

## Donald J. Siegel

Mechanical Engineering Department  
Materials Science & Engineering  
Applied Physics Program  
University of Michigan

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**Research interests:** Materials and systems for energy storage; sustainable transportation; high-throughput materials discovery; computational materials science; thermodynamics, kinetics, and transport properties of materials; multi-scale modeling; Integrated Computational Materials Engineering.

### Education and Training

Case Western Reserve University	Physics	B.S.	1995
Univ. of Illinois at Urbana-Champaign	Physics	Ph.D.	2001
Univ. of Illinois at Urbana-Champaign	Certificate in Computational Sci. & Eng.		2001

### Professional Experience and Affiliations

2018 – present	Associate Chair for Graduate Education, Department of Mechanical Engineering, University of Michigan
2015 – present	Associate Professor, Mechanical Engineering, Materials Science & Engineering, and Applied Physics Program, University of Michigan
2013 – present	Senior Investigator & Member of the Directorate, Joint Center for Energy Storage Research (JCESR)
2012 – present	Affiliate Member, U.S. DRIVE Hydrogen Storage Technical Team
2010 – present	Member, UM Institute for Computational Science & Engineering
2009 – present	Faculty Fellow, University of Michigan Energy Institute
2015 – 2016	VELUX Visiting Professor, Dept. of Energy Conversion & Storage, Technical University of Denmark
2009 – 2015	Assistant Professor, Mechanical Eng. & Applied Physics, University of Michigan
2005 – 2009	Technical Expert & Group Leader, Ford Motor Company
2004 – 2005	National Acad. of Sciences/NRC Postdoctoral Fellow, U.S. Naval Research Lab
2001 – 2004	Postdoctoral Researcher, Sandia National Laboratories (DOE “L” clearance)

### Honors, Awards, and Notoriety

KAIST BK21 Lectureship, 2019  
'Hot Article' Award, *Energy & Environmental Science*, **11**, 2784 (2018)  
U.S. Department of Energy, Secretary of Energy's Achievement Award, 2018  
(For scientific & operational leadership of the Joint Center for Energy Storage Research, JCESR)  
*Chemistry of Materials* Reviewer Award, 2017 (presented to top 1% of reviewers)  
ACS Editors' Choice Article designation:  
Kiyabu, Lowe, Ahmed, & Siegel, *Chemistry of Materials*, DOI:10.1021/acs.chemmater.7b05230  
ACS 'Most Read Article' designation:  
March 2018: Kiyabu, *et al.*, *Chemistry of Materials*, DOI:10.1021/acs.chemmater.7b05230  
May 2017: Park and Siegel, *Chemistry of Materials*, DOI:10.1021/acs.chemmater.7b01166  
September 2017: Sharafi *et al.*, *Chemistry of Materials*, DOI:10.1021/acs.chemmater.7b03002  
Invited Panelist and Writer, *Basic Research Needs for Next Generation Electrical Energy Storage*,  
US Department of Energy, Office of Science, Basic Energy Sciences, 2017  
UM Mechanical Engineering Department Achievement Award, 2016  
Thompson-Reuters Web of Science Highly Cited Papers (4 papers), 2015  
VELUX Visiting Professor – Technical University of Denmark, 2015  
NAE Gilbreth Lecturer, 2014

NSF CAREER Award, 2013  
 SAE Ralph R. Teetor Educational Award, 2013  
 ‘Hot Article’ Award, *Energy & Environmental Science*, **6**, 2370 (2013)  
 Frontiers of Engineering Fellow, U.S. National Academy of Engineering, 2012 (Germany) & 2018 (Kuwait)  
 Elected Member of the Exec. Committee: APS Group on Energy Research and Applications, 2011  
 Kavli Frontiers of Science Fellow, U.S. National Academy of Science, 2011 (Indonesia) & 2013 (India)  
 Elected Member of the Exec. Committee: APS Forum on Industrial & Applied Physics, 2010  
 TMS/Japan Institute of Metals International Scholar Award, 2009  
 U.S. Council for Automotive Research Team Award, 2009  
 Top Papers 2008 Award, *Journal of Physics: Condensed Matter*  
 TMS Young Leader Professional Development Award, 2008  
 Inventor of the Month Award, Ford Research and Advanced Engineering, 2008  
 Publication *Agnew. Chem. Int. Ed.*, **47**, 882 (2008) featured in *Chemical & Eng. News*, 1/28/08, p67.  
 U.S. Council for Automotive Research Special Recognition Award, 2008  
 U.S. National Academies/National Research Council Fellow, 2004  
*Acta Materialia* Outstanding Referee Honorarium, 2004  
 Materials Research Society Graduate Student Award, 2001  
 NSF Travel Fellowship – Lyon, France, 1997.  
 Consecutive Outstanding Teaching Awards, UIUC Physics Department, 1995 & 1996.  
 Senior Scholar Award, Case Western Reserve University Physics Department, 1995  
 U.S. Department of Education National Science Scholar, 1991-1995

**Publications** (Google Scholar statistics: ~5,000 citations, h-index = 40. ORCID: 0000-0001-7913-2513)

1. A. Ahmed, S. Seth, J. Purewal, A. G. Wong-Foy, M. Veenstra, A. J. Matzger, and D. J. Siegel, *Exceptional Hydrogen Storage Achieved by screening Nearly Half a Million Metal-Organic Frameworks*, *Nature Communications*, **10**, 1568 (2019). DOI: 10.1038/s41467-019-09365-w
2. X. Liu, Y. Chen, Z. D. Hood, C. Ma, S. Yu, A. Sharafi, H. Wang, K. An, J. Sakamoto, D. J. Siegel, Y. Cheng, N. H. Jalarvo and M. Chi, *Elucidating the Mobility of  $H^+$  and  $Li^+$  ions in  $(Li_{6.25-x}H_xAl_{0.25})La_3Zr_2O_{12}$  via Correlative Neutron and Electron Spectroscopy*, *Energy & Environmental Science*, **12**, 945-951 (2019). DOI: 10.1039/c8ee02981d
3. K. Nagy, S. Kazemiabnavi, K. Thornton, and D. J. Siegel, *Thermodynamic Overpotentials and Nucleation Rates for Electrodeposition on Metal Anodes*, *ACS Applied Materials & Interfaces*, **11**, 7954-7964 (2019): DOI: 10.1021/acsami.8b19787
4. K. Kim and D. J. Siegel, *Correlating Lattice Distortions, Ion Migration Barriers, and Stability in Solid Electrolytes*, *J. Mater. Chem. A*, **7**, 3216-3227 (2019). DOI: 10.1039/C8TA10989C
5. S. Yu and D. J. Siegel, *Grain Boundary Softening: A Potential Mechanism for Lithium Metal Penetration Through Stiff Solid Electrolytes*, *ACS Applied Materials & Interfaces*, **10**, 38151-38158 (2018). DOI: 10.1021/acsami.8b17223
6. E. Kazyak, K-H Chen, A. L. Davis, S. Yu, A. J. Sanchez, J. Lasso, A. R. Bielinski, T. Thompson, J. Sakamoto, D. J. Siegel, and Neil P. Dasgupta, *Atomic Layer Deposition and First Principles Modeling of Glassy  $Li_3BO_3$ - $Li_2CO_3$  Electrolytes for Solid-State Li-Metal Batteries*, *Journal of Materials Chemistry A*, **6**, 19425-19437 (2018). DOI: 10.1039/c8ta08761j
7. J. G. Smith, G. Vardar, C. W. Monroe, and D. J. Siegel, *Experimental and Computational Investigation of Nonaqueous  $Mg/O_2$  Batteries*. Chapter 11 in *Metal-Air Batteries: Fundamentals and Applications*, Xin-bo Zhang, Editor. Wiley-VCH Verlag GmbH & Co. KGaA. (2018) DOI: 10.1002/9783527807666.ch11

