# Hieu Anh Doan

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## Summary

I am a research chemical engineer who specializes in using computation to aid materials development and discovery. My toolset includes high-throughput quantum mechanical simulations, chemical informatics, machine learning, and most importantly, fundamental physics and chemistry. I have extensive experience in managing multiple projects independently as well as collaboratively in multidisciplinary teams.

## Skills

**Programming** Python, C/C++, Java, Fortran, shell scripting
**Modeling** VASP, Gaussian, Aspen, MATLAB, COMSOL
**Data Science** R, Pandas, Scikit-learn, Numpy, Scipy

## Experience

**Postdoctoral Appointee** *2018-present*
Argonne National Laboratory - Materials Science Division *Lemont, IL*
My current interest is in utilizing high-throughput Density Functional Theory simulations and active learning (e.g. Bayesian Optimization) for accelerated discovery of new functional materials relevant to energy storage and catalysis. Projects:

- Electrolyte design for sustainable redox flow batteries
- Catalyst stability optimization for biomass conversion
- Chemical reaction pathways prediction

**Postdoctoral Fellow** *2016-2018*
Northwestern University - Inorganometallic Catalyst Design Center *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 (published in ***Science***)
- Performed computational screening to guide experimental evaluations of improved palladium catalysts for methane slip reduction in natural gas vehicles (funded by ***Shell***)
- 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

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|---|---|---|
| 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 24$^{th}$ North American Catalysis Society Meeting | *Pittsburgh, PA* |
| 2015 | Invited for a special topic talk at the Gordon Research Conference | *Ventura, CA* |
| 2007 | Summer undergraduate research fellowship | *Houston, TX* |

## Selected Talks

**Quantum Chemistry Informed Active Learning to Guide the Development and Discovery of Energy Storage Materials** *Mar. 2020*
JCESR Webinar *Argonne, IL*

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

**Theoretical Insights into Selective Oxidation of Methane to Methanol on Porphyrin-supported Copper Nanoclusters** *Jun. 2017*
North American Catalysis Society Metting *Denver, CO*

**Importance of the Material Gap in Complete Methane Oxidation over Pd Catalysts** *Sep. 2015*
American Institute of Chemical Engineers Annual Meeting *Salt Lake, UT*

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

## Publications

1. 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." *Proceedings of the National Academy of Sciences*. In review.
2. 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.
3. 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.
4. 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.
5. 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.

6. 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.
7. 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.
8. 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.
9. 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.
10. 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.
11. 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.
12. 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.