Thang D. Pham

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Summary

Postdoctoral researcher specializing in agentic AI systems for scientific discovery. Experience designing multi-agent workflows and scalable agentic pipelines on HPC systems. Proven ability to integrate AI with simulation, data, and scientific software to enable autonomous, large-scale discovery workflows.

Work Experience

Postdoctoral Researcher, Argonne National Laboratory Dec 2024 – Present

- Led the development of ChemGraph, a multi-agent AI system for planning, reasoning, and executing scientific workflows via natural language, enabling scalable execution across 512-Aurora-node workloads.
- Built and deployed agentic AI systems to interface with simulation codes (DFT/MC/MLIP), databases (APIs, RAG), HPC schedulers, and workflow engines.
- Developed an evaluation framework for agent performance in scientific applications, including early-stage assessment of tool-calling capabilities on ALCF inference service.
- Collaborated with scientists to integrate their domain-specific tools into agentic workflows, enabling automated spectroscopy (UV-vis, XANES, IR) and materials discovery pipelines.

Graduate Researcher, Northwestern University Sep 2019 – Sep 2024

- Developed AI-driven discovery systems combining simulation, ML, and optimization for autonomous materials design with experimental validation.
- Designed and implemented sequential decision-making frameworks (Bayesian optimization, evolutionary algorithms) to optimize materials' performance.
- Co-developed CoRE MOF Database (40,000+ materials) for data-driven workflows.

Projects

ChemGraph. Agentic AI framework for computational chemistry workflows GitHub
PACMOF2. ML models for predicting atomic charges in porous materials GitHub
MOFA. MOF generation at scale GitHub

Education

2019 - 2024 PhD in Chemical and Biological Engineering at Northwestern University
2015 - 2019 B.S in Chemical Engineering at Worcester Polytechnic Institute

Skills

Programming	Python, Bash, C
Agentic Systems	LangChain, LangGraph, smolagents
Machine Learning	PyTorch, LLMs, vLLM, RAG, GraphRAG
HPC and Distributed Systems	Slurm, PBS, Globus, Parsl, EnsembleLauncher
HPC Platforms	ALCF (Aurora, Polaris), NERSC (Perlmutter), TACC (Stampede2)
Simulation Packages	DFT (VASP, CP2K, Gaussian), Molecular Simulation (LAMMPS, RASPA), Machine Learning Interatomic Potentials (MACE, UMA)

Publications

[1] Sarah N. Elliott, Rosmi Reji, Qingzhi Chen, Xin Zheng, Simah Riaz, Xiaoli Yan, Thang Pham, Eliu Huerta, Ksenija D. Glusac, and Murat Keçeli. "Data-Driven Discovery of Structure–Reactivity Relationships in Oxidative Addition at Zerovalent Nickel Centers". In: *ChemRxiv* 2026.0601 (2026). DOI: 10.26434/chemrxiv.15004105/v1.

[2] Vitor F. Grizzi, Thang Duc Pham, Luke N. Pretzie, Jiayi Xu, Murat Keceli, and Cong Liu. *ChemGraph-XANES: An Agentic Framework for XANES Simulation and Curation*. 2026. arXiv: 2604.16205 [cond-mat.mtrl-sci].

[3] Thang Duc Pham, Harikrishna Tummalapalli, Fakhrul Hasan Bhuiyan, Álvaro Vázquez Mayagoitia, Christine Simpson, Riccardo Balin, Venkatram Vishwanath, and Murat Keçeli. *Multi-Agent Orchestration for High-Throughput Materials Screening on a Leadership-Class System*. 2026. arXiv: 2604.07681 [cs.AI].

[4] Aritra Roy, Kevin Shen, Andrew MacBride, Awwal Oladipupo, Mudassra Taskeen, Wojtek Treyde, Ruaa A. E. A. Abakar, Ahmad D. Abbas, Elsayed Abdelfatah, Abbas A. Abdullahi, Seham S. Abyah, Chahd Rahyl Adjmi, Fariha Agbere, Savyasanchi Aggarwal, Muhammad Ahmed, Tasnim Ahmed, Motasem Ajlouni, Mattias Akke, Hussein AlAdwan, Anwaar S. Alazani, Zahra A. Alharbi, Wajd A. Aljulyhi, Mohammed A. AlKubaish, Fatima A. Almahri, Sayed A. Almohri, David Obeh Alobo, Mohammed Alouni, Azizah S. Alqahtani, Omar Alsaigh, Husain Althagafi, Md. Aqib Aman, Lena Ara, Arifin, Ignacio Arretche, Abdulaziz Ashy, Syeda A. Asim, Amro Aswad, Adeel Atta, Sören Auer, Abdullah al Azmi, Toheeb Balogun, Suvo Banik, Viktoriia Baibakova, Shakira A. Baksh, Neus G. Bastús, Christina J. Bayard, Adib Bazgir, Louis Beal, Lejla Biberić, Wahid Billah, Ankita Biswas, Joshua Bocarsly, Montassar T. Bouzidi, Esma B. Boydas, Youssef Briki, Cailin Buchanan, Mauricio Cafiero, Damien Caliste, Yi Cao, Rafael E. Castañeda, Sruthy K. Chandy, Benjamin Charmes, Shayantan Chaudhuri, Yiming Chen, Alexander Chen, Jieneng Chen, Min-Hsueh Chiu, Defne Circi, Cinthya H. Contreras, Yoann Cure, Nathan Daelman, Roshini Dantuluri, Thomas Davy, William Dawson, Leonid Didukh, Rui Ding, Aminu R. Doguwa, Claudia Draxl, Sathya Edamadaka, Oulaya Elargab, Christina Ertural, Matthew L. Evans, Edvin Fako, Hossam Farag, Nur A. Fathurrahman, Merve Fedai, Rodrigo P. Ferreira, Giuseppe Fisicaro, Thomas Frank, Sasi K. Gaddipati, Abhijeet Gangan, Jennifer Garland, James Garrick, Luigi Genovese, Maryam Ghadrdran, Sandip Giri, Maxime Goulet, Jeremy Goumaz, Sara U. Gracia, et al. *From Knowledge to Action: Outcomes of the 2025 Large Language Model (LLM) Hackathon for Applications in Materials Science and Chemistry*. 2026. arXiv: 2605.03205 [cond-mat.mtrl-sci].

