintaining its predictive power.

1. Joonho Lee, **H. Q. Pham**, David R. Reichman, **J. Chem. Theory Comput.**, 2022, 18, 12, 7024 **(Front Cover, ACS Editors' Choice)**.
2. **H. Q. Pham**, Runsheng Ouyang, and Dingshun Lv, **J. Chem. Theory Comput.**, 2024, 20, 9, 3524.
3. Yifei Huang, Zhen Guo, **H. Q. Pham**, Dingshun Lv, **arXiv**, 2024, .

Computational chemistry applied to Topological Insulator | Perovskites | MOFs | COFs: I have applied advanced computational techniques — periodic quantum chemistry, Wannier-based tight-binding models, and Grand Canonical Monte Carlo simulations — to study materials like reticular frameworks, topological materials, and photovoltaics. My research identifies new materials with exotic properties for potential industrial use.

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.

Fast Quantum Chemistry on GPU: To position quantum chemistry as a key industrial technology, especially beyond widely-used DFT, speed is critical. Leveraging GPUs can accelerate quantum chemistry, making it more practical for real-world applications. I am focused on optimizing advanced methods, like random phase approximation and quantum embedding, to bring quantum chemistry closer to industrial use by harnessing GPU power.

Software Development and Expertise: I have led and contributed to developing tools and open-source software, enabling efficient quantum chemical methods in chemistry and materials science. Additionally, I have extensive experience using a wide range of computational chemistry packages to tackle complex, real-world challenges in chemistry and materials science, including PySCF, VASP, CRYSTAL, Gaussian, Quantum Espresso, Wannier90, and Materials Studio.

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

Software Portfolio

Main developer: pDMET | MCU | pyWannier90

Contributor: PySCF | iPie | tools-seekpath

Proficiency in: Python | Cupy | MPI | C/C++ | Fortran90

Honors & Awards

Vietnam Education Foundation (VEF) Fellowship, VEF (declined) *2015*

Grant: VNU C2013-50-03, Vietnam National University Ho Chi Minh City *2013*

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*

Service to The Community

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

Teaching

University of Minnesota, Twin Cities *Sep 2015 - Dec 2016*

Courses: General chemistry laboratories (undergraduate), Guest Lecture for Computational chemistry (graduate).

Viet Nam National University Ho Chi Minh City - University of Science *Oct 2011 - Jul 2015*

Courses: General chemistry laboratories, Physical chemistry laboratories, Computational chemistry laboratories (undergraduate).

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*

Oral and Poster Presentations

The 4th International Workshop on Nanotechnology and Application – Vung Tau, Vietnam *Nov. 2014*

Chimie et Matériaux Avancés pour Environnement - CMAE2015 – Hanoi, Vietnam *Jun. 2015*

256th ACS National Meeting – Boston, MA, USA *Aug. 2018*

APS March Meeting 2019 – Boston, MA, USA *Mar. 2019*

The 3th International Workshop on Nanotechnology and Application – Vung Tau, Vietnam *Nov. 2011*

2016 All-Hands Meeting and Reaction Mechanisms Workshop – St. Paul, MN, USA *Aug. 2016*

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*