8. M. D. Allendorf, Z. Hulvey, T. Gennett, A. Ahmed, T. Autrey, J. Camp, H. Furukawa, M. Haranczyk, M. Head-Gordon, A. Karkamkar, D.-J. Liu, J. R. Long, K. R. Meihaus, I. H. Nayyar, R. Nazarov, D. J. Siegel, V. Stavila, J. J. Urban, S. P. Veccham and B. C. Wood, *An Assessment of Strategies for the Development of Solid-State Adsorbents for Vehicular Hydrogen Storage*, *Energy & Environmental Science*, **11**, 2784-2812 (2018). DOI: 10.1039/c8ee01085d
9. J. Lowe and D. J. Siegel, *Reaction Pathways for Solvent Decomposition on Magnesium Anodes*, *Journal of Physical Chemistry C*, **122**, 10714–10724 (2018). DOI: 10.1021/acs.jpcc.8b01752
10. S. Kiyabu, J. S. Lowe, A. Ahmed, and D. J. Siegel, *Computational Screening of Hydration Reactions for Thermal Energy Storage: New Materials and Design Rules*, *Chemistry of Materials*, **30**, 2006-2017 (2018). DOI: 10.1021/acs.chemmater.7b05230 **ACS Editors' Choice Selection. Designated an ACS Most Read Article for March 2018.**
11. Haesun Park, Nitin Kumar, Marko Melander, Tejs Vegge, Juan Maria Garcia Lastra, and D. J. Siegel, *Adiabatic and Nonadiabatic Charge Transport in Li-S Batteries*, *Chemistry of Materials*, **30**, 915-928 (2018). DOI: 10.1021/acs.chemmater.7b04618
12. J. Wolfenstine, J. L. Allen, J. Sakamoto, D. J. Siegel, and H. Choe, *Mechanical Behavior of Li-ion-conducting Crystalline Oxide-based solid Electrolytes: A Brief Review*, *Ionics*, **24**, 1271-1276 (2018), DOI: 10.1007/s11581-017-2314-4
13. D. Samuel, C. Steinhauser, J. G. Smith, A. Kaufman, M. D. Radin, J. Naruse, H. Hiramatsu, and D. J. Siegel, *Ion Pairing and Diffusion in Magnesium Electrolytes Based on Magnesium Borohydride*, *ACS Applied Materials & Interfaces*, **9**, 43755-43766 (2017). DOI: 10.1021/acsami.7b15547
14. S. Yu and D. J. Siegel, *Grain Boundary Contributions to Li-ion Transport in the Solid Electrolyte  $\text{Li}_7\text{La}_2\text{Zr}_2\text{O}_{12}$  (LLZO)*, *Chemistry of Materials*, **29**, 9636-9647 (2017). DOI: 10.1021/acs.chemmater.7b02805
15. Alauddin Ahmed, Yiyang Liu, Justin Purewal, Ly D. Tran, Antek G. Wong-Foy, Mike Veenstra, Adam J. Matzger, and D. J. Siegel, *Balancing Gravimetric and Volumetric Hydrogen Density in MOFs*, *Energy & Environmental Science*, **10**, 2459-2471 (2017). DOI: 10.1039/C7EE02477K
16. T. Vegge, J. M. Garcia-Lastra, and D. J. Siegel, *Lithium-Oxygen Batteries: At a Crossroads?*, *Current Opinion in Electrochemistry*, **6**, 100-107 (2017). DOI: 10.1016/j.coelec.2017.10.014
17. A. Sharafi, E. Kazyak, A. L. Davis, S. Yu, T. Thompson, D. J. Siegel, N. P. Dasgupta, and J. Sakamoto, *Surface Chemistry Mechanism of Ultra-Low Interfacial Resistance in the Solid-State Electrolyte  $\text{Li}_7\text{La}_2\text{Zr}_2\text{O}_{12}$* , *Chemistry of Materials*, **29**, 7961-7968 (2017). DOI: 10.1021/acs.chemmater.7b03002 **Designated an ACS Most Read Article for September 2017.**
18. Y. Ming, N. Kumar, and D. J. Siegel, *Water Adsorption and Insertion in MOF-5*, *ACS Omega*, **2**, 4921-4928 (2017). DOI: 10.1021/acsomega.7b01129
19. A. Sharafi, S. Yu, M. Naguib, M. Lee, C. Ma, H. M. Meyer, J. Nanda, M. Chi, D. J. Siegel, and J. Sakamoto, *Impact of Air Exposure and Surface Chemistry on Li- $\text{Li}_7\text{La}_2\text{Zr}_2\text{O}_{12}$  Interfacial Resistance*, *Journal of Materials Chemistry A*, **5**, 13475-13487 (2017). DOI:10.1039/c7ta03162a
20. H. Park and D. J. Siegel, *Tuning the Adsorption of Polysulfides in Lithium-Sulfur Batteries with Metal-Organic Frameworks*, *Chemistry of Materials*, **29**, 4932-4939 (2017). DOI:10.1021/acs.chemmater.7b01166 **Designated an ACS Most Read Article for May 2017.**
21. J. G. Smith, J. Naruse, H. Hiramatsu, and D. J. Siegel, *Intrinsic Conductivity in Magnesium-Oxygen Battery Discharge Products:  $\text{MgO}$  and  $\text{MgO}_2$* , *Chemistry of Materials*, **29**, 3152–3163 (2017). DOI: 10.1021/acs.chemmater.7b00217
22. J. Zhong, D. J. Siegel, L. G. Hector, and J. B. Adams, *Atomistic Simulations of Adhesion, Indentation and Wear at the Nanoscale*, Ch. 25 in “Applied Nanoindentation in Advanced

- Materials,” Atul Tiwari and Sridhar Natarajan, Editors. John Wiley & Sons, 601-645, (2017). DOI:10.1002/9781119084501.ch25
23. T. Thompson, S. Yu, L. Williams, R. D. Schmidt, R. Garcia-Mendez, J. Wolfenstine, J. L. Allen, E. Kioupakis, D. J. Siegel, and J. Sakamoto, *Electrochemical Window of the Li-ion Solid Electrolyte Li<sub>1-x</sub>La<sub>x</sub>Zr<sub>2</sub>O<sub>7</sub>*, ACS Energy Letters **2**, 462-468 (2017). DOI:10.1021/acseenergylett.6b00593
  24. G. Vardar, J. G. Smith, T. Thompson, K. Inagaki, J. Naruse, H. Hiramatsu, A. Sleightholme, J. Sakamoto, D. J. Siegel, C. W. Monroe, *A Mg/O<sub>2</sub> Battery Based on the MACC Electrolyte*, Chemistry of Materials, **28**, 7629-7637 (2016). DOI: 10.1021/acs.chemmater.6b02488
  25. A. F. Chadwick, G. Vardar, S. DeWitt, A. E. S. Sleightholme, C. W. Monroe, D. J. Siegel, and K. Thornton, *Computational Model of Magnesium Deposition and Dissolution for Property Determination via Cyclic Voltammetry*, Journal of the Electrochemical Society, **163**, A1813-A1821 (2016). DOI: 10.1149/2.0031609jes
  26. Y. Ming, J. Purewal, J. Yang, C. Xu, M. Veenstra, M. Gaab, U. Müller, and D. J. Siegel, *Stability of MOF-5 in a Hydrogen Gas Environment Containing Fueling Station Impurities*, International Journal of Hydrogen Energy, **41**, 9374 (2016). DOI: 10.1016/j.ijhydene.2016.03.155
  27. N. Kumar and D. J. Siegel, *Interface-Induced Renormalization of Electrolyte Energy Levels in Magnesium Batteries*, Journal of Physical Chemistry Letters, **7**, 874-881 (2016). DOI: 10.1021/acs.jpcclett.6b00091
  28. J. G. Smith, J. Naruse, H. Hiramatsu, and D. J. Siegel, *Theoretical Limiting Potentials in Mg/O<sub>2</sub> Batteries*, Chemistry of Materials, **28**, 1390-1401 (2016). DOI: 10.1021/acs.chemmater.5b04501
  29. S. Yu, R. D. Schmidt, R. Garcia-Mendez, E. Herbert, N. J. Dudney, J. B. Wolfenstine, J. Sakamoto, and D. J. Siegel, *Elastic Properties of the Solid Electrolyte Li<sub>1-x</sub>La<sub>x</sub>Zr<sub>2</sub>O<sub>7</sub> (LLZO)*, Chemistry of Materials, **28**, 197-206 (2015). DOI: 10.1021/acs.chemmater.5b03854
  30. G. Vardar, E. G. Nelson, J. G. Smith, J. Naruse, H. Hiramatsu, B. M. Bartlett, A. E. S. Sleightholme, D. J. Siegel, and Charles W. Monroe, *Identifying the Discharge Product and Reaction Pathway for a Secondary Mg/O<sub>2</sub> battery*, Chemistry of Materials, **27**, 7564 (2015). DOI:10.1021/acs.chemmater.5b03608
  31. M. D. Radin, C. W. Monroe, and D. J. Siegel, *Impact of Space Charge Layers on Sudden Death in Li/O<sub>2</sub> Batteries*, Journal of Physical Chemistry Letters, **6**, 3017 (2015). DOI:10.1021/acs.jpcclett.5b01015
  32. H. S. Koh, M. K. Rana, A. Wong-Foy, and D. J. Siegel, *Predicting Methane Storage in Open-Metal-Site MOFs*, Journal of Physical Chemistry C, **119**, 13451 (2015). DOI:10.1021/acs.jpcc.5b02768
  33. S. Yang and D. J. Siegel, *Intrinsic Conductivity in Sodium-air Battery Discharge Phases: Sodium Superoxide vs. Sodium Peroxide*, Chemistry of Materials, **27**, 3852 (2015). DOI:10.1021/acs.chemmater.5b00285
  34. M. D. Radin and D. J. Siegel, *Non-Aqueous Metal-Air Batteries: Past, Present, and Future*, Chapter 18 in “Rechargeable Batteries: Materials, Technologies and New Trends.” Z. Zhang and S. S. Zhang, Editors. Springer (Switzerland), 511 (2015). DOI: 10.1007/978-3-319-15458-9\_18
  35. Nitin Kumar, Maxwell D. Radin, Brandon C. Wood, Tadashi Ogitsu, and Donald J. Siegel, *Surface-Mediated Solvent Decomposition in Li-air Batteries: Impact of Peroxide and Superoxide Surface Terminations*, Journal of Physical Chemistry C, **119**, 9050 (2015). DOI:10.1021/acs.jpcc.5b00256
  36. Y. Ming, J. Purewal, J. Yang, C. Xu, R. Soltis, J. Warner, M. Veenstra, M. Gaab, U. Mueller, and D. J. Siegel, *Kinetic Stability of MOF-5 in Humid Environments: Impact of Powder*