[5] Harikrishna Tummalapalli, Christine M. Simpson, Riccardo Balin, Vitali A. Morozov, Thang D. Pham, Murat Keceli, and Thomas D. Uram. *Overcoming Orchestration Bottlenecks at Exascale: A Decentralized, Policy-Driven Approach for Sim-AI Ensembles*. 2026. arXiv: 2607.12211 [cs.DC].

[6] Jiayang Liu, Xiaoliang Wang, Xiyang Liu, Zi-Ming Ye, Thang D. Pham, Filip Formalik, Manuel Tsotsalas, Omar K. Farha, and Randall Q. Snurr. "Identification of Metal–Organic Frameworks for CO2 Capture from Humid Flue Gas: Integrating Molecular Simulation, Machine Learning, and Experimental Synthesis". In: *Journal of the American Chemical Society* 148.32 (Aug. 2026), pp. 34821–34829. ISSN: 0002-7863. DOI: 10.1021/jacs.6c10566.

[7] Haofan Yang, Qianhui Wang, Thang D. Pham, Zhiwei Wang, Haomiao Xie, Yongjie Xu, Filip Formalik, Davide M. Proserpio, Charlotte L. Stern, Alice Li, Xavier C. Krull, Andrew I. Cooper, Randall Q. Snurr, and Joseph T. Hupp. "Side-arm sterics direct conformation, topology, and function in zirconium metal–organic frameworks". In: *Journal of Materials Chemistry A* 14.29 (May 2026), pp. 18627–18635. ISSN: 2050-7488. DOI: 10.1039/d6ta02142e.

[8] Thang D. Pham, Aditya Tanikanti, and Murat Keçeli. "ChemGraph as an agentic framework for computational chemistry workflows". In: *Communications Chemistry* (Jan. 2026). ISSN: 2399-3669. DOI: 10.1038/s42004-025-01776-9.

[9] Guobin Zhao, Logan M. Brabson, Saumil Chheda, Ju Huang, Haewon Kim, Kunhuan Liu, Kenji Mochida, Thang D. Pham, Prerna, Gianmarco G. Terrones, Sunghyun Yoon, Lionel Zoubritzky, François-Xavier Coudert, Maciej Haranczyk, Heather J. Kulik, Seyed Mohamad Moosavi, David S. Sholl, J. Ilja Siepmann, Randall.Q. Snurr, and Yongchul G. Chung. "CoRE MOF DB: A curated experimental metal-organic framework database with machine-learned properties for integrated material-process screening". In: *Matter* 8.6 (June 2025). ISSN: 2590-2393. DOI: 10.1016/j.matt.2025.102140.

[10] Thang D. Pham and Randall Q. Snurr. "Implementation of Genetic Algorithms to Optimize Metal-Organic Frameworks for CO2 Capture". In: *Langmuir* 41.7 (Feb. 2025), pp. 4585–4593. ISSN: 0743-7463. DOI: 10.1021/acs.langmuir.4c04386.

[11] Thang D. Pham, Faramarz Joodaki, Filip Formalik, and Randall Q. Snurr. "Predicting Partial Atomic Charges in Metal–Organic Frameworks: An Extension to Ionic MOFs". In: *The Journal of Physical Chemistry C* 128.40 (Oct. 2024), pp. 17165–17174. ISSN: 1932-7447. DOI: 10.1021/acs.jpcc.4c04879.

[12] Thang D. Pham, Debabrata Sengupta, Omar K. Farha, and Randall Q. Snurr. "Investigation of Anionic Metal–Organic Frameworks with Extra-Framework Cations for Room Temperature Hydrogen Storage". In: *Chemistry of Materials* 36.8 (Apr. 2024), pp. 3794–3802. ISSN: 0897-4756. DOI: 10.1021/acs.chemmater.4c00126.

