Hung **Pham**

Postdoctoral Research Scientist

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Education and Training

Columbia University — *New York, NY, USA*

Postdoc, Advisor: David Reichman — *June 2021 - Current*

Project: Adapting auxiliary-field quantum Monte Carlo (AF-QMC) to periodic solid state problems of relevance to energy storage materials.

University of Minnesota, Twin Cities — *Minneapolis, MN 55455, USA*

Ph.D. in Chemistry, Advisor: Laura Gagliardi — *Sep 2015 - May 2021*

Thesis: Developing density matrix embedding theory (DMET) for strong correlation in periodic systems.

Vietnam National University Ho Chi Minh City - University of Science — *Ho Chi Minh, Vietnam*

B.S. in Chemistry, Honor program, Advisor: Nguyen-Nguyen Pham-Tran — *Sep 2007 - Oct 2011*

Thesis: Applying grand canonical Monte Carlo (GCMC) and periodic density functional theory (DFT) to metal organic frameworks (MOFs).

Employments

Center for Molecular and NanoArchitecture (MANAR) — *Ho Chi Minh, Vietnam*

Research Assistant — *Oct 2011 - Jul 2015*

Project: Structural modeling and crystal topological analysis for framework materials (MOFs, COFs, ZIFs).

Institute for Computational Science and Technology (ICST) — *Ho Chi Minh, Vietnam*

Research Assistant — *Oct 2011 - Jul 2015*

Project: Gas storage and electronic structures of MOFs and COFs.

Teaching Experiences

University of Minnesota, Twin Cities — *Minneapolis, MN, USA*

Teaching Assistant — *Sep 2015 - Dec 2016*

Courses: General chemistry laboratories, Computational chemistry.

VNUHCM-US — *Ho Chi Minh, Vietnam*

Teaching Assistant — *Oct 2011 - Jul 2015*

Courses: General chemistry laboratory, Physical chemistry laboratory, Computational chemistry laboratory.

Research Grants

10/2013 - 10/2014 **VNU C2013-50-03 , Vietnam National University Ho Chi Minh City,** Investigating effect of linker on electronic band structure of Covalent Organic Framework using DFT calculations ($4,360) — *Vietnam*

Honors & Awards

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

2008 **Lawrence S. Ting Scholarship,** Lawrence Ting Memorial Fund — *Vietnam*

2008-2011 **Academic Excellent Scholarship,** VNUHCM-US — *Vietnam*

Software Development

MCU

Description

A Python package to analyze the periodic wave functions from electronic structure calculations. MCU supports a variety of electronic structure codes, such as: VASP, Quantum Espresso, CRYSTAL, ELK, PySCF, etc.

pyWannier90

Description

A Python interface for wannier90 used to construct the maximally-localized Wannier functions. pyWannier90 currently supports PySCF and VASP.

pDMET

Description

A program to study electronic structure of periodic systems and materials by means of density matrix embedding theory. pDMET utilizes electron integrals and quantum-chemistry solvers from PySCF.

Skills

Programming
- Python, C/C++, Fortran90, OpenMP
- Git, LaTeX

Softwares
- Electronic structure: PySCF, VASP, CRYSTAL, Gaussian, Quantum Espresso, wannier90
- Visualization: Crystal Maker, Materials Studio, Gaussview

