PRATEEK MEHTA

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PROFESSIONAL SUMMARY

- Chemical Engineering PhD candidate 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 **7 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**

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

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 BO_2 Oxide Polymorphs for Epitaxial Growth Candidates. ***ACS Applied Materials & Interfaces***, 2014, 6, 3630

AWARDS

Outstanding Graduate Student 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 — **2018**
Chemical Engineering Graduate Research Symposium, University of Notre Dame

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: Numerical and Statistical Analysis** — **2017**
  Notre Dame Graduate Student Union, Top 3 across all graduate programs
- **Outstanding Teaching Assistant: Numerical and Statistical Analysis** — **2017**
  Department of Chemical and Biomolecular 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 Institute on Heterogeneous Catalysis, Stanford University
- **Battery Division Travel Award** — **2015**
  227^{th} Electrochemical Society Meeting

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

- **N**umerical 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