

Hieu A. Doan

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Summary

Chemical engineer with 8+ years of R&D experience in designing materials with targeted functionalities. Strong expertise in employing state-of-the-art computational modeling and data science to guide the discovery of new heterogeneous catalysts. Adept at managing simultaneous projects independently and collaboratively in multidisciplinary environments.

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 focus is to utilize high-throughput computational screening and machine learning for discovery of new functional materials relevant to energy storage and catalysis.

Postdoctoral Fellow

2016-2018

NORTHWESTERN UNIVERSITY - INORGANOMETALLIC CATALYST DESIGN CENTER

Evanston, IL

My work focuses on designing optimal catalysts for natural gas conversion by means of cheminformatics, machine learning 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
- Employed machine learning to derive key structure-reactivity relations for methane oxidation catalysts
- 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

R&D Chemical Engineer Intern

MERICHEM

May-Aug. 2008

Houston, TX

As a summer intern, I designed, built and operated a THIOLEX™ pilot plant to remove acid gas and mercaptan compounds from hydrocarbon streams:

- Performed material balances
- Prepared the standard operating procedure
- Analyzed plant performance and proposed optimal operating conditions
- Wrote reports and presented in company meetings

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

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| 2018 | Best fundamental paper award from South Texas Section - AIChE | 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

Theoretical Insights into Selective Oxidation of Methane to Methanol on Porphyrin-supported Copper Nanoclusters

NORTH AMERICAN CATALYSIS SOCIETY MEETING

Jun. 2017

Denver, CO

Importance of the Material Gap in Complete Methane Oxidation over Pd Catalysts

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS ANNUAL MEETING

Sep. 2015

Salt Lake, UT

The Critical Role of Water at the Gold-Titania Interface in Catalytic CO Oxidation

GORDON RESEARCH CONFERENCE

Feb. 2015

Ventura, CA

Publications

1. H. A. Doan, B. Bucior, R. Q. Snurr, "Computational Screening of Metal-organic Frameworks for Direct Conversion of Methane to Methanol." In preparation.
2. 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.
3. 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.
4. 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.
6. 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.

7. 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.
8. 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.
- News coverage : <http://phys.org/news/2014-09-decoding-role-gold-nanocatalysis.html>
9. 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.