Publications

* Corresponding author

1. **H. Q. Pham***, N.-N. Pham-Tran; *Topological Insulating Phase in Single-Layer Pentagonal Covalent Organic Frameworks: A Reticular Design using Metal Phthalocyanine*, **Chem. Mater.**, 2021, Accepted.
2. Q. Sun, ..., **H. Q. Pham**, ..., G. K.-L. Chan; *Recent Developments in the PySCF Program Package*, **J. Chem. Phys**, 2020, 153.
3. **H. Q. Pham**, M. R. Hermes, L. Gagliardi; *Periodic Electronic Structure Calculations with the Density Matrix Embedding Theory*, **J. Chem. Theory Comput.**, 2020, 16, 130.
4. R. Sanner, N. Cherepy, **H. Q. Pham**, V. Young; *Phosphorescent Heteroleptic Iridium (III) Cyclometallates: Improved Syntheses of Acetylacetonate Complexes and Quantum Chemical Studies of Their Excited State Properties*, **Polyhedron**, 2020, 176, 114256.
5. **H. Q. Pham***, D. Q. Le, N.-N. Pham-Tran, Y. Kawazoe, D. Nguyen-Manh; *Electron Delocalization in Single-Layer Phthalocyanine-Based Covalent Organic Frameworks: A First Principle Study*, **RSC Advances**, 2019, 9, 29440.
6. R. Sanner, N. Cherepy, H P. Martinez, **H. Q. Pham**, V. Young; *Highly Efficient Phosphorescence From Cyclometallated Iridium(III) Compounds: Improved Syntheses of Picolinate Complexes and Quantum Chemical Studies of Their Electronic Structures*, **Inorganica Chim. Acta**, 2019, 496, 119040.
7. **H. Q. Pham**, R. J. Holmes, E. S. Aydil, L. Gagliardi; *Lead-Free Double Perovskites $Cs_2InCuCl_6$ and $(CH_3NH_3)_2InCuCl_6$: Electronic, Optical, and Electrical Properties*, **Nanoscale**, 2019, 11, 11173.
8. **H. Q. Pham**, V. Bernales, L. Gagliardi; *Can Density Matrix Embedding Theory with the Complete Active Space Self-Consistent Field Solver Describe Single and Double Bond Breaking in Molecular Systems?*, **J. Chem. Theory Comput.**, 2018, 14, 1960.
9. D. Ray, C. Clarke, **H. Q. Pham**, J. Borycz; T. Zhang, E. S. Aydil, R. J. Holmes, L. Gagliardi; *A Computational Study of Structural and Electronic Properties of Lead-Free $CsMI_3$ Perovskites (M = Ge, Sn, Pb, Mg, Ca, Sr, Ba)*, **J. Phys. Chem. C**, 2018, 122, 7838.
10. P. T. K. Nguyen, H. T. D. Nguyen, **H. Q. Pham**, J. Kim, K. E. Cordova, H. Furukawa; *Synthesis and Selective CO_2 Capture Properties of a Series of Hexatopic Linker-Based Metal–Organic Frameworks*, **Inorg. Chem.**, 2015, 54 (20), 10065.
11. T. L. H. Doan, H. L. Nguyen, **H. Q. Pham**, N.-N. Pham-Tran, T. N. Le, K. E. Cordova; *Tailoring the Optical Absorption of Water-Stable Zr^{IV-} and Hf^{IV-}-Based Metal–Organic Framework Photocatalysts*, **Chem. Asian J.**, 2015, 10, 2660.
12. **H. Q. Pham**, T. Mai, N.-N. Pham-Tran, Y. Kawazoe, H. Mizuseki, D. Nguyen-Manh; *Engineering of Band Gap in Metal–Organic Frameworks by Functionalizing Organic Linker: A Systematic Density Functional Theory Investigation*, **J. Phys. Chem. C**, 2014, 118 (9), 4567.

Invited talks

MolSSI Workshop for Python Simulation Software — *Pasadena, CA, USA*

Jun. 2018

- Multiconfigurational Wave Function Methods for Periodic Systems via Density Matrix Embedding Theory.

Oral Presentations

The 4th International Workshop on Nanotechnology and Application - IWNA *Vung Tau, Vietnam*

Oral *Nov. 2013*

- Engineering of Band Gap in Metal–Organic Frameworks by Functionalizing Organic Linker.

Chimie et Matériaux Avancés pour Environnement - CMAE2015 *Hanoi, Vietnam*

Oral *Jun. 2015*

- Engineering of Band Gap in Crystalline Framework Materials via Functionalizing Organic Linker.

256th ACS National Meeting *Boston, MA, USA*

Oral *Aug. 2018*

- Multiconfigurational Wave Function Methods for Periodic Systems via Density Matrix Embedding Theory.

APS March Meeting 2019 *Boston, MA, USA*

Oral *Mar. 2019*

- Density Matrix Embedding Theory for Strongly Correlated Solids.

Poster Presentations

The 3th International Workshop on Nanotechnology and Application - IWNA *Vung Tau, Vietnam*

Poster *Nov. 2011*

- Mixed-linker based zeolitic imidazolate frameworks: Solvothermal synthesis and Computer simulation.

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

Poster *Aug. 2016*

- Metal exchange in the zirconia node of NU-1000 for catalysis.

Minnesota Supercomputing Research Exhibition 2017 *Minneapolis, MN, USA*

Poster *Oct. 2017*

- Metal exchange in the zirconia node of NU-1000 for catalysis.

Minnesota Workshop on ab initio Modeling in Solid State Chemistry with Crystal 2017 *Minneapolis, MN, USA*

Poster *Jul. 2017*

- A Novel Double Perovskite $Cs_2InCuCl_6$: First-principles Study on Electronic, Optical, and Electrical Transport Properties.

Service to The Community

Reviewing activities

- Journal of Chemical Theory and Computation, ACS
- Solid State Communications, Elsevier
- New Journal of Chemistry, RSC