

# HUNG Q. PHAM

## Computational Chemist

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## EXPERIENCE

### Research Assistant

**University of Minnesota** 📍 Minneapolis, USA (Jan 2017 – Present)

- General Chemistry Laboratory

**VNUHCM-US** 📍 Ho Chi Minh, Vietnam (Oct 2011 – Jul 2015)

- General Chemistry Laboratory, Physical Chemistry Laboratory

### Teaching Assistant

**University of Minnesota** 📍 Minneapolis, USA (Sep 2015 – Dec 2016)

- Developing electronic structure theories for periodic systems.

**VNUHCM-US** 📍 Ho Chi Minh, Vietnam (Oct 2011 – Jul 2015)

- First-principle calculations on framework materials (MOFs, COFs).

## 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  $\text{Cs}_2\text{InCuCl}_6$  and  $(\text{CH}_3\text{NH}_3)_2\text{InCuCl}_6$ : 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  $\text{CsMl}_3$  Perovskites ( $M = \text{Ge, Sn, Pb, Mg, Ca, Sr, Ba}$ )*, **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  $\text{CO}_2$  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  $\text{Zr}^{\text{IV}}$ - and  $\text{Hf}^{\text{IV}}$ -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. 🔗

## EDUCATION

### Ph.D. in Chemistry

**University of Minnesota, USA**

📅 Sep. 2015 – Dec. 2020

### B.S. in Chemistry

**VNUHCM-US, Vietnam**

📅 Sep. 2007 – Oct. 2011

## AREA OF INTEREST

- Wave function theories for condensed phases
- Quantum embedding theory
- Density functional theory
- Semiconducting, framework materials

## HONORS & AWARDS

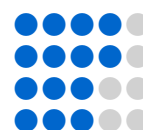
- 🏆 **Vietnam Education Foundation (VEF) Fellowship (Withdraw)**  
VEF, Vietnam (2015)
- 🏆 **Lawrence S. Ting Scholarship**  
Lawrence Ting Memorial Fund, Vietnam (2008)
- 🏆 **Academic Excellent Scholarship**  
VNUHCM-US, Vietnam (2008, 2010, 2011)

## SKILLS

PySCF VASP CRYSTAL Gaussian  
Materials Studio Crystal Maker  
OpenMP Git Scikit-learn Scipy  
Numpy Matplotlib

## LANGUAGES

Python  
C/C++  
Fortran  
Shell script



## REVIEWING ACTIVITY

- Journal of Chemical Theory and Computation, ACS 🔗
- Solid State Communications, Elsevier 🔗