

HIEU A. DOAN

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SUMMARY

A passionate computational scientist with extensive experience in leveraging molecular simulation, high-performance computing, and machine learning for large-scale virtual screening of molecular and crystalline materials. Received two “Best Fundamental Paper Awards” from the American Institute of Chemical Engineers and two “Best Paper Awards” from the Joint Center for Energy Storage Research.

PROFESSIONAL EXPERIENCE

Computational Materials Scientist

Argonne National Laboratory | Lemont, IL

May 2022 - Present

- Design active learning workflows for accelerated discovery of battery materials, reducing experiment time from decades to months
- Develop machine learning models in Python to predict solubility of solids in organic solvents based on physicochemical and quantum-mechanical descriptors
- Tune graph neural networks to accurately predict properties of crystal structures for catalytic applications

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 desired redox potential, solubility, and fluorescence
- Collaborated with chemists and roboticists to design an automated experiment for measuring battery performance
- Performed DFT calculations at scale to create a database of 20,000 optimized structures of adsorbed oxygen on doped metal carbide catalysts

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)

Machine Learning

Deep learning, multi-objective Bayesian optimization

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 CH₄ 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

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| 2023 | Poster Session Award from the 5 th 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 24 th North American Catalysis Society Meeting |
| 2014 | Best Fundamental Paper award from the American Institute of Chemical Engineers |

SELECT PRESENTATIONS

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

The Critical Role of Water at the Gold-Titania Interface in Catalytic CO Oxidation

Gordon Research Conference (Invited) | Ventura, CA

Feb 2015

PUBLICATIONS

27. B. Wang, H. A. Doan, S. Son, D. P. Abraham, S. E. Trask, A. Jansen, C. Liao, "ML-guided Design for New Electrolyte Additives Supporting High-performance 5V LiNi_{0.5}Mn_{1.5}O₄ Cathodes". In preparation.
26. C. Li, J. H. Miller, N. J. LiBretto, A. L. Rein, H. A. Doan, M. Zhou, G. R. Hafenstine, D. R. Vardon, S. Habas, R. S. Assary, "Molecular-level Insights into the Reaction Mechanisms of Reductive Etherification for Production of Sustainable Biofuels". In preparation.
25. X. Li, X. Wu, H. A. Doan, Z. Yang, R. Amine, M. Li, M. V. Bracamonte, C. Su, K. Amine, "Acidity Governed Rules in Electrochemical Performance of Fluorinated Benzenes for High Voltage Lithium Metal Batteries". **Angewandte Chemie**. Submitted.
24. J. Noh*, H. A. Doan*, H. Job, L. A. Robertson, L. Zhang, R. S. Assary, K. Mueller, V. Murugesan, Y. Liang, "An Integrated High-throughput Robotic Platform and Active Learning Approach for Accelerated Discovery of Optimal Electrolyte Formulations". **Nature Communication**. Accepted. *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 Mo₂C 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/TiO₂ Catalysts: Effects on Kinetics, Poisoning Mechanism, and Estimation of the Number of Catalytic Active Sites." **ACS Catalysis** 2, 684-694, 2012.