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
- Excellent written and oral communication skills: 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. This environment is now used by the majority of our research group.
- 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

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

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

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

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

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 ACS Catalysis, Journal of Physical Chemistry C, Journal of Physical Chemistry Letters

Teaching Assistant

- Numerical and Statistical Analysis, Advanced Thermodynamics, Computational Chemistry, Transport Phenomena

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

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
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