*Densification, Humidity Level, and Exposure Time*, Langmuir, **31**, 4988 (2015).  
DOI:10.1021/acs.langmuir.5b00833

37. L. D. Griffith, A. E. S. Sleightholme, J. F. Mansfield, D. J. Siegel, and C. W. Monroe, *Correlating Li/O<sub>2</sub> Cell Capacity and Product Morphology with Discharge Current*, ACS Applied Materials & Interfaces, **7**, 7670 (2015). DOI: 10.1021/acsami.5b00574
38. H. Park, H. S. Koh, and D. J. Siegel, *First-Principles Study of Redox End-Members in Lithium-Sulfur Batteries*, Journal of Physical Chemistry C, **119**, 4675 (2015). DOI: 10.1021/jp513023v
39. M. D. Radin, C. W. Monroe, and D. J. Siegel, *How Dopants can Enhance Charge Transport in Li<sub>2</sub>O<sub>2</sub>*, Chemistry of Materials **27**, 839 (2015). DOI: 10.1021/cm503874c
40. Y. Ming, H. Chi, R. Blaser, C. Xu, J. Yang, M. Veenstra, M. Gaab, U. Müller, C. Uher, D. J. Siegel, *Anisotropic Thermal Transport in MOF-5 Composites*, International Journal of Heat and Mass Transfer **82**, 250 (2015). DOI: 10.1016/j.ijheatmasstransfer.2014.11.053
41. G. Vardar, A. Sleightholme, J. Naruse, H. Hiramatsu, D. J. Siegel, and C. W. Monroe, *Electrochemistry of Magnesium Electrolytes in Ionic Liquids for Secondary Batteries*, ACS Applied Materials & Interfaces **6**, 18033 (2014). DOI: 10.1021/am5049064
42. A. Biswas, D. J. Siegel, and D. N. Seidman, *Compositional Evolution of Q-Phase Precipitates in an Aluminum Alloy*, Acta Materialia **75**, 322 (2014). DOI: 10.1016/j.actamat.2014.05.001
43. F. Tian, M. D. Radin, and D. J. Siegel, *Enhanced Charge Transport in Amorphous Li<sub>2</sub>O<sub>2</sub>*, Chemistry of Materials **26**, 2952 (2014). DOI: 10.1021/cm5007372
44. N. Kumar, K. Leung, and D. J. Siegel, *Crystal Surface and State of Charge Dependencies of Electrolyte Decomposition on LiMn<sub>2</sub>O<sub>4</sub> Cathode*, Journal of the Electrochemical Society **161**, E3059 (2014). DOI: 10.1149/2.009408jes
45. M. K. Rana, H. S. Koh, H. Zuberi, and D. J. Siegel, *Methane Storage in Metal Substituted MOFs: Thermodynamics, Usable Capacity, and the Impact of Enhanced Binding Sites*, Journal of Physical Chemistry C **118**, 2929 (2014). DOI: 10.1021/jp4104273
46. J. Nanda, S. K. Martha, W. D. Porter, H. Wang, N. J. Dudney, M. D. Radin, and D. J. Siegel, *Thermophysical Properties of LiFePO<sub>4</sub> Cathodes with Carbonized Pitch Coatings and Organic Binders: Experiments and First-Principles Modeling*, Journal of Power Sources **251**, 8 (2014). DOI: 10.1016/j.jpowsour.2013.11.022
47. Y. Ming, J. Purewal, D. Liu, A. Sudik, C. Xu, J. Yang, M. Veenstra, K. Rodes, R. Soltis, J. Warner, M. Gaab, U. Muller, and D. J. Siegel, *Thermophysical Properties of MOF-5 Powders*, Microporous and Mesoporous Materials **185**, 235 (2014). DOI: 10.1016/j.micromeso.2013.11.015
48. J. Goldsmith, A. G. Wong-Foy, M. J. Cafarella, and D. J. Siegel, *Theoretical Limits of Hydrogen Storage in Metal-Organic Frameworks: Opportunities and Challenges*, Chemistry of Materials **25**, 3373 (2013). DOI: 10.1021/cm401978e
49. M. D. Radin and D. J. Siegel, *Charge Transport in Lithium Peroxide: Relevance for Rechargeable Metal-Air Batteries*, Energy & Environmental Science **6**, 2370 (2013). DOI: 10.1039/C3EE41632A. Part of Themed Issue: "Post Li-ion Batteries." **Thompson Reuters Web of Science Highly Cited Paper (Sept/Oct 2015)**.
50. M. K. Rana, H. S. Koh, J. Hwang, and D. J. Siegel, *Thermodynamic Screening of Metal-Substituted MOFs for Carbon Capture*, Physical Chemistry Chemical Physics **15**, 4573 (2013). DOI: 10.1039/C3CP50622C
51. C. Xu, J. Yang, M. Veenstra, A. Sudik, J. J. Purewal, Y. Ming, B. J. Hardy, J. Warner, S. Maurer, U. Mueller, and D. J. Siegel, *Hydrogen Permeation and Diffusion in Densified MOF-5 Pellets*,

International Journal of Hydrogen Energy, **38**, 3268 (2013).

DOI:10.1016/j.ijhydene.2012.12.096

52. T. J. Wallington, J. E. Anderson, D. J. Siegel, M. A. Tamor, S. A. Mueller, S. L. Winkler, and O.J. Nielsen, *Sustainable Mobility, Future Fuels, and the Periodic Table*, Journal of Chemical Education **90**, 440 (2013). DOI: 10.1021/ed3004269
53. J. Purewal, D. Liu, A. Sudik, M. Veenstra, J. Yang, S. Maurer, U. Muller, and D. J. Siegel, *Improved Hydrogen Storage and Thermal Conductivity in High-Density MOF-5 Composites*, Journal of Physical Chemistry C, **116**, 20199 (2012) DOI:10.1021/jp305524f
54. (Invited Article in Special Issue: First Principles Computations) M. D. Radin, F. Tian, and D. J. Siegel, *Electronic Structure of  $Li_2O_2$  (0001) Surfaces*. Journal of Materials Science **47**, 7564 (2012). DOI: 10.1007/s10853-012-6552-6
55. D. Liu, J. J. Purewal, J. Yang, A. Sudik, S. Maurer, U. Mueller, J. Ni, and D. J. Siegel, *MOF-5 Composites Exhibiting Improved Thermal Conductivity*. International Journal of Hydrogen Energy **37**, 6109 (2012).
56. M. D. Radin, J. F. Rodriguez, F. Tian, and D. J. Siegel, *Lithium Peroxide Surfaces are Metallic, Lithium Oxide Surfaces are Not*. Journal of the American Chemical Society, **134**, 1093-1103 (2012). **Thompson Reuters Web of Science Highly Cited Paper (Sept/Oct 2015)**.
57. M. K. Rana, H. S. Koh, J. Hwang, and D. J. Siegel, *Comparing van der Waals Density Functionals for  $CO_2$  Adsorption in Metal Organic Frameworks*, Journal of Physical Chemistry C, **116**, 16957 (2012). DOI: 10.1021/jp3051164
58. J. Purewal, D. Liu, J. Yang, A. Sudik, D. J. Siegel, S. Maurer, and U. Muller, *Increased volumetric hydrogen uptake in MOF-5 by powder densification*. International Journal of Hydrogen Energy **37**, 2723 (2012). **Thompson Reuters Web of Science Highly Cited Paper (Sept/Oct 2015)**.
59. M. D. Radin, J. F. Rodriguez, and D. J. Siegel, *Lithium Peroxide Surfaces and Point Defects: Relevance for Li-air Batteries*, Proceedings of the Battery Congress, Vol. **60**, p. 6-16, (2011). Ann Arbor, MI April 11-12 (2011).
60. A. Biswas, D. J. Siegel, C. Wolverton, and D. N. Seidman, *Precipitates in Al-Cu alloys revisited: Atom-probe tomographic experiments and first-principles calculations of compositional evolution and interfacial segregation*. Acta Materialia **59**, 6187 (2011).
61. (Invited Review) J. Yang, A. Sudik, C. Wolverton, and D. J. Siegel, *High capacity hydrogen storage materials: Attributes for automotive applications and techniques for materials discovery*, Chemical Society Reviews **39**, 656 (2010). **Thompson Reuters Web of Science Highly Cited Paper (Sept/Oct 2015)**.
62. A. Biswas, D. J. Siegel, and D. N. Seidman, *Simultaneous Segregation at Coherent and Semi-coherent Heterophase Interfaces*. Physical Review Letters **105**, 076102 (2010).
63. S. J. Moura, J. B. Siegel, D. J. Siegel, H. K. Fathy, and A. G. Stefanopoulou, *Education on Vehicle Electrification: Battery Systems, Fuel Cells, and Hydrogen*, Proceedings of the IEEE Vehicle Power and Propulsion Conference (VPPC10). DOI: 10.1109/VPPC.2010.5729150
64. A. Sudik, J. Yang, D. J. Siegel, C. Wolverton, R. O. Carter, and A. Drews, *Impact of Stoichiometry on the Hydrogen Storage Properties of  $LiNH_2$ - $LiBH_4$ - $MgH_2$  Ternary Composites*, Journal of Physical Chemistry C **113**, 2004 (2009).
65. J. Yang, A. Sudik, D. J. Siegel, D. Halliday, A. Drews, R. O Carter, C. Wolverton, G. J. Lewis, J. W. A. Sachtler, J. J. Low, S. A. Faheem, D. A. Lesch, and V. Ozolins, *A Self-Catalyzing Hydrogen Storage Material*, Angewandte Chemie International Edition **47**, 882 (2008).

