HIEU A. DOAN

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SUMMARY

I am a chemical engineer who is passionate about using computational methods to guide materials development and discovery. Atomic-scale modeling, materials informatics, and machine learning form my main tool set. My current research interest is in efficient data generation and utilization for accelerating materials discovery for catalysis and energy storage applications. Among the recognitions for my work are 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.

TECHNICAL SKILLS

Modeling and Simulation	Density Functional Theory (VASP/Gaussian), Microkinetic Modeling
Machine Learning	Principal Component Analysis, Bayesian Optimization, Graph Neural Network
Programming Language	Python, C/C++, Java, Fortran, shell scripting
Software Package	PyTorch, TensorFlow, Scikit-learn, RDKit, Pandas, NumPy, SciPy

EXPERIENCE

Assistant Scientist

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

In my current role, I spearhead several projects that underscore my dedication to innovation and sustainable technologies. I am working closely with engineers and chemists to develop automated discovery workflows for battery materials, harnessing the synergy of molecular simulations, electrochemical experiments, and machine learning. Additionally, I am driving initiatives focused on the accelerated screening of biomass conversion catalysts, employing high-throughput density functional theory simulations coupled with deep learning.

Postdoctoral Appointee

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

I started developing an interest in combining high-throughput molecular simulations and machine learning to expedite the discovery of innovative functional materials, especially in the realms of energy storage and catalysis. My projects spanned a wide range of applications, including the discovery of materials for sustainable redox flow batteries, the comprehensive screening of catalysts for biomass conversion, and the development of a self-driving laboratory dedicated to electrolyte design.

Postdoctoral Fellow

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

Throughout my research appointment, I pursued the fundamental understanding and subsequent optimal design of catalysts for natural gas conversion, leveraging the power of molecular simulations and materials informatics. My efforts led to an evaluation of the potential of supported metal oxide nanoclusters for the direct conversion of methane to methanol. Simultaneously, I engaged in high-throughput computational screenings of metal-organic frameworks, targeting efficient natural gas utilization.

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

I combined quantum mechanical simulations and kinetic models to advance our understanding of catalysts for carbon monoxide and methane oxidation. Specifically, I carried out density functional theory calculations and microkinetic modeling to investigate the performance of multifunctional catalytic materials, unravel the mechanism behind CO oxidation over gold/titania catalysts, and guide the design of palladium catalysts for natural gas vehicles. Beyond research, I 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

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
2008	Provost Undergraduate Research Scholarship
2008	AMOCO Foundation Scholarship
2008	Julie Ryan Academic Scholarship
2008	University of Houston Competitive Scholarship
2007	Summer Undergraduate Research Fellowship
2007	Herman Krause Academic Scholarship

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

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.