HIEU A. DOAN

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SUMMARY

A passionate computational scientist with over 10 years of experience in leveraging molecular simulation, high-performance computing, and machine learning for scientific research. Specialized in the virtual screenings and design of experiments for catalysts and energy storage materials, contributing to significant advancements in closed-loop discovery of optimal battery electrolytes. Recognized with two 'Best Paper' awards from the Joint Center for Energy Storage Research, a Department of Energy's Energy Innovation Hub for designing and building next-generation battery materials.

PROFESSIONAL EXPERIENCE

Computational Materials Scientist

Argonne National Laboratory | Lemont, IL — May 2022 - Present

- Develop and apply machine learning models to learn on computational (DFT) and experimental characterization data (CV, NMR)
- Combine high-throughput atomistic modeling with graph neural networks to aid inverse design of optimal catalytic materials for biomass utilization
- Leverage automated materials preparation and characterization platforms to design and execute closed-loop active learning workflows for accelerated electrolyte discovery

Postdoctoral Appointee

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

- Developed a multi-objective Bayesian optimization algorithm to identify redox flow battery electrolytes with multiple desired criteria
- Collaborated with chemists and roboticists to design an automated experiment for measuring battery performance
- Performed high-throughput first-principles calculations to create a database of 20,000 catalyst structures and built a graph neural network model for accelerated property prediction.

Postdoctoral Fellow

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

- Evaluated the potential of supported pure and mixed copper oxide nanoclusters for the direct conversion of methane to methanol via density functional theory 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, deep neural network, graph neural network
Programming Language	Python, shell scripting
Software Package	PyTorch, Scikit-learn, RDKit, Pandas, NumPy, SciPy

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

- Performed density functional theory calculations and microkinetic modeling to investigate the multifunctionality of bimetallic transition metal catalysts, unravel the mechanism behind CO oxidation over gold/titania, and guide the design of palladium catalysts for methane slip reduction in natural gas vehicles.
- Mentored new team members, oversaw undergraduate research projects, and contributed to tutoring and grading for courses such as "Chemical Engineering Thermodynamics" and "Design, Safety & Reliability."

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

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

SELECT PRESENTATIONS

Ketonization of Hexanoic Acids over ZrO_2 Catalysts: Insights from First-principles Calculations and DRIFTS Experiments
American Chemical Society Meeting | New Orleans, LA — Mar 2024

Accelerating the Evaluation of Crucial Descriptors in Computational Catalyst Screening via Graph Neural Network
American Chemical Society Meeting | Indianapolis, IN Mar 2023

Accelerated Discovery of Energy Storage Materials via Multi-objective Bayesian Optimization
American Institute of Chemical Engineers Midwest Regional Conference | Virtual Mar 2022

Active Learning via Bayesian Optimization for the Discovery of Energy Storage Materials
nanoHUB Tutorial Series on Machine Learning (Invited) | Virtual Jun 2021

Warp Jumping in the Molecular Universe with Active Learning
Argonne AI and HPC Seminar (Invited) | Lemont, IL Dec 2020

Toward the Optimal Design of Molybdenum Carbide Catalysts for Biomass Conversion
American Chemical Society Meeting (Invited) | San Diego, CA Aug 2019

PUBLICATIONS

24. 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.

23. A. Jain, I. A. Shkrob, H. A. Doan, K. Adams, J. S. Moore, R. S. Assary, "Active Learning Guided Computational Discovery of Plant-based Redoxmers for Organic Non-aqueous Redox Flow Battery". **ACS Applied Materials & Interfaces**, 15, 58309-58319, 2023. Editors' Choice.

22. L. Gao, B. Wang, H. A. Doan, Y. Du, I. A. Shkrob, C. Liao, "Trimer Quinoxalines as Organic Cathode Materials for Lithium-Ion Batteries." **Journal of The Electrochemical Society**, 170, 110520, 2023.

21. A. Jain, I. A. Shkrob, H. A. Doan, L. A. Robertson, L. Zhang, R. S. Assary, "In Silico Discovery of a New Class of Anolyte Redoxmers for Non-aqueous Redox Flow Batteries." **Digital Discovery**, 2, 1197-1208, 2023.

20. H. A. Doan, X. Wang, R. Q. Snurr, "Computational Screening of Supported Metal Oxide Nanoclusters for Methane Activation: Insights into Homolytic versus Heterolytic C-H Bond Dissociation." **Journal of Physical Chemistry Letters**, 14, 5018-5024, 2023.

19. 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.

18. H. A. Doan, C. Li, L. Ward, M. Zhou, L. A. Curtiss, R. S. Assary, "Dataset for Accelerating Catalysts Screening via Machine-Learned Local Coordination Graph Representations." **Materials Data Facility**, 2022.