66. C. Wolverton, D. J. Siegel, A. R. Akbarzadeh, and V. Ozolins, *Discovery of Novel Hydrogen Storage Materials: An Atomic Scale Computational Approach*, Journal of Physics: Condensed Matter **20**, 064228 (2008). (Chosen for JPCM “Top Papers 2008.”)
67. D. J. Siegel, C. Wolverton, and V. Ozolins, *Thermodynamic Guidelines for the Prediction of Hydrogen Storage Reactions and their Application to Destabilized Hydride Mixtures*, Physical Review B **76**, 134102 (2007).
68. D. J. Siegel, C. Wolverton, and V. Ozolins, *First Principles Study of the Crystal Structure and Dehydrogenation Pathways of  $LiBNH_n$* , Physical Review B **75**, 014101 (2007).
69. J. Yang, A. Sudik, D. J. Siegel, D. Halliday, A. Drews, R. Carter, C. Wolverton, G. J. Lewis, J. W. A. Sachtler, J. J. Low, S. A. Faheem, D. A. Lesch, V. Ozolins, *Hydrogen Storage Properties of  $2 LiNH_2 + LiBH_2 + MgH_2$* , Journal of Alloys and Compounds **446-447**, 345 (2007).
70. G. J. Lewis, J. W. A. Sachtler, J. J. Low, D. A. Lesch, S. A. Faheem, P. M. Dosek, L. M. Knight, C. M. Jensen, J. Yang, A. Sudik, D. J. Siegel, C. Wolverton, V. Ozolins, and S. Zhang, *High-Throughput Screening of the Ternary  $LiNH_2$ - $MgH_2$ - $LiBH_2$  Phase Diagram*, Journal of Alloys and Compounds **446-447**, 355 (2007).
71. D. J. Siegel, Generalized Stacking Fault Energies, Ductilities, and Twinnabilities of Ni and Selected Ni Alloys, Applied Physics Letters **87**, 121901 (2005).
72. D. J. Siegel and J. C. Hamilton, *Computational Study of C Segregation and Diffusion within a Ni Grain Boundary*, Acta Materialia **53**, 87 (2005). DOI: 10.1016/j.actamat.2004.09.006
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81. L. G. Hector, Jr., G. A. Nitowski, S. M. Opalka, L. Weiserman, D. J. Siegel, H. Yu, J. B. Adams, *Investigation of Vinyl Phosphonic Acid/Hydroxylated  $\alpha$ - $Al_2O_3$ (0001) Reaction Enthalpies*, Surface Science **494**, 1 (2001).
82. (Invited article) J. B. Adams, L. G. Hector, Jr, D. J. Siegel, H. Yu, J. Zhong, Y. T. Cheng, *Adhesion, Lubrication, and Wear on the Atomic Scale*, Surface and Interface Analysis **31**, 619 (2001).
83. D. J. Siegel, L. G. Hector, Jr, and J. B. Adams, *Stoichiometry and Adhesion of Al/WC*, Materials Research Society Symposium Proceedings **677**, AA.4.26, (2001).

84. D. J. Siegel, L. G. Hector, Jr, and J. B. Adams, *Electronic Structure and Bonding at the Al-Terminated Al/Al<sub>2</sub>O<sub>3</sub> Interface: A First-Principles Study*, Materials Research Society Symposium Proceedings **654**, AA 4.2, (2001).
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86. L.G. Hector, Jr., D. J. Siegel, and J.B. Adams, *Atomistic Simulation of Adhesion and Adhesive Transfer at Metal/Metal-Oxide Interfaces*, Proc. INTEGRATION OF MATERIAL, PROCESS AND PRODUCT DESIGN, N. Zabaras, R. Becker, S. Ghosh, and L Lalli, Eds., p.39-46 (1999) A. A. Balkema Publishers, Leiden, Netherlands, ISBN: 90-5809-101-5
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### Patents, Patent Applications, and Invention Disclosures

1. Patent US 7,790,133: *Multi-component Hydrogen Storage Material* , Assigned 9/7/2010. Inventors: Faheem; Syed A., Lewis; Gregory J., Sachtler; J.W. Adriaan, Low; John J., Lesch; David A., Dosek; Paul M., Wolverton; Christopher M., Siegel; Donald J., Sudik; Andrea C., Yang; Jun
2. Patent US 8,038,980: *Hydrogen Storage Materials Containing Ammonia Borane* , Assigned 10/18/2011. Inventors: Yang; Jun, Sudik; Andrea, Siegel; Donald J., Hirano; Shinichi, Drews; Andrew Robert, Wolverton; Christopher Mark
3. Patent US 8,418,841: *Method of Enhancing Thermal Conductivity in Hydrogen Storage Systems*, Assigned 4/16/2013. Inventors: Yang; Jun, Siegel; Donald J., Pulskamp; Andrea, Drews; Andrew Robert, Hirano; Shinichi, Wolverton; Christopher Mark
4. Patent US 8,790,616: *Hybrid Hydrogen Storage System and Method of Using the Same*, Assigned 7/29/2014. Inventors: Pulskamp; Andrea, Yang; Jun, Siegel; Donald J., Veenstra; Michael Jon
5. Patent US 8,883,117: *Method of Enhancing Thermal Conductivity in Hydrogen Storage Systems*, Assigned 11/11/2014. Inventors: Yang; Jun, Siegel; Donald J., Pulskamp; Andrea, Drews; Andrew Robert, Hirano; Shinichi, Wolverton; Christopher Mark
6. Patent US 8,899,096: *High-throughput modular hydrogen storage engineering properties analyzer*, Assigned 12/2/2014. Inventors: Del Zio; Michael Robert, Yang; Jun, Pulskamp; Andrea, Hirano; Shinichi, Siegel; Donald J.
7. Patent US 8,968,942 *Metal oxygen battery containing oxygen storage materials*. Assigned 3/3/2015. Inventors: Pulskamp; Andrea, Drews; Andrew Robert, Siegel; Donald J., Blakemore; Bruce C., Brost; Ronald D., Yang; Jun, Hirano; Shinichi, Tamor; Michael A.
8. Patent US 9,960467B2: *Magnesium Oxygen Battery*. Assigned 5/1/2018. Inventors: Junichi Naruse, Donald Siegel, Jeffrey Smith, Gulin Vardar, and Charles Monroe. Published June 1<sup>st</sup>, 2017.
9. USPTO Application 12/233,246; Publication #US20100068134 A1: *Methods of Enhancing Kinetic Properties of Hydrogen Storage Materials by Self-Catalysis*, Published 3/18/2010
10. USPTO Application 61/097,999; Publication #US20100233076 A1: *Hydrogen Storage Materials*, Published 9/16/2010
11. USPTO Application 14/955,484; Publication #US2016285108A1: *Rechargeable Magnesium Oxygen Battery*, Filed 12/1/2015. Inventors: Junichi Naruse, Donald Siegel, Jeffrey Smith, Gulin Vardar, and Charles Monroe. Published September 29, 2016.



