

PRATEEK MEHTA

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PROFESSIONAL SUMMARY

- Chemical Engineering PhD with expertise in modeling and simulation to solve energy related problems
- Performed successful computational research in a number of multi-disciplinary environments across academia, industry, and government laboratories
- Authored **9 publications** in leading peer-reviewed journals and delivered **22 presentations** at national and international scientific meetings
- Work recognized by several awards by professional scientific societies and by the University of Notre Dame
- Proficient in use of programming and data analytics tools (**Python, Numpy, Scipy, Pandas, Matplotlib, Jupyter, scikit-learn, MATLAB, Fortran, Linux**) as well as scientific computational chemical engineering packages (**VASP, Quantum Espresso, COMSOL, LAMMPS, GAMS, Aspen Plus, etc**)

EDUCATION

🎓 PhD in Chemical Engineering

Advisor: William Schneider

University of Notre Dame

GPA: 4.0/4.0

📅 May 2019

📍 Notre Dame, IN

- Thesis: Computational design of multifunctional catalytic systems (metal/support interfaces and plasma-enabled catalysis)
- Used a combination of quantum mechanical simulations and kinetic modeling for the design of improved catalysts
- Computational predictions were used to guide and interpret by measurements from experimental collaborators
- Developed a numerically exact method to calculate free energies of catalytic reactions
- Built a Python-based research environment for efficient execution of computational workflows, including calculation automation, data organization and analysis. My approach to database-driven reproducible research was highlighted in an editorial in *Nature Catalysis*.
- My research was highlighted on the US Department of Energy (DoE) website and the DoE *Basic Research Needs for Catalysis Science to Transform Energy Technologies* Report

🎓 M.S. in Chemical Engineering

Advisor: John Kitchin

Carnegie Mellon University

GPA: 4.0/4.0

📅 Dec 2013

📍 Pittsburgh, PA

- Specialized MS program with emphasis on development of computational skills applicable to chemical engineering
- Thesis: Computational identification of metal oxide polymorphs that can be synthesized as thin-films

🎓 B. Tech. in Chemical Engineering

National Institute of Technology

GPA: 7.7/10.0

📅 May 2012

📍 Durgapur, India

INTERNSHIPS

Visiting Scholar

Advisor: Annemie Bogaerts, Richard van de Sanden

University of Antwerp and the Dutch Institute for Fundamental Energy Research

📅 Apr–Jun 2018

📍 Antwerp, Belgium and Eindhoven, Netherlands

- Built reactor models of plasma-phase and plasma-catalytic ammonia synthesis using Fortran- and Python-based kinetic modeling

Computational Chemistry and Materials Science Intern

Advisor: Brandon Wood

Lawrence Livermore National Laboratory

📅 Summer 2016

📍 Livermore, CA

- Used ab-initio molecular dynamics simulations and graph theoretical hop analyses to isolate structure-property relationships that result in extraordinary ionic conductivity in solid-state battery electrolytes

Computational Materials Intern

Advisor: Boris Kozinsky

Robert-Bosch LLC

📅 Jan–July 2014

📍 Cambridge, MA

- Performed classical and ab-initio molecular dynamics simulations to identify factors controlling Li-ion mobility in solid-state battery electrolytes
- Developed an automated Python-based infrastructure for high-throughput computational screening of promising electrolytes from an initial dataset of over 1500 materials

Undergraduate Research Fellow

Advisor: Frerich Keil

Hamburg University of Technology

📅 2011

📍 Hamburg, Germany

- Learned principles of density functional theory and used them to model adsorption of organic molecules on surfaces

