# Donald J. Siegel


Walker Department of Mechanical Engineering
Texas Materials Institute
Oden Institute for Computational Engin. & Sciences
University of Texas at Austin

204 E. Dean Keeton St.; ETC II 5.160
Austin, TX 78712-1591; 512-471-0796
Donald.Siegel@austin.utexas.edu
http://umich.edu/~djsiege


**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; machine learning; Integrated Computational Materials Engineering.

## Education and Training

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|---|---|---|---|
| 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

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|---|---|
| 2021 – present | Professor and Department Chair, Walker Department Mechanical Engineering, Cockrell School of Engineering, University of Texas at Austin |
| 2021 – present | Core Member, Oden Institute for Computational Engineering and Sciences, University of Texas at Austin |
| 2021 – present | Core Member, Texas Materials Institute, University of Texas at Austin |
| 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 |
| 2019 – 2021 | Professor, Mechanical Engineering, Materials Science & Engineering, and Applied Physics Program, University of Michigan |
| 2018 – 2021 | Associate Chair for Graduate Education, Department of Mechanical Engineering, University of Michigan |
| 2010 – 2021 | Member, Michigan Institute for Computational Science & Engineering (MICDE) |
| 2009 – 2021 | Faculty Fellow, University of Michigan Energy Institute |
| 2015 – 2019 | Associate Professor, Mechanical Engineering, Materials Science & Engineering, and Applied Physics Program, University of Michigan |
| 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 |

## Honors, Awards, and Notoriety

Temple Foundation Endowed Professorship #4, Univ. of Texas at Austin (2021)
Cockrell Family Chair for Departmental Leadership #4, UT Austin (2021)
E. & M. Ulsoy Citation Leader Award, UM Mechanical Engineering Department (2021)
Preview article by Glasby and Moghadam, *Hydrogen storage in MOFs: Machine learning for finding a needle in a haystack* (10.1016/j.patter.2021.100305), highlights our publication in *Patterns* (10.1016/j.patter.2021.100291)
Listed among the top 1% of global scientists in the field of materials research (Ioannidis et al., *Updated Science-Wide Author Databases of Standardized Citation Indicators, PLoS Biology* **18**, e3000918. DOI:10.1371/journal.pbio.3000918 )
Editors' Highlight: *Nature Communications*, **11,** 1483 (2020)

Ted Kennedy Family Faculty Team Excellence Award, UM College of Engineering (2020)
Editors' Highlight: *Nature Communications*, **10,** 1568 (2019)
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 Mater*
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: ~9,500 citations, h-index = 53. ORCID: 0000-0001-7913-2513)

1. K. Kim and D. J. Siegel, *Machine Learning Reveals Factors that Control Ion Mobility in Anti-perovskite Solid Electrolytes*, Journal of Materials Chemistry A, Accepted Manuscript (2022). DOI: 10.1039/d2ta03613d
2. K. Nath, A. Ahmed, D. J. Siegel and A. J. Matzger, *Computational Identification and Experimental Demonstration of High-Performance Methane Sorbents*, Angewandte Chemie International Edition, e202203575, (2022). DOI:10.1002/anie.202203575