12. USPTO Application 14/955,618; *Magnesium Oxygen Battery*, Filed 12/1/2015. Inventors: Junichi Naruse and Donald Siegel.
13. USPTO Provisional Patent Application 623/738,385; *Systems And Methods For Improved Solid-State Electrolytes*, Filed 09/28/2018. Inventors: D.J. Siegel and K. Kim.
14. (Invention Disclosure) *Efficient Carbon Capture Materials*, UM Office of Tech Transfer file #5625. Siegel is lead inventor.
15. (Invention Disclosure) *Improved Performance in Rechargeable Metal-Air Batteries via Fermi-Level Tuning*, UM Office of Tech Transfer file #5597. Siegel is lead inventor.
16. (Invention Disclosure) *Materials for High-Density Natural Gas Storage*, UM Office of Tech Transfer file #6077. Siegel is lead inventor.
17. (Invention Disclosure) *Thermal Energy Storage Materials*, UM Office of Tech Transfer file #2018-364. Siegel is lead inventor.

**Grants and Contracts** (Siegel's share of total funds awarded: \$7,387,760)

1. National Science Foundation, "Planning Grant: Engineering Research Center for Comprehensive Energy Storage Solutions in Electrified Transportation (CESSET)," \$100,000, 9/1/18 – 8/31/19. Siegel is Co-PI; my share: ~\$8,000.
2. U.S. Department of Energy, "Joint Center for Energy Storage Research Renewal (JCESR 2.0)." Siegel is PI for UM's portion of the Center. \$120,000,000; UM's share: \$6,488,181; Siegel's share: \$1,980,757; 7/1/2018 – 6/30/23.
3. U.S. Army, Tank Automotive Research Development and Engineering Center, Automotive Research Center, "Computational Discovery of Materials for Energy Storage: High Throughput Screening and Machine Learning," ~\$440,000 total, \$145,403 for Y1. 5/1/2018 – 4/30/21. Siegel is PI; my share: \$440,000.
4. U.S. Department of Energy, "Optimized Hydrogen Adsorbents via Machine Learning and Crystal Engineering," \$1,110,828 total, \$250,000 Y1. 9/1/2017 – 8/31/2020. Siegel is PI; my share: \$450,000.
5. Advanced Research Projects Agency – Energy (ARPA-e), "Transitioning Advanced Ceramic Electrolyte into Solid-State EV Batteries," \$3,500,000. Project period 6/2016 – 6/2019. Siegel is Co-PI; my share: \$270,000.
6. U.S. Department of Energy/Savannah River National Laboratory, "Hydrogen Storage Engineering Center of Excellence (Extension)," \$17,534. 11/2/2015 – 12/31/2016. Siegel is PI.
7. U.S. Department of Energy, "Hydrogen Adsorbents with High Volumetric Density: New Materials and System Projections," \$1,040,000. 9/1/2015 – 8/31/2018. Siegel is PI; my share: \$350,000.
8. National Science Foundation, "MRI: Development of a Configuration for Real Time Coupling of Data and High-Performance Computing," \$2,422,972, 9/1/2015 – 8/31/2018. Siegel is Co-I.
9. Villum Foundation, Visiting Professor Fellowship, 400,000 Danish Kroner (~\$60,000), 8/1/2015 – 7/30/2016. Siegel is PI. Awarded to host institution, Danish Technical University (DTU).
10. Nordea Foundation, Residence Program, 390,300 DKK (~\$60,000), 8/1/2015 – 7/30/2016. Siegel is PI. Housing grant during sabbatical. Awarded to host institution, DTU.
11. U.S. Department of Energy, "Solid Electrolytes for Solid-State and Lithium-Sulfur Batteries," \$1,220,000. October 2014 – September 2017. Siegel is co-PI; my share: \$255,000.
12. Ford Motor Company, "Battery Safety: Modeling and Characterization of Li-ion Batteries," \$200,000, 5/1/14 – 4/30/2018. Siegel is PI.

13. National Science Foundation, Energy for Sustainability Program, "CAREER: First-Principles Modeling of Gas Evolution Reactions in Lithium Batteries," \$400,000, 6/1/14 – 5/31/19. Siegel is PI.
14. National Science Foundation, Energy for Sustainability Program, "GOALI: Experimentally Validated Multiscale Modeling of Li/O<sub>2</sub> Cathodes," \$399,735, 9/1/13 – 8/31/17. Siegel is co-PI; my share \$163,000.
15. U.S. Department of Energy, "Joint Center for Energy Storage Research," \$120,000,000, May 2012 – June 2018. Siegel is co-PI; my share: \$~820,000. Includes \$33,500 increment from Director's Fund awarded August 2014.
16. Lawrence Livermore National Lab, Grand Challenge Computing Grant of 170,000,000 CPU hours. Siegel is co-PI.
17. Denso Corporation, "Rechargeable Mg-air Batteries," \$604,404, Jan. 2013 – Jan 2016. Siegel is PI; my share: \$275,000.
18. U.S. China Clean Energy Research Center for Clean Vehicles (CERC-CV) and Sandia National Laboratories, "Li-ion Battery Aging and Internal Degradation Mechanisms," \$232,580, Jan. 2013 – Jan. 2015. Siegel is co-PI: my share \$232,580.
19. UM MCubed program, "Data-mining for Optimal Metal-Organic Frameworks," \$60,000, Jan. 2013 – June 2014. Siegel is PI: my share: \$20,000.
20. National Institutes of Standards and Technology, "Neutron Imaging of Prototype Hydrogen Storage Devices based on Adsorbent Media," Siegel is PI. 3 days of neutron imaging beam time in January 2013.
21. Robert Bosch Corporation, "Multi-scale Modeling of Li-Air Batteries," \$300,000, Dec. 2011 – Dec. 2013. Siegel is PI; my share: \$150,000.
22. Michigan Memorial Phoenix Energy Institute, "Cyber-Discovery of High Performance CO<sub>2</sub> Adsorbents," \$80,000, Sept. 2011 – Aug. 2013. Siegel is co-PI; my share: \$26,650.
23. U.S. Department of Energy, "CERC-CV: U.S.-China Clean Energy Research Center for Clean Vehicles," \$25,000,000, Oct. 2010 – April 2016. Siegel is co-PI; Siegel's share: \$400,000.
24. UM-SJTU Collaboration on Renewable Energy Science and Technology, "High-Capacity Li-Air Batteries for Electric Vehicle Applications," \$200,000, Sept. 2010 – Aug. 2013. Siegel is PI; my share: \$100,000.
25. Ford Motor Company & U.S. Department of Energy, "Hydrogen Storage Engineering Center of Excellence," \$754,300, Oct. 2009 – June 2015. Siegel is PI; my share: \$754,300.
26. U.S. Department of Energy, "Transportation Electrification Education Partnership for Green Jobs and Sustainable Mobility," \$2,500,000, Oct. 2009 – Sept. 2012. Siegel is co-PI; my share: \$15,000.

### **Invited Presentations**

1. Electrochemical Society (ECS) Fall Meeting, Symposium A07 "Solid State Batteries," October 13-17, 2019, Atlanta, GA.
2. XIX International Congress of the Mexican Hydrogen Society, Materials Institute Research (IIM) Morelia Unit, Mexican National Autonomous University, October 1-4, 2019, Morelia City, Michoacán, Mexico.
3. 2nd World Conference on Solid Electrolytes for Advanced Applications: Garnets and Competitors, September 24-27, 2019, Shizuoka, Japan.
4. Moscow State University – Skoltech 4<sup>th</sup> International Conference of Young Scientists,