PUBLICATIONS

9. **P. Mehta**, P. Barboun, D.B. Go, J.C. Hicks, W.F. Schneider, Catalysis Enabled by Plasma Activation of Strong Chemical Bonds: a review. *ACS Energy Letters*, 2019, in press, doi:10.1021/acseenergylett.9b00263
8. F.A. Herrera, G. Brown, P. Barboun, N. Turan, **P. Mehta**, W.F. Schneider, J.C. Hicks D.B. Go, The Impact of Transition Metal Catalysts on Macroscopic Dielectric Barrier Discharge (DBD) Characteristics in an Ammonia Synthesis Plasma Catalysis Reactor. *Journal of Physics D: Applied Physics*, 2019, 52, 224002
7. **P. Mehta**, P. Barboun, F. Herrera, J. Kim, P. Rumbach, D.B. Go, J.C. Hicks, W.F. Schneider, Overcoming Ammonia Synthesis Scaling Relations with Plasma-enabled Catalysis. *Nature Catalysis*, 2018, 1, 269
6. A. Bajpai*, **P. Mehta*** (* = co-first author), K. Frey, A. Lehmer, W.F. Schneider, Benchmark First-Principles Calculations of Adsorbate Free Energies. *ACS Catalysis*, 2018, 8, 1945
5. K. Kweon, J. Varley, P. Shea, N. Adelstien, **P. Mehta**, T.W. Heo, T. Udovic, V. Stavila, B.C. Wood. Structural, Chemical, and Dynamical Frustration: Origins of Superionic Conductivity in Closo-borate Solid Electrolytes. *Chemistry of Materials*, 2017, 29, 9142
4. **P. Mehta**, J. Greeley, W.N. Delgass, W.F. Schneider. Adsorption Energy Correlations at the Metal-Support Boundary. *ACS Catalysis*, 2017, 7, 4707
3. J. Varley, K. Kweon, **P. Mehta**, P. Shea, T. Heo, T. Udovic, V. Stavila, B.C. Wood. Understanding Ionic Conductivity Trends in Polyborane Solid Electrolytes from Ab Initio Molecular Dynamics. *ACS Energy Letters*, 2017, 2, 250
2. B. Kozinsky, S. Akhade, P. Hirel, A. Hashibon, C. Elsasser, **P. Mehta**, A. Logeat, U. Eisele. Effects of Sublattice Symmetry and Frustration on Ionic Transport in Garnet Solid Electrolytes. *Physical Review Letters*, 2016, 116, 055901
1. **P. Mehta**, P.A. Salvador, J.R. Kitchin. Identifying Potential BO₂ Oxide Polymorphs for Epitaxial Growth Candidates. *ACS Applied Materials & Interfaces*, 2014, 6, 3630

AWARDS

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|---|---|------|
| 🏆 | Eli J. and Helen Shaheen Graduate School Award | 2019 |
| | Top graduating PhD in Engineering, University of Notre Dame | |
| 🏆 | Outstanding Dissertation Award | 2019 |
| | Department of Chemical and Biomolecular Engineering, University of Notre Dame | |
| 🏆 | ACS Meeting Registration Award | 2019 |
| | Catalysis Division, American Chemical Society | |

	Best Research Poster Chemical Engineering Graduate Research Symposium, University of Notre Dame	2018
	CRE Travel Award Catalysis and Reaction Engineering Division, American Institute of Chemical Engineers	2018
	Joseph F. Downes Memorial Award University of Notre Dame	2018
	CRC Award for Computational Sciences and Visualization Center for Research Computing, University of Notre Dame	2018
	CoMSEF Graduate Student Award Computational and Molecular Science and Engineering Forum, American Institute of Chemical Engineers	2017
	ACS Meeting Registration Award Catalysis Division, American Chemical Society	2017
	Richard J. Kokes Award North American Catalysis Society, NAM 25	2017
	Outstanding Teaching Assistant: Numerical and Statistical Analysis Notre Dame Graduate Student Union, Top 3 across all graduate programs	2017
	Outstanding Teaching Assistant: Numerical and Statistical Analysis Department of Chemical and Biomolecular Engineering, University of Notre Dame	2017
	Best Research Poster Lawrence Livermore National Laboratory, Summer Scholars Symposium	2016
	CCMS Fellowship Lawrence Livermore National Laboratory	2016
	California Initiative Grant Notre Dame Career Center	2016
	Eilers Graduate Fellowship Center for Sustainable Energy, University of Notre Dame	2016
	Best Research Poster SUNCAT Institute on Heterogeneous Catalysis, Stanford University	2015
	Battery Division Travel Award 227 th Electrochemical Society Meeting	2015