3. J. G. Smith and D. J. Siegel, *Ion Migration Mechanisms in the Sodium Sulfide Solid Electrolyte* $Na_{3-x}Sb_{1-x}W_xS_4$, Chemistry of Materials, **34**, 4166-4171 (2022). DOI:10.1021/acs.chemmater.2c00526
4. K. Kim, Y. Li, P.-C. Tsai, F. Wang, S.-B. Son, Y.-M. Chiang, D. J. Siegel, *Exploring the Synthesis of Alkali-metal Anti-perovskites*, Chemistry of Materials, **34**, 947–958 (2022). DOI:10.1021/acs.chemmater.1c02150
5. S. Yu and D. J. Siegel, *Atomic-Scale Simulations of the Solid Electrolyte* $Li_7La_3Zr_2O_{12}$, Chapter 15 in *Transition Metal Oxides for Electrochemical Energy Storage,* 1st Ed. J. Nanda and V. Augustyn, Editors, 375-391, (2022) WILEY-VCH GmbH. DOI: 10.1002/9783527817252.ch15
6. J. Cabana, T. Alaan, G. W. Crabtree, M. C. Hatzell, K. Manthiram, D. A. Steingart, I. Zenyuk, F. Jiao, A. Vojvodic, J. Y. Yang, N. P. Balsara, K. A. Persson, D. J. Siegel, C. L. Haynes, J. Mauzeroll, M. Shen, B. J. Venton, N. Balke, J. Rodríguez-López, D. R. Rolison, R. Shahbazian-Yassar, V. Srinivasan, S. Chaudhuri, A. Couet, and J. Hattrick-Simpers, *NGenE 2021: Electrochemistry Is Everywhere,* ACS Energy Letters, **7**, 368–374 (2022). DOI:10.1021/acsenergylett.1c02608
7. S. Kuthuru, D. Aulakh, J. Purewal, D. J. Siegel, M. Veenstra, and A. J. Matzger, *Optimizing Hydrogen Storage in MOFs through Engineering of Crystal Morphology and Control of Crystal Size,* Journal of the American Chemical Society, **143**, 10727-10734 (2021). DOI:10.1021/jacs.1c04926
8. D. J. Siegel, L. Nazar, Y.-M. Chiang, C. Fang, and N. P. Balsara, *Establishing a Unified Framework for Ion Solvation and Transport in Liquid and Solid Electrolytes,* Trends in Chemistry, **3**, 807-818 (2021). DOI: 10.1016/j.trechm.2021.06.004
9. A. Ahmed and D. J. Siegel, *Predicting Hydrogen Storage in MOFs via Machine Learning*, Patterns, **2**, 100291 (2021). DOI: 10.1016/j.patter.2021.100291
10. K. Kim and D. J. Siegel, *Multivalent Ion Transport in Anti-Perovskite Solid Electrolytes,* Chemistry of Materials, **33**, 2187–2197 (2021). DOI: 10.1021/acs.chemmater.1c00096
11. H. Park, S. Yu, and D. J. Siegel, *Predicting Charge Transfer Stability Between Sulfide Solid Electrolytes and Li Metal Anodes*, ACS Energy Letters, **6**, 150-157 (2020). DOI:10.1021/acsenergylett.0c02372
12. M. R. Fuhst and D. J. Siegel, *Gas Evolution in Li-ion Batteries: Modeling Ethylene Carbonate Decomposition on* $LiCoO_2$ *in the Presence of Surface Magnetism*, Journal of Physical Chemistry C, **124,** 24097-24104 (2020). DOI:10.1021/acs.jpcc.0c07550 (2020).
13. J. Lowe and D. J. Siegel, *Modeling the Interface Between Lithium Metal and its Native Oxide*, ACS Applied Materials & Interfaces, **12,** 46015-46026 (2020) DOI: 10.1021/acsami.0c12468
14. F. Wang, H. A. Evans, K. Kim, L. Yin, Y. Li, P.-C. Tsai, J. Liu, S. H. Lapidus, C. M. Brown, D. J. Siegel, and Y.-M. Chiang, *Dynamics of Hydroxyl Anions Promotes Lithium Ion Conduction in Anti-perovskite* $Li_2OHCl$, Chemistry of Materials, **32,** 8481-8491 (2020), DOI: 10.1021/acs.chemmater.0c02602
15. L. Yin, M. Murphy, K. Kim, L. Hu, J. Cabana, D. J. Siegel, and S. H. Lapidus, *Synthesis of Antiperovskite Solid Electrolytes: Comparing* $Li_3SI$, $Na_3SI$, *and* $Ag_3SI$, Inorganic Chemistry, **59**, 11244–11247 (2020), DOI: 10.1021/acs.inorgchem.0c01705
16. K.S. Nagy and D. J. Siegel, *Anisotropic Elastic Properties of Battery Anodes*, Journal of the Electrochemical Society, **167**, 110550 (2020), DOI: 10.1149/1945-7111/aba54c
17. L. Trahey, F. R. Brushett, N. P. Balsara, G. Ceder, L. Cheng, Y.-M. Chiang, N. T. Hahn, B. J. Ingram, S.D. Minteer, J.S. Moore, K.T. Mueller, L.F. Nazar, K.A. Persson, D.J. Siegel, K. Xu, K. R. Zavadil, V. Srinivasan, G. W. Crabtree, *Energy storage emerging: A perspective from the*

*Joint Center for Energy Storage Research,* Proceedings of the National Academy of Sciences, **117**, 12550-12557 (2020), DOI: 10.1073/pnas.1821672117