- September 15-18, Moscow, Russia.
5. XXI Mendeleev Congress of General and Applied Chemistry, Symposium on “Elemental Materials for Electrochemical Energy,” September 9-13, 2019, St. Petersburg, Russia.
  6. American Chemical Society (ACS) Fall Meeting, Symposium on “Advances in Fundamental Research for Energy Storage Beyond Lithium Ion,” August 25-29, 2019, San Diego, CA.
  7. ECS ECEE 2019: Electrochemical Conference on Energy and the Environment: Bioelectrochemistry and Energy Storage, symposium on “Mass and Charge Transfer across Electrochemical Interfaces,” July 21-26, 2019, Glasgow, Scotland.
  8. ICE 2019: International Conference on Electroceramics, July 14-19, 2019, Lausanne, Switzerland.
  9. Gordon Research Conference on Hydrogen-Metal Systems, session on “Advancements in Porous Materials for Hydrogen Adsorption,” June 30-July 5, 2019, Barcelona, Spain.
  10. ‘NGenE’ Next Generation Electrochemistry Summer Institute, University of Illinois at Chicago, June 3-7, 2019, Chicago, IL.
  11. MRS 2019 Spring Meeting, Symposium S-19 ES04 “Solid-State Electrochemical Energy Storage,” April 22-26, 2019, Phoenix, AZ.
  12. Argonne National Laboratory, Materials Science Division Colloquium, April 4, 2019, Argonne, IL.
  13. American Chemical Society (ACS) 257<sup>th</sup> National Meeting, symposium on “Innovative Chemistry and Materials for Electrochemical Energy Storage,” March 31-April 4, 2019, Orlando, FL.
  14. TMS 2019 Annual Meeting, 5<sup>th</sup> Symposium on Advanced Materials for Energy Conversion and Storage, March 10-14, 2019, San Antonio, TX.
  15. Korea Institute of Science and Technology, Center for Energy Storage Research, February 20, 2019, Seoul, South Korea.
  16. Seoul National University, School of Chemical and Biological Engineering, February 19, 2019, Seoul, South Korea.
  17. Korea Advanced Institute of Science & Technology (KAIST), Department of Chemistry – School of Molecular Science, BK21 Lectureship, February 18, 2019, Daejeon, South Korea.
  18. University of Illinois at Urbana-Champaign, Materials Science and Engineering Department Colloquium, November 12, 2018, Urbana, IL.
  19. 3<sup>rd</sup> National Conference on Materials for Energy Conversion and Storage, October 18-20, 2018, IIT-BHU, Varanasi, India
  20. 2<sup>nd</sup> Bosch Energy Research Network (BERN) Symposium on Innovative Energy Research, September 6-7, 2018, Sunnyvale, CA.
  21. Electrochemical Society (ECS) Fall Meeting, “12<sup>th</sup> Solid State Ionic Devices (SSID 12) Symposium,” September 30 - October 4, 2018, Cancun, Mexico.
  22. Electrochemical Society (ECS) Fall Meeting, symposium on “Batteries and Energy Storage,” September 30 - October 4, 2018, Cancun, Mexico.
  23. American Chemical Society’s 256<sup>th</sup> National Meeting, symposium on “Electrochemical Interfaces,” August 19-23, 2018, Boston, MA.
  24. American Chemical Society’s 256<sup>th</sup> National Meeting, symposium on “Nanoscience of Energy Storage,” August 19-23, 2018, Boston, MA.
  25. 3<sup>rd</sup> Li-SM<sup>3</sup> Conference: Lithium-Sulfur Batteries: Mechanisms, Modelling and Materials, April

- 25-26, 2018, Chicago, IL.
26. TMS 2018 Spring Meeting, Symposium on “Materials for Energy Conversion and Storage,” March 11-15, 2018, Phoenix, AZ.
  27. Northwestern University, Materials Science and Engineering Department Seminar, September 26, 2017. Evanston, IL.
  28. Indian Institute of Science Education and Research (IISER-BPR), September 4, 2017, Berhampur, India.
  29. 1<sup>st</sup> World Congress on Lithium Garnets, Competitors and Beyond for Advanced Batteries, September 6-9, 2017, Puducherry, India.
  30. Telluride Science Research Center, Computational Materials Chemistry Workshop, August 7-11, 2017, Telluride, CO.
  31. Bosch Energy Research Network Symposium on Innovative Energy Research, July 27-28, 2017, Palo Alto, CA.
  32. Waterloo Institute for Nanotechnology, University of Waterloo, May 8, 2017, Waterloo, ON, Canada.
  33. MRS 2017 Spring Meeting, Symposium on “Mechanics of Energy Storage and Conversion,” April 17-21, 2017, Phoenix, AZ.
  34. TMS 2017 Annual Meeting & Exhibition, Symposium on “Advanced Materials for Energy Conversion and Storage,” February 26 – March 2, San Diego, CA.
  35. TMS 2017 Annual Meeting & Exhibition, Symposium on “Computational Materials Discovery and Optimization – From Bulk to Materials Interfaces and 2D Materials,” February 26 – March 2, San Diego, CA.
  36. XXV International Materials Research Congress (IMRC), August 14-19, 2016. Cancun, Mexico.
  37. Danish Battery Society Annual Symposium, April 7<sup>th</sup>, 2016. Copenhagen, Denmark.
  38. Technical University of Denmark (DTU), Department of Energy Conversion and Storage Department Colloquium, February 1<sup>st</sup>, 2016, Lyngby, Denmark.
  39. University of Florida Material Science/Mechanical & Aerospace Engineering Seminar, December 7<sup>th</sup>, 2015, Gainesville, FL.
  40. Nordic Battery Conference (NORDBATT2), December 2-3, 2015, Trondheim, Norway.
  41. Lithium Battery Power 2015, November 17-19, 2015, Baltimore, MD.
  42. Electrochemical Society (ECS) Fall Meeting, October 11-16, 2015, Phoenix, AZ.
  43. NSF workshop on “Rise of Data in Materials Research,” June 29-30, 2015, College Park, MD.
  44. Telluride Science Research Center, Computational Materials Chemistry Workshop, June 23-27, 2015, Telluride, CO.
  45. American Ceramic Society – 11<sup>th</sup> International Conference on Ceramic Materials and Components for Energy and Environmental Applications (CMCEE), June 14-19, 2015, Vancouver, British Columbia, Canada.
  46. American Chemical Society National Meeting, symposium on “Natural Resource Capture, Storage and Energy Conversion,” March 22-26, 2015, Denver, CO.
  47. American Chemical Society National Meeting, symposium on “2D Materials for Energy and Fuel,” March 22-26, 2015, Denver, CO.
  48. U.S. Department of Energy Hydrogen Storage Workshop, January 27-29, 2015, National Renewable Energy Laboratory, Golden, CO.

49. University of Michigan Transportation Research Institute (UMTRI), Automotive Futures Conference: *Inside China: Understanding China's Current and Future Automotive Industry*, November 12, 2014, Ann Arbor, MI.
50. The Battery Show, September 16-18, 2014, Novi, MI.
51. U.S.-China Electric Vehicle and Battery Technology Workshop, August 18-19, 2014, Seattle, WA.
52. Telluride Science Research Center, Battery Materials Workshop, July 14-18, 2014, Telluride, CO.
53. 1<sup>st</sup> International Symposium on Sustainable Secondary Battery Manufacturing and Recycling, June 29-July 4, 2014, Cancun, Mexico
54. U.S. Nat. Congress on Theoretical and Applied Mechanics, June 15-20, 2014, East Lansing, MI
55. SIT Investment Associates' Annual Client Workshop, Feb. 13-16, 2014, Carlsbad, CA
56. Gilbreth Lecture: NAE National Meeting, Feb. 6, 2015, Irvine, CA
57. American Ceramic Society -- Electronic Materials & Applications Conference, January 22-24, 2014, Orlando, FL.
58. 8th U.S.-China Electric Vehicle and Battery Technology Workshop, September 20-22, 2013, Chengdu, China.
59. The Battery Show, September 17-19, 2013 Novi, Michigan.
60. 2nd ReLiable Li-Air Workshop, September 9-10, 2013 Copenhagen, Denmark
61. Denso Research Laboratories, August 23, 2013, Nisshin, Japan.
62. RIKEN Advanced Science Institute, August 22, 2013, Wako, Japan.
63. American Chemical Society National Meeting, "Chemical Mechanisms in Advanced Materials," September 8-12, 2013, Indianapolis.
64. Beyond Lithium Ion VI Conference, June 4-6, 2013, Boulder, Colorado.
65. U.S. National Academy of Sciences Indo-American Frontiers of Science Symposium, April 7-10, 2013, Agra, India.
66. Detroit Section of the Electrochemical Society, February 20, 2013, Southfield, MI.
67. U.S. Dept. of Energy, Adsorbent Hydrogen Storage Workshop, Nov. 27, 2012, Washington, D.C.
68. Denso International America Inc., Research and Engineering Division, June 29, 2012, Southfield, MI.
69. WHEC 2012, World Hydrogen Energy Conference, June 3-7, 2012, Toronto, Canada.
70. 5th US-China Electric Vehicle and Battery Technology Workshop, April 16-17, 2012, Hangzhou, China.
71. U.S. National Academy of Engineering-Alexander von Humboldt German-American Frontiers of Engineering Symposium, March 28-31, 2012, Potsdam, Germany.
72. American Chemical Society National Meeting, "Integrating Theory and Experiment for Discovering the Fundamental Chemistry of the Li-air and Other Metal-air Battery Systems," March 25-29, 2012, San Diego.
73. TMS 2012 Annual Meeting, "Solid-State Interfaces II: Toward an Atomic-Scale Understanding of Structure, Properties, and Behavior Through Theory and Experiment," March 11-15, 2012, Orlando.

