

Alexander J. Hoffman

Curriculum Vitae

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Education

University of Florida
Ph.D. in Chemical Engineering, 2022

Gainesville, FL

College of William and Mary
B.S. in Chemistry, 2015

Williamsburg, VA

Research Experience

Postdoctoral Associate
Department of Materials Science and Engineering, 2022–present
Advisor: Rafael Gómez-Bombarelli

Massachusetts Institute of Technology
Cambridge, MA

Graduate Research Assistant
Department of Chemical Engineering, 2017–2022
Advisor: David Hibbitts
Thesis: *Using Probe Species and Reactions to Study Catalyst Active Site Structures and Develop Density Functional Theory Models*

University of Florida
Gainesville, FL

Master's Thesis Researcher
Department of Chemical Engineering, 2016–2017
Advisor: David Hibbitts

University of Florida
Gainesville, FL

Publications

†These authors contributed equally to this work.

§Undergraduate or Master student mentee.

*Corresponding author.

Journal Articles

1. S. Nystrom[†]; [A. Hoffman[†]](#); D. Hibbitts*. Tuning Brønsted acid strength by altering site proximity in CHA framework zeolites. *ACS Catal.*, **2018**. DOI: [10.1021/acscatal.8b02049](https://doi.org/10.1021/acscatal.8b02049)

2. A. Hoffman; M. DeLuca; D. Hibbitts*. Restructuring of MFI framework zeolite models and their associated artifacts in density functional theory calculations. *J. Phys. Chem. C*, **2019**. ACS Editors' Choice. DOI: [10.1021/acs.jpcc.8b12230](https://doi.org/10.1021/acs.jpcc.8b12230)
3. M. DeLuca; P. Kravchenko; A. J. Hoffman; D. Hibbitts*. Mechanism and kinetics of methylating C₆–C₁₂ methylbenzenes with methanol and dimethyl ether in H-MFI zeolites. *ACS Catal.*, **2019**. Front Cover Feature. DOI: [10.1021/acscatal.9b00650](https://doi.org/10.1021/acscatal.9b00650)
4. J. Di Iorio; A. J. Hoffman; C. Nimlos; S. Nystrom; D. Hibbitts*; R. Gounder*. Mechanistic origins of the high-pressure inhibition of methanol dehydration rates in small-pore acidic zeolites. *J. Catal.*, **2019**. DOI: [10.1016/j.jcat.2019.10.012](https://doi.org/10.1016/j.jcat.2019.10.012)
5. M. C. Allen[†]; A. J. Hoffman[†]; T-W. Liu[§]; M. Webber; D. Hibbitts*; T. J. Schwartz*. Highly selective cross-etherification of 5-hydroxymethylfurfural with ethanol. *ACS Catal.*, **2019**. DOI: [10.1021/acscatal.0c01328](https://doi.org/10.1021/acscatal.0c01328)
6. A. J. Hoffman; J. S. Bates; J. R. Di Iorio; S. Nystrom; C. T. Nimlos; R. Gounder*; D. Hibbitts*. Rigid Arrangements of Ionic Charge in Zeolite Frameworks Conferred by Specific Al Distributions Preferentially Stabilize Alkanol Dehydration Transition States. *Angew. Chem. Int. Ed.*, **2020**. DOI: [10.1002/anie.202007790](https://doi.org/10.1002/anie.202007790)
7. C. Nimlos[†]; A. J. Hoffman[†]; Y. Hur; J. Di Iorio; D. Hibbitts*; R. Gounder*. Experimental and Theoretical Assessments of Aluminum Proximity in MFI Zeolites and its Alteration by Organic and Inorganic Structure-Directing Agents. *Chem. Mater.*, **2020**. DOI: [10.1021/acs.chemmater.0c03154](https://doi.org/10.1021/acs.chemmater.0c03154)
8. L. Kilburn[‡]; M. DeLuca[†]; A. J. Hoffman; S. Patel; D. Hibbitts*. Comparing Alkene Disproportionation and Formaldehyde-mediated Diene Formation Routes in Methanol-to-Olefins Catalysis in MFI and CHA. *J. Catal.*, **2021**. DOI: [10.1016/j.jcat.2021.05.010](https://doi.org/10.1016/j.jcat.2021.05.010)
9. A. J. Hoffman; C. Asokan; N. Gadinas; P. Kravchenko; A. Getsoian; P. Christopher*; D. Hibbitts*. Theoretical and Experimental Characterization of Adsorbed CO and NO on γ -Al₂O₃-Supported Rh Nanoparticles. *J. Phys. Chem. C*, **2021**. DOI: [10.1021/acs.jpcc.1c05160](https://doi.org/10.1021/acs.jpcc.1c05160)
10. G. Marsden; P. Kostetsky; R. Sekiya[§]; A. J. Hoffman; S. Lee; R. Gounder; D. Hibbitts; and L. J. Broadbelt*. Quantifying Effects of Active Site Proximity on Rates of Methanol Dehydration to Dimethyl Ether over CHA Zeolites through Microkinetic Modeling. *ACS Materials Au*, **2021**. DOI: [10.1021/acsmaterialsau.1c00057](https://doi.org/10.1021/acsmaterialsau.1c00057)
11. E. E. Bickel; A. J. Hoffman; S. Lee; H. E. Snider; C. T. Nimlos; N. K. Zamiechowski; D. Hibbitts; R. Gounder*. Altering the Arrangement of Framework Al Atoms in MEL Zeolites Using Mixtures of Tetrabutylammonium and Sodium Structure-Directing Agents. *Chem. Mater.*, **2022**. DOI: [10.1021/acs.chemmater.2c01083](https://doi.org/10.1021/acs.chemmater.2c01083)
12. A. J. Hoffman[†], C. Asokan[†], N. Gadinas, E. Schroeder, G. Zakem, S. V. Nystrom, A. Getsoian, P. Christopher*, D. Hibbitts*. Experimental and theoretical characterization of Rh single-atoms supported on γ -Al₂O₃ with varying hydroxyl content during NO reduction by CO. *ACS Catal.*, **2022**. DOI: [10.1021/acscatal.2c02813](https://doi.org/10.1021/acscatal.2c02813)