18. J. G. Smith and D. J. Siegel, *Low-Temperature Paddlewheel Effect in Glassy Solid Electrolytes*, Nature Communications, **11**, 1483 (2020), DOI: 10.1038/s41467-020-15245-5
19. R. Garcia-Mendez, J. G. Smith, J. C. Neuefeind, D. J. Siegel and J. Sakamoto, *Correlating Macro and Atomic Structure with Elastic Properties and Ionic Transport of Glassy $Li_2S$-$P_2S_5$ (LPS) Solid Electrolyte for solid-State Li Metal Batteries,* Advanced Energy Materials 2000335, (2020). DOI: 10.1002/aenm.202000335
20. N. R. Mathiesen, S. Yang, J. M. García-Lastra, T. Vegge, and D. J. Siegel, *Charge Transport in Alkali-Metal Superoxides: A Systematic First-Principles Study*, Chemistry of Materials, **31**, 9156-9167 (2019), DOI: 10.1021/acs.chemmater.9b03592
21. K. Kim and D. J. Siegel, *Predicting Wettability and the Electrochemical Window of Lithium Metal/Solid Electrolyte Interfaces*, ACS Applied Materials & Interfaces, **11**, 39940-39950 (2019), DOI: 10.1021/acsami.9b13311
22. S. Yu, H. Park, and D. J. Siegel, *Thermodynamic Assessment of Coating Materials for Solid-State Li, Na, and K Batteries,* ACS Applied Materials & Interfaces, **11**, 36607-36615 (2019), DOI: 10.1021/acsami.9b11001
23. J. Purewal, M. Veenstra, D. Tamburello, A. Ahmed, A. J. Matzger, A. G. Wong-Foy, S. Seth, Y. Liu, D. J. Siegel, *Estimation of System-Level Hydrogen Storage for Metal-Organic Frameworks with High Volumetric Storage Density,* International Journal of Hydrogen Energy, 44, 15135-15145 (2019). DOI: 10.1016/j.ijhydene.2019.04.082
24. 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
25. 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
26. 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
27. 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
28. 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
29. 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
30. 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
31. 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

32. 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
33. 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.**
34. 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
35. 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
36. 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
37. S. Yu and D. J. Siegel, *Grain Boundary Contributions to Li-ion Transport in the Solid Electrolyte $Li_7La_3Zr_2O_{12}$ (LLZO)*, Chemistry of Materials, **29**, 9636-9647 (2017). DOI: 10.1021/acs.chemmater.7b02805
38. 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
39. 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
40. 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 $Li_7La_3Zr_2O_{12}$*, Chemistry of Materials, **29**, 7961-7968 (2017). DOI: 10.1021/acs.chemmater.7b03002 **Designated an *ACS Most Read Article* for September 2017.**
41. 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
42. 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-$Li_7La_3Zr_2O_{12}$ Interfacial Resistance*, Journal of Materials Chemistry A, **5,** 13475-13487 (2017). DOI:10.1039/c7ta03162a
43. H. Park and D. J. Siegel, *Tuning the Adsorption of Polysulfides in Lithum-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.**
44. J. G. Smith, J. Naruse, H. Hiramatsu, and D. J. Siegel, *Intrinsic Conductivity in Magnesium-Oxygen Battery Discharge Products: MgO and $MgO_2$*, Chemistry of Materials, **29**, 3152–3163 (2017). DOI: 10.1021/acs.chemmater.7b00217
45. 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

46. 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 $Li_7La_3Zr_2O_{12}$,* ACS Energy Letters **2**, 462-468 (2017). DOI:10.1021/acsenergylett.6b00593
47. 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/$O_2$ Battery Based on the MACC Electrolyte*, Chemistry of Materials, **28**, 7629-7637 (2016). DOI: 10.1021/acs.chemmater.6b02488
48. 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
49. 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
50. 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.jpclett.6b00091
51. J. G. Smith, J. Naruse, H. Hiramatsu, and D. J. Siegel, *Theoretical Limiting Potentials in Mg/$O_2$ Batteries*, Chemistry of Materials, **28**, 1390-1401 (2016). DOI: 10.1021/acs.chemmater.5b04501
52. 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 $Li_7La_3Zr_2O_{12}$ (LLZO)*, Chemistry of Materials, **28**, 197-206 (2015). DOI: 10.1021/acs.chemmater.5b03854
53. 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/$O_2$ battery,* Chemistry of Materials, **27,** 7564 (2015). DOI:10.1021/acs.chemmater.5b03608
54. M. D. Radin, C. W. Monroe, and D. J. Siegel, *Impact of Space Charge Layers on Sudden Death in Li/$O_2$ Batteries,* Journal of Physical Chemistry Letters, **6**, 3017 (2015). DOI:10.1021/acs.jpclett.5b01015
55. 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
56. 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
57. 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
58. 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
59. 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

