Hieu Anh Doan, Ph.D.

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Summary of Qualifications

I am a chemical engineer with expertise in using computational simulations and cheminformatics to guide materials development and discovery. Atomic scale modeling, materials science, 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 the *Best Paper Award* from the Joint Center for Energy Storage Research.
Residency status: Legal Permanent Resident/Green Card holder

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*
My interest is 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 work focused 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 *2010-2015*
University of Houston *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 *December 2015*
University of Houston *Houston, TX*

- Dissertation : Computational Screening of Bifunctional Catalysts for CO and CH_4 Oxidation
- Advisor : Professor Lars C. Grabow

B.S. in Chemical Engineering - Magna Cum Laude *December 2009*
University of Houston *Houston, TX*

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

Honors & Awards

2020	Best Paper Award from 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 24th 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

Accelerated Discovery of Energy Storage Materials via Multiobjective Bayesian Optimization *March. 2022*
AIChE Midwest Regional Conference *Virtual*

Active Learning via Bayesian Optimization for Discovery of Energy Storage Materials *June. 2021*
nanoHUB Tutorial Series on Machine Learning (Invited) *Virtual*

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

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

The Critical Role of Water at the Gold-Titania Interface in Catalytic CO Oxidation *Feb. 2015*
Gordon Research Conference (Invited) *Ventura, CA*

Publications

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. 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.