Hung **Pham**

PH.D. CANDIDATE · COMPUTATIONAL CHEMIST

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"Think differently."

Summary

I am a research assistant at the University of Minnesota developing novel numerical techniques for periodic systems and condensed phases. I have been working on variety of projects from method developments to application of electronic structure theories to condensed phases. These helped me earning skills and expertise in the fields of quantum embedding theories, wave function theories, density functional theory, crystallography, crystal topology, photovotaics and porous materials modeling.

Education

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

PH.D. IN CHEMISTRY, ADVISOR: LAURA GAGLIARDI — *2015 - 2020*

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

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

Experience

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

RESEARCH ASSISTANT — *Nov 2017 - Present*

- Developed density matrix embedding theory for periodic systems.
- Developed density matrix embedding theory using multireference solvers for molecules.
- Designed lead-free perovskites for optoelectronic applications
- Applied time-dependent DFT to study light absorption and emission in the iridium complexes for OLED applications.

TEACHING ASSISTANT — *Sep 2015 - Dec 2016*

- Courses: General Chemistry laboratories, i.e., CHEM 1017, CHEM 1065, CHEM 1066.

VNUHCM-US — *Ho Chi Minh, Vietnam*

RESEARCH ASSISTANT — *Oct 2011 - Jul 2015*

- Investigated the band-gap engineering in metal-organic frameworks.
- Mentored and helped master students learn crystalline and porous materials modeling using DFT and GCMC.

TEACHING ASSISTANT — *Oct 2011 - Jul 2015*

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

Skills

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

Softwares
- PySCF, VASP, CRYSTAL
- Gaussian, ADF
- Crystal Maker, Materials Studio

Coding Projects

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

PERSONAL

- pDMET is a package to compute electronic structure of periodic systems and materials by means of density matrix embedding theory.
- A variety of quantum chemical solvers is supported such as FCI, DMRG, CCSD, CASSCF.
- Compute the ground-state energy and electronic band structures.

MCU (https://github.com/hungpham2017/mcu)

Personal

- MCU is a Python package to analyze the periodic wave functions from DFT calculations.
- It is mainly written to study systems with non-trival band structures but it also supports functions and tools to study crystals and condensed phases.

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

Personal

- pyWannier90 is a python interface for wannier90 used to construct the maximally-localized Wannier functions.
- Available for PySCF and VASP

CAS-DMET (https://github.com/hungpham2017/casdmet)

Personal

- A CASSCF solver module for density matrix embedding theory.

Publications

1. **H. Q. Pham**, M. R. Hermes, L. Gagliardi; *Periodic Density Matrix Embedding Theory: A Wave Function Approach for Strongly Correlated Materials*, , 2019, Manuscript under preparation.

2. **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, Manuscript under revision.

3. 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.

4. **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.

5. **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.

6. 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.

7. 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.

8. 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.

9. **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.

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.

MolSSI Workshop for Python Simulation Software

Pasadena, CA, USA

Oral — *Jun. 2018*

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

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 2011 *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 Cs2InCuCl6: First-principles Study on Electronic, Optical, and Electrical Transport Properties.

Service to the community

Refereeship

- Journal of Chemical Theory and Computation

Honors & Awards

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

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

Referees

Laura Gagliardi

McKnight Presidential Endowed Chair, Distinguished McKnight University Professor, Director

Inorganometallic Catalyst Design Center

- University of Minnesota, Minneapolis, MN 55455, USA

Christopher J. Cramer

Vice President for Research, Distinguished McKnight University Professor

- University of Minnesota, Minneapolis, MN 55455, USA