60. L. D. Griffith, A. E. S. Sleightholme, J. F. Mansfield, D. J. Siegel, and C. W. Monroe, *Correlating Li/$O_2$ Cell Capacity and Product Morphology with Discharge Current*, ACS Applied Materials & Interfaces, **7**, 7670 (2015). DOI: 10.1021/acsami.5b00574
61. 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
62. M. D. Radin, C. W. Monroe, and D. J. Siegel, *How Dopants can Enhance Charge Transport in $Li_2O_2$,* Chemistry of Materials **27**, 839 (2015). DOI: 10.1021/cm503874c
63. 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
64. 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
65. 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
66. F. Tian, M. D. Radin, and D. J. Siegel, *Enhanced Charge Transport in Amorphous $Li_2O_2$*, Chemistry of Materials **26**, 2952 (2014). DOI: 10.1021/cm5007372
67. N. Kumar, K. Leung, and D. J. Siegel, *Crystal Surface and State of Charge Dependencies of Electrolyte Decomposition on $LiMn_2O_4$ Cathode*, Journal of the Electrochemical Society **161**, E3059 (2014). DOI: 10.1149/2.009408jes
68. 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
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72. 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).**
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84. (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).**

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88. 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).

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91. D. J. Siegel, C. Wolverton, and V. Ozolins, *First Principles Study of the Crystal Structure and Dehydrogenation Pathways of $Li_4BN_3H_{10}$*, Physical Review B **75**, 014101 (2007).
92. 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 $LiNH_2$ + $LiBH_4$ + $MgH_2$*, Journal of Alloys and Compounds **446-447**, 345 (2007).
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95. 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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101. D. J. Siegel, L. G. Hector, Jr, and J. B. Adams, *First-Principles Study of Metal–carbide/nitride Adhesion: Al/VC vs. Al/VN*, Acta Materialia **50**, 619 (2002).
102. D. J. Siegel, L. G. Hector, Jr, and J. B. Adams, *Adhesion, Stability, and Bonding at Metal/Metal-Carbide Interfaces: Al/WC*, Surface Science **498**, 321 (2002).
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107. D. J. Siegel, L. G. Hector, Jr, and J. B. Adams, *Electronic Structure and Bonding at the Al-Terminated Al/Al2O3 Interface: A First-Principles Study*, Materials Research Society Symposium Proceedings **654**, AA 4.2, (2001).
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110. P.L. Taylor and D. J. Siegel, *Approach to Equilibrium in Cholesteric Liquid Crystals*, Condensed Matter & Materials Physics (CMMP'95) Proc. Institute of Physics, London, p.93 (1996).

**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 1st, 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. U.S. Patent Application 17/581,356; *Salt Hydrate Compositions for Thermal Energy Storage Systems*, Filed 01/21/22. Inventors: D. J. Siegel and Steven Kiyabu.
15. (Invention Disclosure) *Efficient Carbon Capture Materials*, UM Office of Tech Transfer file #5625. Siegel is lead inventor.
16. (Invention Disclosure) *Improved Performance in Rechargeable Metal-Air Batteries via Fermi-Level Tuning,* UM Office of Tech Transfer file #5597. Siegel is lead inventor.
17. U.S. Patent Application 63/331,559; *High-Performance Metal-Organic Frameworks as Methane Sorbents and Computational Identification Methods,* Filed 04/15/2022. Inventors: Donald Siegel, Alauddin Ahmed, Karabi Nath and Adam Matzger