74. Electronic Materials & Applications Conference, symposium on “Energy Storage Materials and Systems,” Jan. 18-20, 2012, Orlando.
75. 4th US-China Electric Vehicle and Battery Technology Workshop, August 4-5, 2011, Argonne, IL.
76. Frontiers of Energy Materials Workshop, Penn State, May 18, 2011.
77. General Motors R&D Center, Warren, MI, Aug. 10, 2011.
78. MS&T 2011, “7th Annual Symposium on Phase Stability, Diffusion, Kinetics, and Their Applications (PSDK),” October 2011, Columbus.
79. TMS 2011 Annual Meeting, 10th Symposium on “Computational Thermodynamics and Kinetics of Materials,” March 2011, San Diego
80. Chemistry Department Seminar, University of Detroit Mercy, Nov. 9, 2010.
81. MRS 2010 Spring Meeting, Symposium Y: “Computational Approaches to Materials for Energy,” April 2010, San Francisco
82. School of Mechanical, Aerospace, Chemical, and Materials Engineering, Arizona State University, Nov. 13, 2009, Tempe, AZ
83. Physics Department Colloquium, Case Western Reserve University, Oct. 1, 2009, Cleveland, OH.
84. XVIII International Materials Research Congress 2009, August 16-21, Cancun, Mexico.
85. NIST Workshop on Atomistic Simulations for Industrial Needs, April 27-28, 2009, Gaithersburg, MD.
86. Japan Institute of Metals 2009 Spring Meeting, Session S1: “Hydrogen Storage Materials,” March 28-30, Tokyo, Japan.
87. APS 2009 March Meeting, Invited Session: “Computational Design of Hydrogen Storage Materials,” March 16-20, Pittsburgh, PA.
88. Chemical Engineering and Materials Science Dept. Colloquium, Michigan State University, March 5, 2009, East Lansing, MI.
89. MRS 2009 Spring Meeting “Symposium HH: Quantitative Characterization of Nanostructured Materials,” April 13-17, San Francisco, CA.
90. MS&T’08 Conference “Discovery and Optimization of Materials through Computational Design,” October 5-9, Pittsburgh, PA.
91. NIST Workshop “Atomistic Simulations for Industrial Needs,” April 28-29, 2008, Gaithersburg, MD.
92. MRS 2008 Spring Meeting “DOE Theory Focus Session on Hydrogen Storage Materials,” March 24, San Francisco.
93. TMS Annual Meeting: “Career Forum,” March 2008, New Orleans.
94. University of Michigan, Guest Lecture for MSE 250, Materials for Energy, Nov. 2007.
95. Erwin Schrodinger Institute–University of Vienna, Theory Meets Industry Workshop, 12 June 2007
96. University of Michigan, Materials Science and Engineering Colloquium, 2 February 2007
97. Lawrence Livermore National Laboratory, Metals and Alloys Group, 14 April 2005

98. University of Texas at El Paso, Department of Physics Colloquium, 6 April 2005
99. Ford Research Laboratory, Physical and Environmental Sciences Department, 4 April 2005
100. Pacific Northwest National Laboratory, Energy Science and Technology Directorate, Jan. 2005
101. University of Tennessee, Department of Materials Science and Engineering, October 2004
102. Oak Ridge National Laboratory, Joint Institute for Computational Sciences, October 2004
103. CECAM Workshop on Oxide-Metal Interfaces: Progress and Challenges, October 2001, Lyon, France
104. Advances in Surface Engineering—Fundamentals and Applications, Materials Research Society Meeting, November 2001, Boston, MA
105. NIST Workshop on Modeling and Simulation of Structure Formation in Liquid Crystals, Polymers, and their Mixtures, June 1995, Gaithersburg, MD

**Ph.D. Committees Chaired/Co-chaired (with graduation/expected graduation date)**

1. Maxwell Radin (Physics), September 2014, “First-principles and Continuum Modeling of Charge Transport in Li-O<sub>2</sub> Batteries.” Chair.
2. Hyun Seung Koh (Mech. Eng), September 2014, “Computational Discovery of Metal-Organic Frameworks for Carbon Capture and Natural Gas Storage.” Chair.
3. Yang Ming (Physics), August 2015 “Robustness and Thermophysical Properties of MOF-5: A Prototypical Hydrogen Storage Material.” Chair.
4. Gulin Vardar (Mat. Sci.), February 2016, “Rechargeable Magnesium/Oxygen Batteries: Reaction Mechanisms and Their Dependence on Electrolyte Composition.” Co-chair
5. Sheng Yang (Physics), October 2, 2017, “Modeling of Metal-air batteries.” Chair.
6. Jeffrey Smith (Mech. Eng.), September 4, 2018, “First Principles Study of Magnesium/Oxygen Batteries and Glassy Solid Electrolytes.” Chair
7. Seungho Yu (Mech. Eng.), September 10, 2018. “Atomic Scale Simulations of the Solid Electrolyte Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub>.” Chair
8. Haesun Park (Mech. Eng.), December 2018. Chair
9. Jeff Lowe (Chem. Eng.), December 2018. Chair
10. Kyle Nagy (Mech. Eng.), September 2019. Chair
11. Mallory Fuhst (Applied Physics), September 2019. Chair
12. Kwangnam Kim (Mech. Eng.), September 2020. Chair
13. Everardo Olide (Applied Physics), September 2021. Chair
14. Steven Kiyabu (Mechanical Engineering), September 2022. Chair.

**Postdoctoral Researchers Advised/Co-advised**

1. Dr. Justin Purewal (April 2010 – April 2012)
2. Dr. Malay Rana Kumar (May 2011 – present)
3. Dr. Feng Tian (April 2011 – August 2013)
4. Dr. Jacob Goldsmith, co-advised with A. Wong-Foy (Chemistry) and M. Cafarella (CSE) (September 2011 – May 2013)
5. Dr. Nitin Kumar, co-advised with Dr. Kevin Leung, Sandia National Labs (Jan. 2013 – Dec. 2017)

6. Dr. Ram Balachandran (June 2014 – January 2015)
7. Dr. Alauddin Ahmed (September 2015 – present)

### **M.S. Students Advised/Co-advised**

1. Hyun Seung Koh, 2011, Mechanical Engineering. Thesis project: Modeling of Carbon Capture Materials. Currently continuing in my group as a Ph.D. student.
2. Hee Jin Bang, 2012, Energy Systems Engineering. Thesis project: Atomistic Modeling of the solid Li-ion conductor LLZO.
3. Ke Pan, 2012, Mechanical Engineering. Thesis project: Gas capture in nano-confined liquids.
4. Samantha Sunny, 2012-2013, Mechanical Engineering. Thesis project: Solvent decomposition in Li-ion Batteries.
5. Jinhyung Hwang, 2012-2013, Mechanical Engineering. Thesis project: Design and Testing of a Multi-User Metal-Air Battery Test Stand.
6. Haesun Park, 2013-2015, Mechanical Engineering. Thesis project: Modeling Li-S Batteries.

### **Undergraduate Research Projects Directed**

1. UROP: Modeling of Lithium oxide surfaces, Jill Rodriguez, 5/2010 – 4/2011
2. SURE: Modeling of Metal Organic Frameworks for CO<sub>2</sub> Capture, Jinhyung Hwang, 5/2010 – 4/2011.
3. SURE: Modeling Hydrogen Spillover in MOF-5: Chencheng Zhou, 5/2011 – 8/2011.
4. SURE: Methane Capture in M-DOBDC: Haroon Zuberi, 5/2012 – 8/2012.
5. UROP: Gas Capture in Nano-confined Liquids: Brian Tong, 9/2012 – 4/2013.
6. SROP: Thermodynamics and Structure of Mg Anode Surfaces, Kyle Nagy, 6/2013 – 8/2013.
7. UROP: MD Simulations of Heat Transfer in MOF-74: Devon Samuel, 9/2013 – 8/2014.
8. SURE: Simulations of Mg Electrolytes: Aaron Kaufmann, 9/2013-8/2014.
9. MI-LSAMP: Functionalized Metal Organic Frameworks, Fernando Pichardo, 6/2014 – 8/2014.
10. UROP: Development of a Web-Based Crystal Structure Database for Metal-Organic Frameworks: Carl Steinhäuser, 9/2014-8/2015.
11. SURE: Materials for Thermal Energy Storage, Steven Kiyabu, 5/2015 – 8/2017
12. UROP: Atomistic Simulation of Metal-Organic Frameworks, Alan Fong, 9/2016 – 8/2017
13. SURE: Atomistic Simulation of Materials for Energy Storage, Abby Chapin, 6/2018 – present
14. SURE: Atomistic Simulation of Materials for Energy Storage, Jackson Teener, 5/2018 – present
15. SURE: Atomistic Simulation of Materials for Energy Storage, Justin Stobart, 5/2018 – present

