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

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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

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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

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Master's Dissertation — Advisor: Prof. John Kitchin

Carnegie Mellon University

2012–2013 — Pittsburgh, PA

Identifying metal oxide polymorphs for epitaxial growth candidates

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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, doi:10.1038/s41929-018-0045-1
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
  227^{th} 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 BO_2 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