HUNG Q. PHAM

Computational Chemist

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EXPERIENCE

Research Assistant

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

- Developing and applying electronic structure theories for/to periodic systems.

Center for Molecular and NanoArchitecture (MANAR)
Vietnam (Oct 2011 – Jul 2015)

- Computer modeling and topological analysis on metal-organic frameworks.

Institute for Computational Science and Technology (ICST)
Vietnam (Oct 2011 – Jul 2015)

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

Teaching Assistant

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

- General Chemistry Laboratory (CHEM 1017, CHEM 1065, CHEM 1066)

VNUHCM-US
Vietnam (Oct 2011 – Jul 2015)

- General Chemistry Laboratory, Physical Chemistry Laboratory

CODE DEVELOPMENT

pDMET

- A package to compute electronic structure of periodic systems and materials by means of density matrix embedding theory.

MCU

- A Python package to analyze the periodic wave functions from DFT calculations.

pyWannier90

- A Python interface for wannier90 used to construct the maximally-localized Wannier functions.

ORAL PRESENTATIONS

- APS March Meeting, 2019, Boston, MA, USA
- 256th ACS National Meeting, 2018, Boston, MA, USA
- MolSSI Workshop for Python Simulation Software, Pasadena, CA, USA
- Chimie et Matériaux Avancés pour Environnement (CMAE), 2015, Hanoi, Vietnam
- The 4th International Workshop on Nanotechnology and Application (IWNA), 2013, Vung Tau, Vietnam
- The 3th International Workshop on Nanotechnology and Application (IWNA), 2011, Vung Tau, Vietnam

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
- Perovskites for optoelectronic applications
- Crystalline framework materials.
- 2D materials.

HONORS & AWARDS

Vietnam Education Foundation (VEF) Fellowship (Withdrew)
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

PUBLICATIONS

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

2. 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.

3. **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 Adv.**, 2019, 9, 29440.

4. 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.

5. **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.

6. **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.

7. 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.

8. 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.

9. 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.

10. **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.