

PRATEEK MEHTA

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RESEARCH EXPERIENCE

Doctoral Research Advisor: Prof. William Schneider

University of Notre Dame

📅 2014–present

📍 Notre Dame, IN

Computational modeling of heterogeneous catalysis at metal/oxide interfaces and plasma-enabled catalysis

Visiting Scholar

Advisors: Prof. Annemie Bogaerts and
Prof. Richard van de Sanden

Univ. Antwerp and Dutch Institute for Fundamental Energy Research

📅 Apr–Jun 2018

📍 Antwerp, Belgium & Eindhoven, Netherlands

Modeling of plasma and plasma-catalytic ammonia synthesis

Research Fellow

Advisor: Dr. Brandon Wood

Lawrence Livermore National Laboratory

📅 Summer 2016

📍 Livermore, CA

Discovery of mechanisms of ionic conductivity in solid electrolytes using ab-initio molecular dynamics simulations and graph theory

Computational Materials Intern

Advisor: Dr. Boris Kozinsky

Robert-Bosch LLC

📅 2014

📍 Cambridge, MA

Discovery of descriptors for fast Li-ion mobility in solid-state battery electrolytes using high-throughput computational screening

Master's Dissertation

Advisor: Prof. John Kitchin

Carnegie Mellon University

📅 2012–2013

📍 Pittsburgh, PA

Identifying metal oxide polymorphs for epitaxial growth candidates

Undergraduate Research Fellow

Advisor: Prof. Frerich Keil

Hamburg University of Technology

📅 Summer 2011

📍 Hamburg, Germany

PUBLICATIONS

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, accepted
6. A. Bajpai*, P. Mehta*, K. Frey, A. Lehmer, W.F. Schneider, Benchmark First-Principles Calculations of Adsorbate Free Energies. *ACS Catalysis*, 2018, 8, 1945 (* = co-first author)
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

EDUCATION

🎓 PhD in Chemical Engineering

University of Notre Dame

GPA: 4.0/4.0

📅 2019

📍 Notre Dame, IN

🎓 M.S. in Chemical Engineering

Carnegie Mellon University

GPA: 4.0/4.0

📅 Dec 2013

📍 Pittsburgh, PA

🎓 B. Tech. in Chemical Engineering

National Institute of Technology

GPA: 7.7/10.0

📅 May 2012

📍 Durgapur, India

AWARDS

- 🏆 CoMSEF Graduate Student Award 2017
Computational and Molecular Engineering Forum, American Institute of Chemical Engineers
- 🏆 ACS Meeting Registration Award 2017
Catal. Division, American Chemical Society
- 🏆 Richard J. Kokes Award 2017
North American Catalysis Society, NAM 25
- 🏆 Outstanding Teaching Assistant 2017
Notre Dame Graduate Student Union
Top 3 across all graduate programs
- 🏆 Outstanding Teaching Assistant 2017
Dept. of Chemical Engineering, Notre Dame
- 🏆 Best Research Poster 2016
LLNL Summer Scholars Symposium
- 🏆 CCMS Fellowship 2016
Lawrence Livermore National Laboratory
- 🏆 California Initiative Grant 2016
Notre Dame Career Center
- 🏆 Eilers Graduate Fellowship 2016
Center for Sustainable Energy, Notre Dame
- 🏆 Best Research Poster 2015
SUNCAT Summer Institute, Stanford Univ.
- 🏆 Battery Division Travel Award 2015
227th Electrochemical Society Meeting

SERVICE

- ▶ Instructor 2016–present
Software Carpentry Foundation
- ▶ President 2016–17
Chemical and Biomolecular Engineering Graduate Student Organization
- ▶ Manuscript Reviewer
Journal of Physical Chemistry C
Journal of Physical Chemistry Letters
- ▶ Undergraduate Research Mentor 2015–17
Andrew Lehmer, ND Energy Slatt Fellow

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

CONFERENCE PRESENTATIONS

15. **P. Mehta**, P. Barboun, F. Herrera, J. Kim, P. Rumbach, D.B. Go, J.C. Hicks, W.F. Schneider. Breaking Ammonia Synthesis Scaling Relations with Plasma-enabled Catalysis. *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, NACS, 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 (**selected as best talk of session**). *AIChE Annual Meeting, San Francisco, CA*, 2016
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 (**invited**). *Electrochemical Energy Symposium, Carnegie Mellon University, Pittsburgh, PA*, 2016
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 (**selected as best talk of session**). *AIChE Annual Meeting, Salt Lake City, UT*, 2015
5. **P. Mehta**, B. Kozinsky. Structural Descriptors Controlling Ionic Motion in Solid Electrolytes from Automated Atomistic Computations (**invited**). *Lawrence Livermore National Laboratory, Livermore, CA*, 2015
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 BO₂ Oxide Polymorph Stability. *Pittsburgh-Cleveland Catalysis Society, Spring Meeting*, 2013

TEACHING

- ▶ **Software Carpentry**
Led Fundamentals of Python Programming Workshop at the Federal Reserve Bank of Chicago, 2017
- ▶ **Teaching Assistant**
Numerical and Statistical Analysis
Advanced Thermodynamics
Computational Chemistry
Transport Phenomena

TECHNICAL SKILLS

catalysis

electronic structure

statistical mechanics

Python

MATLAB

shell scripting

VASP

Quantum Espresso

LAMMPS

Atomic Simulation Environment

COMSOL

GAMS

Aspen Plus

Emacs

org-mode

LaTeX

Git

Linux