HIEU A. DOAN

Chicago, IL | (832)-434-4703 | hieu.a.doan@gmail.com | hieuadoan.github.io

SUMMARY

A computational scientist with over 10 years of experience in molecular simulations and high-performance computing (HPC), with the past 5 years dedicated to applying machine learning for accelerated materials discovery and optimization. Recognized for bridging experimental and computational teams to drive data-driven decision-making in research and development.

PROFESSIONAL EXPERIENCE

Computational Materials Scientist

Argonne National Laboratory | Lemont, IL — May 2022 – Apr 2024

- Designed workflows integrating physics-based simulations and graph neural networks to optimize catalyst materials for biomass utilization
- Developed active learning pipelines to accelerate electrolyte screening workflows, reducing discovery timelines significantly
- Collaborated cross-functionally with experimental scientists to improve experimental design and decision-making using data-driven insights

Postdoctoral Appointee

Argonne National Laboratory | Lemont, IL — Nov 2018 – Apr 2022

- Developed Bayesian optimization algorithms for high-throughput molecular screening, integrating multi-objective parameters
- Managed high-throughput simulation workflows on HPC clusters, generating extensive computational datasets for materials discovery

Postdoctoral Fellow

Northwestern University | Evanston, IL — Jul 2016 – Oct 2018

- Conducted high-throughput screening of catalytic nanoclusters and metal-organic frameworks (MOFs) for chemical conversions
- Collaborated closely with experimentalists to validate computational predictions

TECHNICAL SKILLS

Materials Simulation	Density functional theory (DFT using VASP/Gaussian 16), COMSOL
Machine Learning	Bayesian optimization, graph neural network, generative AI
Programming Language	Python, SQL, HTML, CSS, shell scripting
Software Package	PyTorch, Scikit-learn, RDKit, Pandas, NumPy, SciPy, Streamlit
Cloud Computing	HPC, AWS

HONORS

2023	Poster Session Award from the 5th Battery and Energy Storage Conference | AIChE
2022	Best Paper Award from the Joint Center for Energy Storage Research
2020	Best Paper Award from the Joint Center for Energy Storage Research
2019	Best Poster Presentation at the Argonne Postdoctoral Symposium
2018	Best Fundamental Paper Award from the American Institute of Chemical Engineers
2015	Kokes Travel Award for the 24th North American Catalysis Society Meeting
2014	Best Fundamental Paper award from the American Institute of Chemical Engineers

EDUCATION

Ph.D. in Chemical Engineering
University of Houston | Houston, TX — Dec 2015
Dissertation : Computational Screening of Bifunctional Catalysts for CO and CH_4 Oxidation

- Developed expertise in density functional theory simulations, microkinetic modeling, and data analysis for catalyst design
- Mentored team members and contributed to teaching undergraduate courses

B.S. in Chemical Engineering – Magna Cum Laude
University of Houston | Houston, TX — Dec 2009
Honor Thesis : Experimental Analysis of Soot Combustion in Diesel Particulate Filter

SELECTED PUBLICATIONS

5. J. Noh*, H. A. Doan*, H. Job, L. A. Robertson, L. Zhang, R. S. Assary, K. Mueller, V. Murugesan, Y. Liang, "An Integrated Hight-throughput Robotic Platform and Active Learning Approach for Accelerated Discovery of Optimal Electrolyte Formulations". **Nature Communications**, 15, 2757, 2024. *Authors contributed equally.

4. H. A. Doan, C. Li, L. Ward, M. Zhou, L. A. Curtiss, R. S. Assary, "Accelerating the Evaluation of Crucial Descriptors for Catalyst Screening via Message Passing Neural Network." **Digital Discovery**, 2, 59-68, 2023.

3. H. A. Doan, G. Agarwal, H. Qian, M. J. Counihan, J. Rodriguez-Lopez, R. S. Assary, "Quantum Chemistry-Informed Active Learning to Accelerate the Design and Discovery of Sustainable Energy Storage Materials." **Chemistry of Materials** 32, 6338-6346, 2020.

2. H. A. Doan, Z. Li, O. K. Farha, J. T. Hupp, R. Q. Snurr, "Theoretical Insights into Direct Conversion of Methane to Methanol over Supported Dicopper Oxo Nanoclusters." **Catalysis Today** 312, 2-9, 2018.

1. J. Saavedra, H. A. Doan, C. J. Pursell, L. C. Grabow, B. D. Chandler, "The Critical Role of Water at the Gold-Titania Interface in Catalytic CO Oxidation." **Science** 345, 1599-1602, 2014.