PRATEEK MEHTA

@ pmehta1@nd.edu | 412-417-0152 | prtkm.github.io | @prtk_m | linkedin.com/in/prtkm | orcid.org/0000-0001-6233-8072

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, M.C.M van de Sanden
Univ. Antwerp and Dutch Institute for Fundamental Energy Research
Apr-Jun 2018 — Antwerp, Belgium and Eindhoven, Netherlands

Kinetic modeling of plasma-phase 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

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 automated computational screening

Master's Thesis — 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
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

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

CRE Travel Award 2018
Catalysis and Reaction Engineering Division, American Institute of Chemical Engineers

Joseph F. Downes Memorial Award 2018
University of Notre Dame

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

CoMSEF Graduate Student Award 2017
Computational and Molecular Science and 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

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

16. **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
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 (**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

Best Research Poster **2015**
SUNCAT Institute on Heterogeneous Catalysis, Stanford University

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

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 | materials | 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 | FORTRAN