Hung **Pham**

PH.D. CANDIDATE · COMPUTATIONAL CHEMIST

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"Think differently."

Summary

I am a Ph.D. candidate at the University of Minnesota, Twin Cities. My research focus on developing and applying new numerical techniques for periodic systems and strongly correlated materials. Working on variety of projects from theory to applications helps me earning skills and expertise in the fields of quantum embedding theories, wave function theories, density functional theory, condensed matter physics, photovotaics, and crystalline-framework materials. My Google Scholar profile could be found here

Education

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

PH.D. IN CHEMISTRY, ADVISOR: LAURA GAGLIARDI — *2015 - 2021 (expected)*

VNUHCM-US (Vietnam National University Ho Chi Minh City - University of Science) — *Ho Chi Minh, Vietnam*

B.S. IN CHEMISTRY, HONOR PROGRAM — *2007 - 2011*

Experiences

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

RESEARCH ASSISTANT — *Nov 2017 - Present*

- Developed density matrix embedding theory for strongly correlated materials
- In silico design of lead-free perovskites for optoelectronic applications
- Theoretical study of light absorption and emission in the iridium complexes for OLED applications.

TEACHING ASSISTANT — *Sep 2015 - Dec 2016*

- General chemistry laboratories
- Computational chemistry: tutorials for OpenMolcas and CRYSTAL17, lectures on the electronic structures for periodic systems.

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

RESEARCH ASSISTANT — *Oct 2011 - Jul 2015*

- Gas adsorption in metal-organic frameworks and zeolite imidazole framework.
- Structural modeling and topological analysis on crystalline framework materials.

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

RESEARCH ASSISTANT — *Oct 2011 - Jul 2015*

- Band gap engineering in metal-organic frameworks (MOFs).

VNUHCM-US — *Ho Chi Minh, Vietnam*

TEACHING ASSISTANT — *Oct 2011 - Jul 2015*

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

Skills

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

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

Software development

pDMET (https://github.com/hungpham2017/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.

MCU (https://github.com/hungpham2017/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, PySCF, wannier90, etc.

pyWannier90 (https://github.com/hungpham2017/pyWannier90)

Description

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

Publications

1. Q. Sun, ..., **H. Q. Pham**, ..., G. K.-L. Chan; *Recent Developments in the PySCF Program Package*, **J. Chem. Phys**, 2020, 153.

2. **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.

3. 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.

4. **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.

5. 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.

6. **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.

7. **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.

8. 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.

9. 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.

10. 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.

11. **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.

Presentations

The 4th International Workshop on Nanotechnology and Application - IWNA — *Vung Tau, Vietnam*, *Nov. 2013*

Oral

- 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.

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

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*