13. H. Balcom^{†§}, A. J. Hoffman[†], H. Loch[§], D. Hibbitts*. Brønsted Acid Strength Does Not Change for Bulk and External Sites of MFI. *ACS Catal.*, **2023**. DOI: [10.1021/acscatal.3c00076](https://doi.org/10.1021/acscatal.3c00076)
14. S. Ezenwa; H. Montalvo-Castro; A. J. Hoffman; H. Loch[§]; J. Attebery; D.-Y. Jan; M. Schmithorst; B. Chmelka; D. Hibbitts*; R. Gounder*. Synthetic Placement of Active Sites in Zeolites for Selective Toluene Methylation to para-Xylene. *J. Am. Chem. Soc.*, **2024**. DOI: [10.1021/jacs.4c00373](https://doi.org/10.1021/jacs.4c00373)
15. M. Xie; D. Schwalbe-Koda; Y. M. Semanate-Esquivel; E. Bello-Jurado; A. J. Hoffman; O. Santiago Reyes; C. Paris; M. Moliner; R. Gómez-Bombarelli*. An exhaustive mapping of zeolite-template chemical space. *Submitted to Nat. Mater.*, **2024**. Preprint DOI: [10.26434/chemrxiv-2024-d74sw](https://doi.org/10.26434/chemrxiv-2024-d74sw)
16. A. J. Hoffman; M. Xie; R. Gómez-Bombarelli*. Learning descriptors to predict organic structure-directing agent applicability in zeolite synthesis. *Submitted to Micro. Meso. Mater. (Invited paper)*, **2024**. Preprint DOI: [10.26434/chemrxiv-2024-mbg26](https://doi.org/10.26434/chemrxiv-2024-mbg26)
17. S. Kwont[†]; H. Leet[†]; A. J. Hoffman; M. Xie; R. Gómez-Bombarelli; Y. Román-Leshkov*. Synthesizing different lta-cage zeolites with the same organic structure-directing agent. *In preparation*.
18. A. J. Hoffman; C. Paris; M. Xie; M. Moliner; R. Gómez-Bombarelli*. Graph convolutional neural networks for determining aluminum distributions in zeolites. *In preparation*.
19. A. J. Hoffman[†]; N. Kragt[†]; R. Gounder*; D. Hibbitts*. Mapping the catalytic activity of Brønsted acid sites in MFI using methanol dehydration. *In preparation*.