LEADERSHIP AND SERVICE

Manuscript Reviewer


- Peer-reviewer for *Journal of the American Chemical Society*, *ACS Catalysis*, *Journal of Physical Chemistry C*, *Journal of Physical Chemistry Letters* (15 total reviews)

Organization of Professional Meetings

- Co-organizer and chair of the session, *Catalysis for Nitrogen Chemistry*, at the 2019 Annual Meeting of the American Institute of Chemical Engineers (AIChE)
- Chaired the session, *Fundamentals of Catalysis V*, at the 2018 AIChE Annual Meeting
- Co-organizer of the 2019 Catalysis Club of Chicago Annual Symposium

Instructor

Software Carpentry Foundation

 2016–present

- Led *Fundamentals of Python Programming* workshop at the Federal Reserve Bank of Chicago, 2017
- Contributed to development of course material for Python, Matlab, Git, and Linux Shell lessons

President

Chemical and Biomolecular Engineering Graduate Student Organization

📅 2016–2017

📍 University of Notre Dame

- Led the organization of annual graduate research symposium: invited alumni and industrial representatives, moderated alumni panel discussion, and led fundraising and social activities

Undergraduate Research Mentor

Schneider Group

📅 2015–2017

📍 University of Notre Dame

- Mentored Andrew Lehmer (ND Energy Slatt Fellow) and taught him how to use molecular simulations
- Work resulted in one publication with Andrew as co-author

Teaching Assistant

- Numerical and Statistical Analysis, Advanced Thermodynamics, Computational Chemistry, Transport Phenomena

CONTRIBUTED AND INVITED PRESENTATIONS

22. **P. Mehta**, P. Barboun, F. Herrera, J. Kim, P. Rumbach, D.B. Go, J.C. Hicks, W.F. Schneider, Advancing Sustainable Ammonia Synthesis with Plasma-enabled Catalysis. *Chemical Engineering Seminar Series, University of Notre Dame*, Notre Dame, IN, 2018 (**invited**)
21. **P. Mehta**, A. Bajpai, K. Frey, C. Waitt, A. Lehmer, G. Laughlin, W.F. Schneider, Accurate Adsorbate Free Energies from First-Principles. *AIChE Annual Meeting*, Pittsburgh, PA, 2018
20. **P. Mehta**, P. Barboun, F. Herrera, J. Kim, P. Rumbach, D.B. Go, J.C. Hicks, W.F. Schneider, Overcoming Ammonia Synthesis Scaling Relations with Plasma-enabled Catalysis. *AIChE Annual Meeting*, Pittsburgh, PA, 2018
19. **P. Mehta**, P. Barboun, F. Herrera, J. Kim, P. Rumbach, D.B. Go, J.C. Hicks, W.F. Schneider, Advancing Sustainable Ammonia Synthesis with Plasma-enabled Catalysis. *ExxonMobil Research & Engineering*, Clinton, NJ, 2018 (**invited**)
18. **P. Mehta**, P. Barboun, F. Herrera, D.B. Go, J.C. Hicks, W.F. Schneider, Catalyst development for application with plasmas: breaking scaling relations of thermal catalysis. *iPlasmaNano*, New Buffalo, MI, 2018
17. **P. Mehta**, P. Barboun, F. Herrera, J. Kim, P. Rumbach, D.B. Go, J.C. Hicks, W.F. Schneider, Overcoming Ammonia Synthesis Scaling Relations with Plasma-enabled Catalysis. *Gordon Research Conference on Catalysis*, New London, NH, 2018
16. **P. Mehta**, P. Barboun, F. Herrera, J. Kim, P. Rumbach, D.B. Go, J.C. Hicks, W.F. Schneider, Advancing Sustainable Ammonia Synthesis with Plasma-enabled Catalysis. *Dutch Institute for Fundamental Energy Research, Eindhoven, Netherlands*, 2018 (**invited**)
15. **P. Mehta**, P. Barboun, F. Herrera, J. Kim, P. Rumbach, D.B. Go, J.C. Hicks, W.F. Schneider, Ammonia Synthesis Using Plasma Assisted Catalysis: Understanding Rate Enhancements By Excited Species. *AIChE Annual Meeting*, Minneapolis, MN, 2017
14. **P. Mehta**, A. Bajpai, K. Frey, A. Lehmer, W.F. Schneider, Benchmark First-Principles Calculations of Adsorbate Free Energies. *AIChE Annual Meeting*, Minneapolis, MN, 2017
13. **P. Mehta**, A. Bajpai, K. Frey, A. Lehmer, W.F. Schneider. A First-Principles Approach to Adsorbate Free Energies. *American Chemical Society Meeting*, Washington, D.C., 2017
12. **P. Mehta**, J.P. Greeley, W.N. Delgass, W.F. Schneider. Adsorption Energy Correlations at the Metal-Support Boundary. *American Chemical Society Meeting*, Washington, D.C., 2017
11. **P. Mehta**, J.P. Greeley, W.N. Delgass, W.F. Schneider. Adsorption Energy Correlations at the Metal-Support Boundary. *North American Meeting, North American Catalysis Society, Denver, CO*, 2017
10. **P. Mehta**, J. Kim, D. Go, J. Hicks, W.F. Schneider. Ammonia Synthesis Using Plasma Assisted Catalysis: Understanding Rate Enhancements by Excited Species. *Chicago Catalysis Club Meeting, Chicago, IL*, 2017
9. **P. Mehta**, J.P. Greeley, W.N. Delgass, W.F. Schneider. Unraveling the Nature of Boundary Sites on Metal-on-Oxide Catalysts. *AIChE Annual Meeting, San Francisco, CA*, 2016 (**selected as best talk of session**)