[13] Yigitcan Comlek, Thang Duc Pham, Randall Q. Snurr, and Wei Chen. "Rapid design of top-performing metal-organic frameworks with qualitative representations of building blocks". In: *npj Computational Materials* 9.1 (Sept. 2023), p. 170. ISSN: 2057-3960. DOI: 10.1038/s41524-023-01125-1.

[14] Jacob C. Crislip, Jim Vicens, Thang Pham, Yifan Zhang, Geoffrey Tompsett, and Andrew R. Teixeira. "Dominance of heat transfer limitations in conventional sol-gel synthesis of LTA revealed by microcrystallization". In: *Journal of Flow Chemistry* 12.4 (Dec. 2022), pp. 397–408. ISSN: 2063-0212. DOI: 10.1007/s41981-022-00217-1.

[15] Peipei Huang, Jiahao Huang, Junying Li, Thang Duc Pham, Lei Zhang, Jie He, Gary W. Brudvig, N. Aaron Deskins, Anatoly I. Frenkel, and Gonghu Li. "Revealing the Structure of Single Cobalt Sites in Carbon Nitride for Photocatalytic CO2 Reduction". In: *The Journal of Physical Chemistry C* 126.20 (May 2022), pp. 8596–8604. ISSN: 1932-7447. DOI: 10.1021/acs.jpcc.2c01216.

[16] Wei Gong, Yi Xie, Thang Duc Pham, Suchetha Shetty, Florencia A. Son, Karam B. Idrees, Zhijie Chen, Haomiao Xie, Yan Liu, Randall Q. Snurr, Banglin Chen, Bassam Alameddine, Yong Cui, and Omar K. Farha. "Creating Optimal Pockets in a Clathrochelate-Based Metal–Organic Framework for Gas Adsorption and Separation: Experimental and Computational Studies". In: *Journal of the American Chemical Society* 144.8 (Mar. 2022), pp. 3737–3745. ISSN: 0002-7863. DOI: 10.1021/jacs.2c00011.

[17] Thang Duc Pham and N. Aaron Deskins. "Efficient Method for Modeling Polarons Using Electronic Structure Methods". In: *Journal of Chemical Theory and Computation* 16.8 (Aug. 2020), pp. 5264–5278. ISSN: 1549-9618. DOI: 10.1021/acs.jctc.0c00374.

[18] Satish Kumar Iyemperumal, Thang Duc Pham, Jack Bauer, and N. Aaron Deskins. "Quantifying Support Interactions and Reactivity Trends of Single Metal Atom Catalysts over TiO2". In: *The*

Journal of Physical Chemistry C 122.44 (Nov. 2018), pp. 25274–25289. ISSN: 1932-7447. DOI: 10.1021/acs.jpcc.8b05611.

Presentations

[1] *Multi-Agent Orchestration for High-Throughput Materials Screening on a Leadership-Class System.* ISC High Performance 26, The Second International Workshop on Foundational Large Language Models Advances for HPC. Hamburg, Germany, June 2026.

[2] *Agentic Workflows.* 2026 ALCF INCITE GPU Hackathon. Lemont, IL, Apr. 2026.

[3] *Agentic AI Workflows for Scientific Discovery.* Invited talk, DemonHacks, DePaul University. Chicago, IL, Feb. 2026.

[4] *Agentic Workflows.* Advanced Topics in AI for Science: A Student Training Series. Lemont, IL, Oct. 2025.

[5] *ChemGraph: An Agentic Framework for Computational Chemistry.* Trillion Parameter Consortium (TPC25). San Jose, CA, July 2025.

[6] *ChemGraph: An Agentic Framework for Computational Chemistry.* Poster presentation, CELS Staff Poster Presentations. Lemont, IL, July 2025.

[7] *Using Data Mining and Large Language Models for a Large-Scale Comparison of Adsorption from Molecular Simulation and Experiment.* Context, Connections, and Community (C3) Symposium. Evanston, IL, July 2024.

[8] *Predicting Partial Atomic Charges in Metal-Organic Frameworks: An Extension to Ionic MOFs with Extra-framework Ions.* Presentation, CDPM Collaboration Meeting. Minneapolis, MN, Feb. 2024.

[9] *Investigation of Room Temperature Hydrogen Storage Using Anionic Metal-Organic Frameworks with Extra-Framework Cations.* AIChE Annual Meeting 2023. Orlando, FL, Oct. 2023.

[10] *CO2 Capture in Metal-Organic Frameworks via Genetic Algorithms.* AIChE Annual Meeting 2022. Phoenix, AZ, Oct. 2022.

[11] *Optimization Methods for CO2 Capture in Metal-Organic Frameworks.* Poster presentation, FOMMS Meeting 2022. Delavan, WI, July 2022.

[12] *Efficient Strategies for Modeling Polaron.* Major Qualifying Project Presentation. Worcester, MA, May 2019.