Presentations

1. A. Hoffman; J. Di Iorio; S. Nystrom; C. Nimlos; R. Gounder; D. Hibbitts. Methanol dehydration over H-SSZ-13 with controlled site proximity: Effects of site proximity and coverage. *American Chemical Society National Meeting*, **2019**.
2. A. Hoffman; S. Nystrom; J. Di Iorio; C. Nimlos; R. Gounder; D. Hibbitts. Elucidating proximal Brønsted acid site interactions in CHA zeolites during methanol dehydration catalysis. *North American Catalysis Society Meeting*, **2019**.
3. A. Hoffman; J. Di Iorio; S. Nystrom; C. Nimlos; R. Gounder; D. Hibbitts. Acceleration of Methanol Dehydration in H-SSZ-13 by Acid Site Proximity. *American Institute of Chemical Engineers National Meeting*, **2019**.
4. A.J. Hoffman; C. T. Nimlos; A. Petro; P. M. Kester; J. Di Iorio; S. V. Nystrom; R. Gounder; D. Hibbitts*. Assessing the Kinetic Effects of Al Siting on Methanol Dehydration in Different Zeolite Void Environments Using Density Functional Theory. *American Institute of Chemical Engineers National Meeting*, **2020**.

5. A.J. Hoffman; C.T. Nimlos; Y.G. Hur; B.J. Lee; J.R. Di Iorio; D. Hibbitts*; R. Gounder*. Assessing Al proximity in MFI Zeolites Using Both Experiment and Theory. *North-East Corridor Zeolite Association Meeting*, **2020**.
6. A.J. Hoffman; C. Asokan; I. Alfayez; S.V. Nystrom Jr.; P. Kravchenko; A. Getsoian; P. Christopher; D. Hibbitts*. Characterizing Rh Particles and Single-Atoms Supported on γ -Al₂O₃ for NO Reduction Using Probe-Molecule IR Spectroscopy and DFT. *Graduate Association of Chemical Engineers (GRACE) Symposium*, **2021**.
7. A.J. Hoffman; C. Asokan; I. Alfayez; S.V. Nystrom Jr.; P. Kravchenko; A. Getsoian; P. Christopher; D. Hibbitts*. Characterizing Rh Particles and Single-Atoms Supported on γ -Al₂O₃ for NO Reduction Using Probe-Molecule IR Spectroscopy and DFT. *American Institute of Chemical Engineers National Meeting*, **2021**.
8. A.J. Hoffman; N. Gadinias; C. Asokan; E. Schroeder; A. Getsoian; P. Christopher; D. Hibbitts*. Characterizing Rh single-atoms catalysts on γ -Al₂O₃ using CO and NO probe-molecule IR and density functional theory. *American Chemical Society National Meeting*, **2022**.
9. A.J. Hoffman; S. Lee; R.-S. Sekiya; C. Nimlos; R. Gounder; and D. Hibbitts*. Effects of Al position, confinement, and clustering on methanol dehydration rates and kinetics in MFI. *North American Catalysis Society Meeting*, **2022**.
10. A.J. Hoffman; N. Gadinias; C. Asokan; E. Schroeder; A. Getsoian; P. Christopher; D. Hibbitts*. Characterizing Rh single-atoms catalysts on γ -Al₂O₃ using CO and NO probe-molecule IR and density functional theory. *Gordon Research Seminar – Catalysis*, **2022**.
11. A.J. Hoffman; R.-S. Sekiya; J. Di Iorio; C. Nimlos; R. Gounder; D. Hibbitts. Origins of Changes in Methanol Dehydration Turnover Rates on Brønsted Acid Sites in Zeolites with Different Al Distributions. *American Institute of Chemical Engineers National Meeting*, **2022**.
12. A. J. Hoffman; S. Lee; E. Bickel; C. Nimlos; R. Gómez-Bombarelli; R. Gounder; D. Hibbitts*. Mapping Interactions between Cationic Structure-Directing Agents and Framework Anions in Zeolites Using Computational Tools. *American Institute of Chemical Engineers National Meeting*, **2022**.
13. A. J. Hoffman; C. Asokan; N. Gadinias; E. Schroeder; S. V. Nystrom Jr.; A. Getsoian; P. Christopher; D. Hibbitts*. *American Institute of Chemical Engineers National Meeting*, **2022**.
14. A.J. Hoffman; M. Xie; C. París; M. Moliner; R. Gómez-Bombarelli*. Thermodynamics of Al Substitution in CHA and ERI with and without structure-directing agents. *Gordon Research Seminar – Nanoporous Materials*, **2023**.
15. A.J. Hoffman; M. Xie; C. París; M. Moliner; R. Gómez-Bombarelli*. Thermodynamics of Al Substitution in CHA with and without Organic Structure-Directing Agents. *American Institute of Chemical Engineers National Meeting*, **2023**.