8. **P. Mehta**, J. Varley, K. Kweon, P. Shea, and B. Wood. Understanding Ionic Conductivity Trends in Polyborane Solid Electrolytes from Ab Initio Molecular Dynamics. *Electrochemical Energy Symposium, Carnegie Mellon University, Pittsburgh, PA, 2016 (invited)*
7. **P. Mehta**, J.P. Greeley, W.N. Delgass, W.F. Schneider. Unraveling the Nature of Boundary Sites on Metal-on-Oxide Catalysts. *Chicago Catalysis Club Meeting, Chicago, IL, 2016*
6. **P. Mehta**, J.P. Greeley, W.N. Delgass, W.F. Schneider. Energetics at Metal-Oxide Interfaces: Effect on Water Gas Shift Intermediates. *AIChE Annual Meeting, Salt Lake City, UT, 2015 (selected as best talk of session)*
5. **P. Mehta**, B. Kozinsky. Structural Descriptors Controlling Ionic Motion in Solid Electrolytes from Automated Atomistic Computations. *Lawrence Livermore National Laboratory, Livermore, CA, 2015 (invited)*
4. **P. Mehta**, H. Zhu, J.P. Greeley, W.N. Delgass, F.H. Ribeiro, W.F. Schneider. Influence of the Metal-Oxide Interface on Water Gas Shift Intermediates. *SUNCAT Summer Institute, Stanford University, Palo Alto, CA, 2015*
3. **P. Mehta**, H. Zhu, J.P. Greeley, W.N. Delgass, F.H. Ribeiro, W.F. Schneider. Influence of the Metal-Oxide Interface on Water Gas Shift Intermediates. *North American Meeting, NACS, Pittsburgh, PA, 2015*
2. **P. Mehta**, B. Kozinsky. Structural Descriptors Controlling Ionic Motion in Solid Electrolytes from Automated Atomistic Computations. *227th ECS Meeting, Chicago, IL, 2015*
1. **P. Mehta**, J. R. Kitchin. Trends in BO_2 Oxide Polymorph Stability. *Pittsburgh-Cleveland Catalysis Society, Spring Meeting, 2013*