### **Visiting Scholars**

1. Junichi Naruse, Denso Corporation, 11/2013 – 5/2015

### **Service to Government and Professional Organizations**

1. *Elected Office*: Member of the Executive Committee: American Physical Society (APS) Group on Energy Research and Applications (GERA), 2012-2015. Member of the Executive Committee: APS Forum on Industrial & Applied Physics (FIAP), 2010-2013
2. *Symposium Organizer*: 2<sup>nd</sup> World Conference on Solid Electrolytes for Advanced Applications: Garnets and Competitors, September 24-27, 2019, Shizuoka, Japan; Telluride Science Research



Center: “Interfacial Chemistry and Charge Transfer for Energy Storage and Conversion,” July 23-27, 2018, Telluride, CO; Telluride Science Research Center: “Interfacial Chemistry and Charge Transfer for Energy Storage and Conversion,” July 25-29, 2016, Telluride, CO; APS April Meeting Invited Session: “Low Carbon Transportation,” April 2013, Denver, CO; “Battery Congress,” April 11-12, 2011 Michigan League, Ann Arbor, MI; 2011 APS March Meeting Focus Topic Session: “Physics of Energy Storage Materials;” APS 2010 March Meeting Focus Topic session “Hydrogen Storage: Materials, Measurements, & Modeling,” Portland, OR; “High-Density Hydrogen Storage for Automotive Applications: Materials and Methods,” MS&T’07, September 2007, Detroit, MI; “New Insights on Solid-Solid Interfaces from Combined Observation and Modeling,” Materials Research Society Fall Meeting, Boston, MA 2005.

3. *Review Panelist:* U.S. DOE Hydrogen Program and Vehicle Technologies Program Annual Merit Review, 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017; NSF Division of Chemical, Bioengineering, Environmental, and Transport Systems (CBET), 2014, 2015, 2016, 2017; Swiss National Science Foundation, 2014; U.S. DOE Office of Science, Basic Energy Sciences, 2012; U.S. DOE Office of Technology Transitions, Technology Commercialization Fund, 2017.
4. *Invited Panelist and Writer:* U.S. Department of Energy 2017 Report, *Basic Research Needs for Electrical Energy Storage*.
5. *Industry/Gov’t Technical Panels:* Affiliate Member, U.S. DRIVE Hydrogen Storage Technical Team, 2012 – present. Member and co-Chair, DOE FreedomCAR Hydrogen Storage Technical Team, 2007-2009. Ad hoc Member of the Directorate, Joint Center for Energy Storage Research (JCESR), 2015 – present.
6. *Faculty Advisor:* UM Society of Automotive Engineers Student Chapter, 2010 – present
7. *Invited participant:* ARPA-E Electrical Energy Storage for Vehicles Workshop, Nov. 2009, Arlington, VA. NIST workshop on “Measurements Needs for Local Structure Determination in Inorganic Materials,” February 2008, Gaithersberg, MD.
8. *Reviewer:* Science, Nature Materials, Nature Chemistry, Nature Energy, Nature Communications, Journal of Physical Chemistry C, Journal of Chemical Physics, Physical Review Letters, Acta Materialia, Physical Review B, Journal of Physics: Condensed Matter, Surface and Interface Analysis, CALPHAD, SAE Transactions, Journal of Physical Chemistry Letters, Physical Chemistry Chemical Physics, Langmuir, ACS Combinatorial Science, International Journal of Hydrogen Energy, Journal of the American Chemical Society, Nano Letters, Journal of the Electrochemical Society, Journal of Applied Physics, Modeling in Materials Science and Engineering, Journal of Materials Science, Energy & Environmental Science, International Journal of Heat and Mass Transfer, Journal of Materials Chemistry A, Scripta Materialia, Crystal Growth & Design, ACS Applied Materials & Interfaces, Chemistry of Materials, Microporous and Mesoporous Materials, Advanced Functional Materials, Journal of the American Ceramic Society, ChemElectroChem, ChemSusChem, ACS Catalysis, ACS Energy Letters, Journal of Power Sources, npj Computational Materials, Journal of Chemical Theory and Computation, Joule

### Courses Taught at UM

Course #	Course title	Role	Term	Enrollment
ME 235	Thermodynamics I	Sole Instructor	F 18	90
ME 433/533	Advanced Energy Solutions	Sole Instructor	W 18	53
ME 235	Thermodynamics I	Sole Instructor	F 17	62

ME 507	Atomistic Computer Modeling of Materials	Sole Instructor	W 17	19
ME 235	Thermodynamics I	Sole Instructor	F 16	60
	Sabbatical leave		W 16	
	Sabbatical leave		F15	
ME 235	Thermodynamics I	Sole Instructor	W 15	91
ME 499/599-001	Atomistic Computer Modeling of Materials	Sole Instructor	F 14	18
ME 235	Thermodynamics I	Sole Instructor	W 14	88
ME 499/599-001	Atomistic Computer Modeling of Materials	Sole instructor	F 13	12
ME 235	Thermodynamics I	Sole instructor	W 13	93
ME 499/599-001	Atomistic Computer Modeling of Materials	Sole instructor	F 12	19
ME 499/599-007	Atomistic Computer Modeling of Materials	Sole instructor	W 12	35
ME 235	Thermodynamics I	Sole instructor	F 11	118
ME 499/599-001	Vehicle Electrification: Hydrogen and Fuel Cells	Co-Instructor	F 11	27
Modified Duties (paternity leave) – did not teach			W 11	
ME 235	Thermodynamics I	Sole instructor	F 10	73
ME 499/599-007	Vehicle Electrification: Hydrogen and Fuel Cells	Co-Instructor	W 10	43
ME 599-004	Atomistic Computer Modeling of Materials	Sole instructor	F 09	18

### New Courses Introduced at UM

1. **MECHENG 499/599: Vehicle Electrification: Hydrogen and Fuel Cells.** Co-developed with A. Stefanopoulou. This course covers essential aspects of fuel cell vehicle technology, hydrogen fueling infrastructure, storage, and potential benefits & barriers to the use of hydrogen as a vehicular fuel. Emphasis is placed upon system-level modeling and control issues of polymer electrolyte membrane fuel cells and on the principles and design of on-board hydrogen storage systems. Hydrogen generation and distribution technologies are introduced, and life-cycle (well-to-wheels) analyses of petroleum consumption, efficiency, and CO<sub>2</sub> reduction are presented. Lectures are supplemented with fuel cell vehicle demonstrations conducted by local automotive OEMs, and with site visits to hydrogen fueling stations. Requires a basic background in signals and systems or controls (Laplace transforms, time/frequency analysis and control design tools), and basic chemistry and thermodynamics of materials. Mathworks/Matlab will be used. This course was developed under the sponsorship of the U.S. Department of Energy, award no. DE-EE0002119: *Transportation Electrification Education Partnership for Green Jobs and Sustainable Mobility*
2. **MECHENG 507: Atomistic Computer Modeling of Materials. (Cross-listed in MSE)** Computational hardware and algorithms have evolved to the point where they can strongly complement traditional, experiment-based approaches to materials research and development. This course covers the core methods used to simulate matter at the atomic scale, and offers hands-on experience with a number of research-caliber simulation codes on multi-processor clusters. The course provides a *broad-based* and *practical* introduction to atomistic methods, and is meant to serve as a launching-point for students looking to begin independent research in this field. Topics covered include: (i.) Structure of matter and interatomic potentials; (ii.) High-performance

computing; (iii.) Electronic structure methods (Hartree-Fock & Density Functional Theory); (iv.) Molecular dynamics; (v.) Monte Carlo methods; (vi.) Transition state theory; (vii.) Accelerated dynamics and multi-scale modeling. Several applications of the methods are highlighted, ranging from the mechanical properties of solids to the discovery of new materials for energy storage.

### **Short Courses and Outreach Activities**

1. Developed Industry “InterPRO” short-course “Introduction to Electrical Energy Storage” for the UM Certificate in Emerging Automotive Technologies (CEAT). Course has been completed by students from industry (including General Motors) and is offered continuously as a distance learning class.
2. Lecturer at “Vehicle Electrification Boot-Camp” during summers of 2010 and 2011. This is a weeklong program for high school students that introduces them to electric vehicle technologies. Sponsored by a grant from the U.S. Dept. of Energy.
3. Developed a series of 9 YouTube videos for lay audiences on “Batteries of the Future.” These videos have been viewed approximately 250,000 times as of January 2018.  
<http://goo.gl/L1VV0>
4. Co-Developer of UM Women in Science and Engineering – Girls in Science and Engineering (WISE-GISE) Summer Camp module on Energy Storage. This program has been offered during summer 2015, 2016, 2017, and 2018.