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 developing data-driven models and autonomous workflows that drive innovation and enable efficient scientific problem-solving.

PROFESSIONAL EXPERIENCE

Computational Materials Scientist

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

- Leveraged automated materials preparation and characterization platforms to design closed-loop active learning workflows for electrolyte screening, reducing discovery timelines by 10 folds.
- Combined physics-based models with graph neural networks for in silico design of optimal catalytic materials for biomass utilization
- Collaborated with cross-functional teams to integrate theory with experiment for improving catalyst and electrolyte design

Postdoctoral Appointee

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

- Developed a multi-objective Bayesian optimization algorithm to identify optimal organic molecules for battery applications
- Designed and operated high-throughput simulation platforms on HPC for computational material database generation

Postdoctoral Fellow

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

- Evaluated the potential transition metal oxide nanoclusters for the direct conversion of methane to methanol via DFT simulation
- Carried out high-throughput computational screening of metal-organic framework catalysts for methane activation

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 and microkinetic modeling for computational catalyst screening
- Mentored new team members, oversaw undergraduate research projects, and contributed to tutoring and grading for courses in chemical engineering

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.