

Le Nhan Pham

PERSONAL INFORMATION

Research associate

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College of Science and Engineering
Flinders University
Personal homepage: <https://lenhanpham.github.io>

EDUCATION

KU Leuven, Leuven, Belgium

PhD, Chemistry

- Dissertation Title: “Properties of small 3d-metal based clusters: A journey from wave function to density functional methods”

Pre-doctoral program, Chemistry

University of Science, Ho Chi Minh City, Vietnam

M.S., Chemistry

Thesis Topic: “Fabrication of Dye Sensitized Solar Cells (DSSC) Using 620-1H3TBA (Black Dye) and Investigation into Their Performance and Long-term Stability”

University of Quy Nhon, Quy Nhon, Vietnam

B.E., Chemistry

RESEARCH INTERESTS

- 2D nanomaterials and biological materials
- Materials for surface coating
- Molecular dynamics force field development
- Semiconductor clusters doped with transition metals
- Transition metal oxide magnetic materials
- Recovery of rare earth metals in battery

SELECTED PUBLICATIONS

1. C. Zhu, **Pham, L. N.**, X. Yuan, H. Ouyang, M. L. Coote, and X. Zhang, High Electric Fields on Water Microdroplets Catalyze Spontaneous and Fast Reactions in Halogen-Bond Complexes. *J. Am. Chem. Soc.* **2023** [doi:10.1021/jacs.3c08818](https://doi.org/10.1021/jacs.3c08818)
2. S. J. Tonkin, **Pham, L. N.**, J. R. Gascooke, M. R. Johnston, M. L. Coote, C. T. Gibson, and J. M. Chalker, Thermal Imaging and Clandestine Surveillance Using Low-Cost Polymers with Long-Wave Infrared Transparency. *Adv. Opt. Mater.* **2023** [doi:10.1002/adom.202300058](https://doi.org/10.1002/adom.202300058)
3. J. M. M. Pople, T. P. Nicholls, **Pham, L. N.**, W. M. Bloch, L. S. Lisboa, M. V. Perkins, C. T. Gibson, M. L. Coote, Z. Jia, and J. M. Chalker, Electrochemical Synthesis of Poly(Trisulfides). *J. Am. Chem. Soc.* **2023** <https://doi.org/10.1021/jacs.3c03239>

4. **Pham, L. N.;** Walsh, T. Predicting Biomolecule Adsorption on MoS₂ Nanosheets with High Structural Fidelity. *Chem. Sci.* **2022** doi:10.1039/D1SC06814H (*Chem Sci Pick of the Week*)
5. **Pham, L. N.;** Walsh, T. R. Force Fields for Water–Surface Interaction: Is Reproduction of the Experimental Water Contact Angle Enough? *Chem. Commun.* **2021**, 57 (27), 3355–3358. doi:10.1039/d1cc00426c.
6. **Pham, L. N.;** Nguyen, M. T. Another Look at Photoelectron Spectra of the Anion Cr₂O₂⁻: Multireference Characters and Energetic Degeneracy. *J. Chem. Theory Comput.* **2018**, 14, pp 4833-4843. doi:10.1021/acs.jctc.8b00412.

CONFERENCE PRESENTATIONS

1. **Pham, L. N.;** Nguyen, M. T. ScSi₂^{-/0} and TiGe₂^{-/0}: Electronic Structures and Insights into Anion Photoelectron Spectra. *WATOC-2017, Munich Germany*, Poster presentation 2017.
2. **Pham, L. N.;** Hendrickx, M. F.A.; Nguyen, M. T. Electronic Transition in Anion Photoelectron Spectra of VC₂⁻ and ScSi₂⁻ Clusters. *ITN Conference, Leuven Belgium*, Poster presentation 2017.

SKILLS

Chemistry tools: DFT plane-wave methods, multireference (CASSCF/CASPT2, RASSCF/-RASPT2, NEVPT2, MRCI, DMRG) methods, single reference methods (DFT, CCSD(T)), molecular dynamics simulations

Electrochemistry: Cyclic voltammetry (CV), Electrochemical impedance spectroscopy (EIS)

Experience in Use of Computational Codes: Materials Studio (Castep, Dmol³), ADF, Quantum Espresso, VASP, Qbox, CP2K, Gromacs, LAMMPS, Molcas, Molpro, Dalton, Gaussian, Orca, CFOUR, PSI4, Turbomole, QChem, NWChem, ChemPS2.

Computer skills: Python, C++ (beginner), Keras (beginner), TensorFlow (beginner), L^AT_EX, Linux & Windows

WORKING EXPERIENCE

Researcher College of Science and Engineering - Flinders University, from July 2022 to present

Researcher Institute for Frontier Materials (IFM) - Deakin University, from July 2020 to June 2022

Visiting Scholar School of Science (Physics), RMIT University from February 2020 to July 2020

Lecturer Department of Chemistry, Dalat University from 2010 to 2021

**HONORS AND
AWARDS**

July, 2016 - June, 2019: Full PhD Scholarship from University of Leuven (KU Leuven), Leuven, Belgium.

February, 2015 - June, 2016: Full predoctoral Scholarship from University of Leuven (KU Leuven), Leuven, Belgium.

2003 - 2004: Top ten students of the academic year 2003-2004, Quy Nhon University

REFERENCES

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Prof. Tiffany R. Walsh

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