THANG PHAM

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Education

Northwestern University, Evanston, IL
Ph.D in Chemical and Biological Engineering. GPA: 3.90/4.00. Expected: June 2024.
Advisor: Professor Randall Q. Snurr
Worcester Polytechnic Institute (WPI), Worcester, MA
B.S in Chemical Engineering. GPA: 3.96/4.00. May 2019.

Research Experience

Graduate Researcher, Northwestern University, Evanston, IL. 2019 – Present.

- Developed machine learning models to predict partial atomic charges in porous materials and reduced computation cost by three orders of magnitude.
- Designed ionic metal-organic frameworks to store hydrogen at ambient temperature.
- Performed high-throughput screening to determine potential porous materials for direct water capture from air.
- Implemented genetic algorithm and Bayesian optimization to predict potential materials for carbon dioxide capture from flue gas.
- Performed atomistic simulations and collaborated with experimental groups to understand the molecular structures and adsorption properties of porous materials.

Summer Intern, Los Alamos National Laboratory, Los Alamos, NM. June – August 2019.

- Assisted in the development of the non-adiabatic excited-state molecular dynamics (NEXMD) software to simulate photoexcited dynamics of benzene.

Summer Undergraduate Research Fellow, WPI, Worcester, MA. June – August 2018.

- Studied mechanism and kinetics of Zeolite A crystallization in a micro-batch flow reactor.

Undergraduate Researcher, WPI, Worcester, MA. September 2017 – May 2019.

- Developed workflow to model polaron formation in metal oxides using density functional theory.
- Studied photocatalytic CO_2 reduction in carbon nitride and single atom catalysts.
- Investigated the rechargeability of liquid metal-air battery.

Teaching Experience

Teaching Assistant. Northwestern University, Evanston, IL. September 2019 – Present.

- Courses: Thermodynamics, Statistical mechanics, Molecular modeling, Kinetics.

Peer Learning Assistant. WPI, Worcester, MA. August 2017 – May 2019.

- Courses: Fluid mechanics, Heat and mass transfer, Thermodynamics, Separation.

Skills

- Programming languages: Python, Bash, C++, Matlab, SQL
- Modelling software: VASP, Gaussian, LAMMPS, RASPA, CP2K, COMSOL, Aspen Plus
- Programing libraries: Torch, PyTorch Geometric, Scikit-learn, XGBoost, NetworkX, Pymatgen

Professional Services

- Peer reviewer. The journal of physical chemistry. June 2023 – Present.
- Distinguished Trainee Service Award Committee. Northwestern University. May 2023 – Present.
- Graduate Recruitment Representative. Northwestern University. August 2020 – September 2022.
- Tau Beta Pi Honor Society, Member. February 2018 – Present.

Honors and Awards

- Terminal year fellowship. Northwestern University. 2023.
- Predictive science and engineering design fellowship. Northwestern University. 2021.
- Data science fellowship. Northwestern University. 2019.
- Best computation and theory presentation in Gulf coast undergraduate research symposium. Rice University. 2018.
- Undergraduate research fellowship. Worcester Polytechnic Institute. 2018.
- Certificate for outstanding undergraduate research presentation. Northeastern University. 2017.
- Presidential scholarship. Worcester Polytechnic Institute. 2015 – 2019.

Publications

1. **Pham, T. D.**, Snurr, R. Q. Implementation of Genetic Algorithms in Metal-Organic Frameworks for CO_2 Capture. In preparation. Manuscript available upon request.
2. **Pham, T. D.**, Sengupta, D., Farha, O. K., Snurr, R. Q. Investigation of Anionic Metal-Organic Frameworks for Hydrogen Storage at Room Temperature. In preparation. Manuscript available upon request.
3. Comlek, Y., **Pham, T. D.**, Snurr, R. Q., Chen, W. (2023). Rapid Design of Top-Performing Metal-Organic Frameworks with Qualitative Representations of Building Blocks. *npj Computational Materials*, *9*(1), p.170.
4. Wei, G., Xie, Y., **Pham, T. D.**, Shetty, S., Son, F. A., Idrees, K. B. Chen, Z., Xie, H., Liu, Y., Snurr, R. Q., Chen, B., Alameddine, B., Cui, Y., Farha, O. K. (2022). Creating Optimal Pockets in a Clathrochelate-Based Metal–Organic Framework for Gas Adsorption and Separation: Experimental and Computational Studies. *Journal of the American Chemical Society*, *144*(8), 3737-3745.
5. Huang, P., Huang, J., Li, J., **Pham, T. D.**, Zhang, L., He, J., Brudvig, G. W., Deskins, N. A., Frenkel, A. I., Li, G., (2022). Revealing the Structure of Single Cobalt Sites in Carbon Nitride for Photocatalytic CO_2 Reduction. *The Journal of Physical Chemistry C, 126*(20), 8596-8604.
6. Crislip, J. C., Vicens, J., **Pham, T. D.**, Zhang, Y., Tompsett, G., Teixeira, A. R. (2022). Dominance of heat transfer limitations in conventional sol-gel synthesis of LTA revealed by microcrystallization. *Journal of Flow Chemistry*, 1-12.
7. **Pham, T. D.**, & Deskins, N. A. (2020). Efficient method for modeling polarons using electronic structure methods. *Journal of Chemical Theory and Computation*, *16*(8), 5264-5278.
8. Iyemperumal, S. K., **Pham, T. D.**, Bauer, J., & Deskins, N. A. (2018). Quantifying support interactions and reactivity trends of single metal atom catalysts over TiO_2. *The Journal of Physical Chemistry C*, *122*(44), 25274-25289.

Presentations

- Investigation of Room Temperature Hydrogen Storage Using Anionic Metal-Organic Frameworks with Extra-Framework Cations (2023). AIChE Annual Meeting. Orlando, FL. Scheduled.
- CO_2 Capture in Metal-Organic Frameworks via Genetic Algorithms (2022). AIChE Annual Meeting. Phoenix, AZ.
- Implementation of Genetic Algorithms in Metal-Organic Frameworks for CO_2 Capture (2022). Foundations of Molecular Modeling and Simulations (FOMMS). Delavan, WI.
- Efficient Strategies for modeling polaron (2019). Major Qualifying Project presentation. Worcester, MA.
- Quantifying support interactions and reactivity trends of single metal atom catalysts over TiO_2 (2018). Gulf Coast Undergraduate Research Symposium. Houston, TX.
- Photocatalytic Reduction of Carbon Dioxide (2018). ACS Southeastern Regional Conference (SERMACS). Augusta, GA.