Hieu Anh Doan

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Summary of Qualifications

I am a research chemical engineer with expertise in using computational simulations and AI to aid materials development and discovery. I have published 15 scientific papers in peer-reviewed journals such as *Science*, *Journal of the American Chemical Society*, and *Chemistry of Materials*. I have extensive experience working in interdisciplinary research teams including the Joint Center for Energy Storage and Research (JCESR), Consortium of Computational Physics and Chemistry (CCPC Biomass), and Inorganometallic Catalyst Design Center (ICDC UMN).

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, Deep Learning

Experience

Postdoctoral Appointee *2018-present*

Argonne National Laboratory - Materials Science Division *Lemont, IL*

My current interest is in utilizing high-throughput molecular simulations 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

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 of 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

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

1. 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***. Accepted.*Authors contributed equally.
2. 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***. Accepted.
3. 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.

4. 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.
5. 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.
6. 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.
7. 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.
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.
9. 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.
10. 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.
11. 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.
12. 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.
13. 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.
14. 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: G. M. Mullen, C. B. Mullins, "Water's place in Au catalysis." ***Science***. 345, 1564- 1565, 2014.
15. 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.