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 **17 presentations** at national and international scientific meetings
- 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 packages used in high performance computing environments (**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 validated by measurements from experimental collaborators
- Developed a numerically exact method to calculate free energies of catalytic reactions using neural network accelerated quantum mechanical calculations
- 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
- Relevant coursework: Mathematical Modeling of Chemical Engineering Processes, Process Systems Modeling, Analysis and Modeling of Transport Phenomena, Principles of Molecular Simulation, Energy Systems Modeling
- 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-based kinetic modeling

Research Fellow — Advisor: Brandon Wood

Lawrence Livermore National Laboratory

Summer 2016 — Livermore, CA

- Performed large-scale molecular dynamics simulations to evaluate Li-ion mobility in solid-state battery electrolytes
- Developed a Python-module utilizing graph theory for tracking of Li hops as a function of time and related hopping-frequencies to Li diffusivity

Computational Materials Intern — Advisor: Boris Kozinsky

Robert-Bosch LLC

2014 — Cambridge, MA

- Developed an automated Python-based infrastructure for high-throughput computational screening of promising materials for use as solid-state Li-ion battery electrolytes from an initial dataset of over 1500 materials

Undergraduate Research Fellow — Advisor: Frerich Keil

Hamburg University of Technology

Summer 2011 — Hamburg, Germany

- Learned principles of quantum mechanical density functional theory and applied it to model adsorption on catalytic 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

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 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

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

Manuscript Reviewer

- Peer-reviewer for Journal of the American Chemical Society, ACS Catalysis, Journal of Physical Chemistry C, Journal of Physical Chemistry Letters

Teaching Assistant

- **N**umerical and Statistical Analysis, Advanced Thermodynamics, Computational Chemistry, Transport Phenomena

CONFERENCE PRESENTATIONS

17. **P. Mehta**, P. Barboun, F. Herrera, J. Kim, P. Rumbach, 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
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