16. A.J. Hoffman; M. Xie; C. París; M. Moliner; R. Gómez-Bombarelli*. Thermodynamics of Al Substitution in CHA with and without Organic Structure-Directing Agents. *American Chemical Society National Spring Meeting*, **2024**.

Teaching Experience

Department of Chemistry, College of William and Mary

Teaching Assistant, Inorganic Chemistry Lab

Spring 2015

Instructor: J. Molloy

Department of Chemical Engineering, University of Florida

Teaching Assistant, Advanced Chemistry & Biology Lab

Spring & Summer 2019

Instructor: D. Kopelevich

Department of Chemical Engineering, University of Florida

Supervised Teacher, Molecular Basis (Statistical Mechanics)

Fall 2019 & Fall 2020

Instructor: J. Weaver

Department of Materials Science and Engineering, MIT

Co-Instructor, Introduction to Modeling and Simulation

Spring 2024

Awards and Fellowships

Graduate School Preeminence Award (GSPA), University of Florida 2017

Best-in-session Presentation, GRACE Symposium, University of Florida 2021

Kokes Award, North American Catalysis Society 2022

Chemical Engineering PhD Research Excellence Award, University of Florida 2022

Professional Affiliations

American Chemical Society (ACS), Member 2018–present

American Institute of Chemical Engineers (AIChE), Member 2018–present

Phi Kappa Phi Honor Society, Member 2018–2020

Tau Beta Pi Honor Society, Member 2019–present

Materials Research Society, Member 2023–present

Leadership and Service

Women in Science and Engineering, Ambassador 2018–2019

Graduate Association of Chemical Engineers, Social Chair 2018–2019

Graduate Association of Chemical Engineers, Vice President 2019–2020

Graduate Association of Chemical Engineers, President	2020–2021
American Chemical Society CATL division, Seminar organizer at spring meeting	2024
Gordon Research Seminar–Nanoporous Materials, Chair elect	2025

Other Professional Experience

Environmental Protection Agency, Office of Pesticide Programs	2015–2016
Oak Ridge Institute for Science and Education (ORISE) Intern	Fort Meade, MD