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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, 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





- 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
- 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



- 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
- 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
- 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
- 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
- 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
- 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
- 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
- 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
- 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
- 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
- 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
- P. Mehta**, B. Kozinsky. Structural Descriptors Controlling Ionic Motion in Solid Electrolytes from Automated Atomistic Computations (**invited**). *Lawrence Livermore National Laboratory*, Livermore, CA, 2015
- 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
- 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
- P. Mehta**, B. Kozinsky. Structural Descriptors Controlling Ionic Motion in Solid Electrolytes from Automated Atomistic Computations. *227th ECS Meeting*, Chicago, IL, 2015
- P. Mehta**, J. R. Kitchin. Trends in BO₂ 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
227th Electrochemical Society Meeting

SERVICE

-  **Instructor** 2016–present
Software Carpentry Foundation
-  **President** 2016–17
Chemical and Biomolecular Engineering Graduate Student Organization
-  **Manuscript Reviewer**
ACS Catalysis
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
org-mode	Emacs	
TeX	Git	Linux
		FORTRAN