**Grants and Contracts** (Siegel's share of total funds awarded: ~$8,000,000)

1. Graham Sustainability Institute – Carbon Neutrality Acceleration Program (CNAP), "Evaluating Thermal Energy Storage for Deep Decarbonization," $300,000 total. 4/1/2021 – 3/30/2023. Bala Chandran is PI; my share: $100,000.
2. U.S. Department of Energy, "A Systematic Study of Phenomena that Control the Mechanical Integrity and Cycling Stability of Ceramic Membrane Technology," $1,250,000 total. 10/1/2019 – 9/30/2022. Sakamoto is PI; my share: ~$130,000.
3. U.S. Department of Energy, "Optimal Adsorbents for Low-Cost Storage of Natural Gas: Computational Identification, Experimental Demonstration, and System-Level Projection," $1,250,000 total. 11/1/2019 – 10/31/2022. Siegel is PI; my share: $575,000.
4. 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.
5. 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.
6. 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.
7. 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.
8. 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.
9. 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.
10. 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.

11. 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.
12. 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).
13. 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.
14. 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.
15. Ford Motor Company, "Battery Safety: Modeling and Characterization of Li-ion Batteries," $200,000, 5/1/14 – 4/30/2018. Siegel is PI.
16. National Science Foundation, Energy for Sustainability Program, "CAREER: First-Principles Modeling of Gas Evolution Reactions in Lithium Batteries," $400,000, 6/1/14 – 5/31/19. Siegel is PI.
17. National Science Foundation, Energy for Sustainability Program, "GOALI: Experimentally Validated Multiscale Modeling of Li/$O_2$ Cathodes," $399,735, 9/1/13 – 8/31/17. Siegel is co-PI; my share $163,000.
18. 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.
19. Lawrence Livermore National Lab, Grand Challenge Computing Grant of 170,000,000 CPU hours. Siegel is co-PI.
20. Denso Corporation, "Rechargeable Mg-air Batteries," $604,404, Jan. 2013 – Jan 2016. Siegel is PI; my share: $275,000.
21. 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.
22. UM MCubed program, "Data-mining for Optimal Metal-Organic Frameworks," $60,000, Jan. 2013 – June 2014. Siegel is PI: my share: $20,000.
23. 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.
24. Robert Bosch Corporation, "Multi-scale Modeling of Li-Air Batteries," $300,000, Dec. 2011 – Dec. 2013. Siegel is PI; my share: $150,000.
25. Michigan Memorial Phoenix Energy Institute, "Cyber-Discovery of High Performance $CO_2$ Adsorbents," $80,000, Sept. 2011 – Aug. 2013. Siegel is co-PI; my share: $26,650.
26. 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.
27. 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.
28. 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.
29. 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. Texas A&M University, Department of Mechanical Engineering, October 5, 2022, College Station, TX.
2. Telluride Science Research Center Workshop on "Materials Chemistry in Electrochemical Energy Storage," September 26-30, 2022, Telluride, CO.
3. Euromech Colloquium: MULTISCALE MECHANICS, MULTIPHYSICS MODELING AND SIMULATIONS FOR ENERGY STORAGE, August 29-31, 2022, Sirmione, Lake Garda, Italy.
4. Symposium on "Multiscale and Multiphysics Modelling of the Structural and Mechanical Properties of Energy Storage Materials" July 31-August 5, 2022, Yokohama, Japan.
5. 23rd International Conference on Solid State Ionics (SSI-23), July 17-22, Boston, MA.
6. Case Western Reserve University, Department of Mechanical and Aerospace Engineering, April 12, 2022, Cleveland, OH.
7. Purdue University, Mechanical Engineering Department, April 11, 2022, West Lafyette, IN.
8. Gordon Research Conference – *Batteries*, June 5-15, 2022, Ventura, CA.
9. American Chemical Society (ACS) Spring Meeting, Symposium on "Electrolytes and Interfaces in Energy Storage," March 20-24, 2022, San Diego, CA.
10. MRS 2021 Fall Meeting, Symposium on "Advanced Materials for Hydrogen and Fuel Cell Technologies," Nov. 28 – Dec. 3, 2021, Boston, MA.
11. Modeling and Design of Molecular Materials, September 21-24, 2020, Gdańsk, Poland. POSTPONED to Fall 2022.
12. Thailand Machine Learning for Chemistry Competition, October 22nd, 2021.
13. MRS 2021 Spring Meeting, Symposium on "Progress in Understanding Charge Transfer at Electrochemical Interfaces in Batteries," April 18-23, 2021, Seattle, WA.
14. International Workshop on Energy Storage Technology for E-mobility, March 25-27, 2021, Chennai, India. Sponsored by the Energy Science Society of India. (Held virtually due to coronavirus pandemic.)
15. Nano Korea 2020, session on 'Nanotechnology for Next Generation Batteries,' July 1-3, 2020, Goyang – Korea International Exhibition Center (KINTEX), South Korea. Held virtually due to coronavirus pandemic.
16. ~~Solvation Phenomena in Energy Storage, April 27-28, 2020, Berkeley, CA~~. Postponed due to Coronavirus pandemic.
17. 3rd International Conference on Hydrogen & Fuel Cell Technologies, ~~March 20-22, 2020, Hammamet, Tunisia.~~ Postponed and held virtually during Nov. 14-15, 2020 due to coronavirus pandemic.
18. ~~Royal Society of Chemistry, "Understanding Fast-ion Conduction in Solid Electrolytes," Kavli Royal Society Centre, Chicheley Hall, March 16-17, 2020, Buckinghamshire, UK~~. Postponed due to Coronavirus pandemic.
19. Gordon Research Conference – *Batteries*, February 16-21, 2020, Ventura, CA.
20. Technical University of Denmark (DTU), Department of Energy Conversion and Storage Department Colloquium, February 14, 2020, Lyngby, Denmark.
21. Electrochemical Society (ECS) Fall Meeting, Symposium A07 "Solid State Batteries," October 13-17, 2019, Atlanta, GA.

