PRATEEK MEHTA

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RESEARCH EXPERIENCE

Doctoral Research — William F. 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 — Annemie Bogaerts, 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 — 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 — 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 — John Kitchin
Carnegie Mellon University
2012–2013 — Pittsburgh, PA

Identifying metal oxide polymorphs for epitaxial growth candidates

Undergraduate Research Fellow — 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, 1, 269
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

CRC Award for Computational Sciences and Visualization — **2018**
Center for Research Computing, University of Notre Dame

CoMSEF Graduate Student Award — **2017**
Computational and Molecular Engineering Forum, American Institute of Chemical Engineers

ACS Meeting Registration Award — **2017**
Catalysis 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**
Department of Chemical Engineering, University of Notre Dame

Best Research Poster — **2016**
Lawrence Livermore National Laboratory, 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, University of Notre Dame

Best Research Poster — **2015**
SUNCAT Summer Institute, Stanford University

Battery Division Travel Award — **2015**
227^{th} Electrochemical Society Meeting

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

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

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