17. H. Qian*, M. J. Counihan*, H. A. Doan*, A. S. Danis, W. Setwipatanachai, N. S. Purwanto, J. Rodriguez-Lopez, R. S. Assary, J. S. Moore, "Mesolytic Cleavage of Homobenzylic Ethers for Programmable End-of-Life Function in Redoxmers." **Journal of Materials Chemistry A** 10, 7739-7753, 2022. *Authors contributed equally.

16. G. Agarwal*, H. A. Doan*, L. A. Robertson, L. Zhang, R. S. Assary, "Discovery of Energy Storage Molecular Materials using Quantum Chemistry-guided Multiobjective Bayesian Optimization." **Chemistry of Materials** 33, 8133-8144, 2021. *Authors contributed equally.

15. M. Li, S. A. Odom, L. A. Robertson, T. P. Vaid, A. Pancoast, G. Agarwal, H. A. Doan, Y. Wang, M. Suduwella, S. Bheemireddy, R. H. Ewoldt, R. S. Assary, L. Zhang, M. Sigman, S. Minteer, "Experimental Protocols for Studying Organic Non-Aqueous Redox Flow Batteries." **ACS Energy Letters** 6, 3932-3943, 2021.

14. M. Zhou, H. A. Doan, L. A. Curtiss, R. S. Assary, "Identification of Active Metal Carbides and Nitrides Catalytic Facets for Hydrodeoxygenation Reactions." **Journal of Physical Chemistry C** 125, 8630-8637, 2021.

13. Y. Zhao, J. Zhang, G. Agarwal, Z. Yu, R. E. Corman, Y. Wang, L. A. Robertson, Z. Shi, H. A. Doan, R. H. Ewoldt, I. A. Shkrob, R. S. Assary, L. Cheng, V. Srinivasan, S. J. Baninec, L. Zhang, "TEMPO Allegro: Liquid Catholyte Redoxmers for Nonaqueous Redox Flow Batteries." **Journal of Materials Chemistry A** 9, 16769-16775, 2021.

12. G. Agarwal, H. A. Doan, R. S. Assary, "Molecular Structure and Electron Affinity of Metal-Solvent Complexes: Insights from Density Functional Theory Simulations." **Journal of the Electrochemical Society** 167, 5636-5646, 2020.

11. 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.

10. M. Zhou, H. A. Doan, L. A. Curtiss, R. S. Assary, "Effect of Ni Dopant on Furan Activation over Mo_2C Surface: Insights from First-Principles-Based Microkinetic Modeling." **Journal of Physical Chemistry C** 124, 5636- 5646, 2020.

9. P. Jian, H. A. Doan, S. Madireddy, R.S. Assary, P. Balaprakash, "Value-added Chemical Discovery using Reinforcement Learning." **arXiv**, 2019.

8. 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.

7. H. A. Doan, M. K. Sharma, W. S. Epling, L. C. Grabow, "From Active-Site Models to Real Catalysts: Importance of the Material Gap in the Rational Design of Pd Catalysts for Methane Oxidation." **ChemCatChem** 9, 1594-1600, 2017.

6. Q. Yuan, H. A. Doan, L. C. Grabow, S. R. Brankovic, "Finite Size Effects in Sub-monolayer Catalysts Investigated by CO Electrosorption on Pt/Pd(100)." **Journal of the American Chemical Society** 139, 13676-13679, 2017.

5. S. Pellizzeri, I. A. Jones, H. A. Doan, R. Q. Snurr, R. B. Getman, "Using Gas-Phase Clusters to Screen Porphyrin-supported Nanocluster Catalysts for Ethane Oxidation to Ethanol." **Catalysis Letters** 146, 2566-2573, 2016.

4. H-V Tran, H. A. Doan, B. D. Chandler, L. C. Grabow, "Water-assisted Oxygen Activation during Selective Oxidation Reactions." **Current Opinion in Chemical Engineering** 13, 100-108, 2016.

3. L. C. Grabow, Q. Yuan, H. A. Doan, S. R. Brankovic, "Novel 2D RuPt Core-Edge Nanocluster Catalyst for CO Electro-oxidation." **Surface Science** 640, 50-58, 2015.

2. 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.

- Highlight article: "Water's place in Au catalysis." **Science**. 345, 1564- 1565, 2014.

1. B. D. Chandler, S. Kendell, H. Doan, R. Korkosz, L. C. Grabow, C. J. Pursell, "NaBr Poisoning of Au/TiO_2 Catalysts: Effects on Kinetics, Poisoning Mechanism, and Estimation of the Number of Catalytic Active Sites." **ACS Catalysis** 2, 684-694, 2012.