22. Electrochemical Society (ECS) Fall Meeting, Symposium I05 "Crosscutting Materials Innovation for Transformational Chemical and Electrochemical Energy Conversion Technologies," October 13-17, 2019, Atlanta, GA.
23. 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.
24. 2nd World Conference on Solid Electrolytes for Advanced Applications: Garnets and Competitors, September 24-27, 2019, Shizuoka, Japan.
25. Moscow State University – Skoltech 4th International Conference of Young Scientists, September 15-18, Moscow, Russia.
26. XXI Mendeleev Congress of General and Applied Chemistry, Symposium on "Elemental Materials for Electrochemical Energy," September 9-13, 2019, St. Petersburg, Russia.
27. 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.
28. 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.
29. ICE 2019: International Conference on Electroceramics, July 14-19, 2019, Lausanne, Switzerland.
30. Gordon Research Conference on Hydrogen-Metal Systems, session on "Advancements in Porous Materials for Hydrogen Adsorption," June 30-July 5, 2019, Barcelona, Spain.
31. 'NGenE' Next Generation Electrochemistry Summer Institute, University of Illinois at Chicago, June 3-7, 2019, Chicago, IL.
32. MRS 2019 Spring Meeting, Symposium S-19 ES04 "Solid-State Electrochemical Energy Storage," April 22-26, 2019, Phoenix, AZ.
33. Argonne National Laboratory, Materials Science Division Colloquium, April 4, 2019, Argonne, IL.
34. American Chemical Society (ACS) 257th National Meeting, symposium on "Innovative Chemistry and Materials for Electrochemical Energy Storage," March 31-April 4, 2019, Orlando, FL.
35. TMS 2019 Annual Meeting, 5th Symposium on Advanced Materials for Energy Conversion and Storage, March 10-14, 2019, San Antonio, TX.
36. Korea Institute of Science and Technology, Center for Energy Storage Research, February 20, 2019, Seoul, South Korea.
37. Seoul National University, School of Chemical and Biological Engineering, February 19, 2019, Seoul, South Korea.
38. Korea Advanced Institute of Science & Technology (KAIST), Department of Chemistry – School of Molecular Science, BK21 Lectureship, February 18, 2019, Daejeon, South Korea.
39. University of Illinois at Urbana-Champaign, Materials Science and Engineering Department Colloquium, November 12, 2018, Urbana, IL.
40. 3rd National Conference on Materials for Energy Conversion and Storage, October 18-20, 2018, IIT-BHU, Varanasi, India
41. 2nd Bosch Energy Research Network (BERN) Symposium on Innovative Energy Research, September 6-7, 2018, Sunnyvale, CA.

