

Hieu Anh Doan, Ph.D.

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Summary of Qualifications

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. I have published scientific papers in peer-reviewed journals such as *Science*, *Journal of the American Chemical Society*, and *Chemistry of Materials*. I have received several recognitions including 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

Programming Language	Python, C/C++, Java, Fortran, shell scripting
Modeling Software	VASP, Gaussian, Aspen, MATLAB, COMSOL
Data Science Code	Tensorflow, Scikit-learn, Pandas, Numpy, Scipy
Machine Learning Method	Gaussian Process Regression, Multiobjective Active Learning, Graph Neural Network

Experience

Assistant Scientist

2022-present

ARGONNE NATIONAL LABORATORY - MATERIALS SCIENCE DIVISION

Lemont, IL

I am currently leading the following projects:

- Development of autonomous workflows for electrolyte discovery via molecular simulations, electrochemical experiments, and active learning
- Accelerated screening of biomass conversion catalysts via high-throughput density functional theory simulations and graph representation learning
- Mechanistic study of catalytic processes for sustainable aviation fuel production

Postdoctoral Appointee

2018-2022

ARGONNE NATIONAL LABORATORY - MATERIALS SCIENCE DIVISION

Lemont, IL

I was interested in utilizing high-throughput molecular simulations, materials informatics, and machine learning to accelerate the discovery of new functional materials relevant to energy storage and catalysis.

Projects:

- Materials discovery for sustainable redox flow batteries
- Catalyst screening for biomass conversion
- Self-driving laboratory for electrolyte design

Other relevant tasks: Write quarterly progress reports and prepare research proposals for new fundings

Postdoctoral Fellow

2016-2018

NORTHWESTERN UNIVERSITY - DEPARTMENT OF CHEMICAL AND BIOLOGICAL ENGINEERING

Evanston, IL

My research had a focus on designing optimal catalysts for natural gas conversion by means of cheminformatics and molecular simulations:

- Evaluated the prospect of supported metal oxide nanoclusters for direct conversion of methane to methanol
- Performed high-throughput computational screening of metal-organic frameworks for efficient natural gas utilization
- Additional responsibilities: Mentor Ph.D. students, write proposals to acquire research funding and allocations at supercomputing centers

Graduate Research Assistant

UNIVERSITY OF HOUSTON

2010-2015

Houston, TX

I used a combination of quantum mechanical simulations and kinetic modeling to study catalysts and catalytic reactions:

- Developed a microkinetic modeling code for activity prediction of multifunctional catalytic materials
- Conducted a detailed mechanistic study of CO oxidation over gold/titania catalysts to explain experimental observations
- Performed computational screening to guide experimental evaluations of improved palladium catalysts for methane slip reduction in natural gas vehicles
- Other responsibilities: Train new group members, supervise undergraduate research projects, conduct tutoring sessions and grade assignments and exams for the following courses (20-30 students/class): Chemical Engineering Thermodynamics, Design, Safety&Reliability

Education

Ph.D. in Chemical Engineering

UNIVERSITY OF HOUSTON

December 2015

Houston, TX

- Dissertation : Computational Screening of Bifunctional Catalysts for CO and CH₄ Oxidation
- Advisor : Professor Lars C. Grabow

B.S. in Chemical Engineering - Magna Cum Laude

UNIVERSITY OF HOUSTON

December 2009

Houston, TX

- Honor Thesis : Experimental Analysis of Soot Combustion in Diesel Particulate Filter
- Advisor : Professor Dan Luss

Honors & Awards

2022	Best Paper Award from the Joint Center for Energy Storage Research (JCESR)	Argonne, IL
2020	Best Paper Award from the Joint Center for Energy Storage Research (JCESR)	Argonne, IL
2019	Best Poster Presentation at the Argonne Postdoctoral Symposium	Argonne, IL
2018	Best Fundamental Paper Award from the American Institute of Chemical Engineers	Houston, TX
2015	Kokes Travel Award for the 24 th North American Catalysis Society Meeting	Pittsburgh, PA
2014	Best Fundamental Paper award from the American Institute of Chemical Engineers	Houston, TX
2008	Provost Undergraduate Research Scholarship	Houston, TX
2008	AMOCO Foundation Scholarship	Houston, TX
2008	Julie Ryan Academic Scholarship	Houston, TX
2008	University of Houston Competitive Scholarship	Houston, TX
2007	Summer Undergraduate Research Fellowship	Houston, TX
2007	Herman Krause Academic Scholarship	Houston, TX

Select Presentations

Accelerating the Evaluation of Crucial Descriptors in Computational Catalyst Screening via Graph Neural Network

AMERICAN CHEMICAL SOCIETY SPRING MEETING

March, 2023

Indianapolis, IN

Accelerated Discovery of Energy Storage Materials via Multiobjective Bayesian Optimization

AIChE MIDWEST REGIONAL CONFERENCE

March, 2022

Virtual

Active Learning via Bayesian Optimization for Discovery of Energy Storage Materials

NANO HUB TUTORIAL SERIES ON MACHINE LEARNING (INVITED)

June, 2021

Virtual

Warp Jumping in the Molecular Universe with Active Learning

ARGONNE AI AND HPC SEMINAR (INVITED)

Dec. 2020

Argonne, IL

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***, Lily A. Robertson, Lu 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. Minter, "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.