42. Electrochemical Society (ECS) Fall Meeting, "12th Solid State Ionic Devices (SSID 12) Symposium," September 30 - October 4, 2018, Cancun, Mexico.
43. Electrochemical Society (ECS) Fall Meeting, symposium on "Batteries and Energy Storage," September 30 - October 4, 2018, Cancun, Mexico.
44. American Chemical Society's 256th National Meeting, symposium on "Electrochemical Interfaces," August 19-23, 2018, Boston, MA.
45. American Chemical Society's 256th National Meeting, symposium on "Nanoscience of Energy Storage," August 19-23, 2018, Boston, MA.
46. 3rd Li-SM$^3$ Conference: Lithium-Sulfur Batteries: Mechanisms, Modelling and Materials, April 25-26, 2018, Chicago, IL.
47. TMS 2018 Spring Meeting, Symposium on "Materials for Energy Conversion and Storage," March 11-15, 2018, Phoenix, AZ.
48. Northwestern University, Materials Science and Engineering Department Seminar, September 26, 2017. Evanston, IL.
49. Indian Institute of Science Education and Research (IISER-BPR), September 4, 2017, Berhampur, India.
50. 1st World Congress on Lithium Garnets, Competitors and Beyond for Advanced Batteries, September 6-9, 2017, Puducherry, India.
51. Telluride Science Research Center, Computational Materials Chemistry Workshop, August 7-11, 2017, Telluride, CO.
52. Bosch Energy Research Network Symposium on Innovative Energy Research, July 27-28, 2017, Palo Alto, CA.
53. Waterloo Institute for Nanotechnology, University of Waterloo, May 8, 2017, Waterloo, ON, Canada.
54. MRS 2017 Spring Meeting, Symposium on "Mechanics of Energy Storage and Conversion," April 17-21, 2017, Phoenix, AZ.
55. TMS 2017 Annual Meeting & Exhibition, Symposium on "Advanced Materials for Energy Conversion and Storage," February 26 – March 2, San Diego, CA.
56. 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.
57. XXV International Materials Research Congress (IMRC), August 14-19, 2016. Cancun, Mexico.
58. Danish Battery Society Annual Symposium, April 7th, 2016. Copenhagen, Denmark.
59. Technical University of Denmark (DTU), Department of Energy Conversion and Storage Department Colloquium, February 1st, 2016, Lyngby, Denmark.
60. University of Florida Material Science/Mechanical & Aerospace Engineering Seminar, December 7th, 2015, Gainesville, FL.
61. Nordic Battery Conference (NORDBATT2), December 2-3, 2015, Trondheim, Norway.
62. Lithium Battery Power 2015, November 17-19, 2015, Baltimore, MD.
63. Electrochemical Society (ECS) Fall Meeting, October 11-16, 2015, Phoenix, AZ.
64. NSF workshop on "Rise of Data in Materials Research," June 29-30, 2015, College Park, MD.
65. Telluride Science Research Center, Computational Materials Chemistry Workshop, June 23-27, 2015, Telluride, CO.

66. American Ceramic Society – 11th International Conference on Ceramic Materials and Components for Energy and Environmental Applications (CMCEE), June 14-19, 2015, Vancouver, British Columbia, Canada.
67. American Chemical Society National Meeting, symposium on "Natural Resource Capture, Storage and Energy Conversion," March 22-26, 2015, Denver, CO.
68. American Chemical Society National Meeting, symposium on "2D Materials for Energy and Fuel," March 22-26, 2015, Denver, CO.
69. U.S. Department of Energy Hydrogen Storage Workshop, January 27-29, 2015, National Renewable Energy Laboratory, Golden, CO.
70. 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.
71. The Battery Show, September 16-18, 2014, Novi, MI.
72. U.S.-China Electric Vehicle and Battery Technology Workshop, August 18-19, 2014, Seattle, WA.
73. Telluride Science Research Center, Battery Materials Workshop, July 14-18, 2014, Telluride, CO.
74. 1st International Symposium on Sustainable Secondary Battery Manufacturing and Recycling, June 29-July 4, 2014, Cancun, Mexico
75. U.S. Nat. Congress on Theoretical and Applied Mechanics, June 15-20, 2014, East Lansing, MI
76. SIT Investment Associates' Annual Client Workshop, Feb. 13-16, 2014, Carlsbad, CA
77. Gilbreth Lecture: NAE National Meeting, Feb. 6, 2015, Irvine, CA
78. American Ceramic Society -- Electronic Materials & Applications Conference, January 22-24, 2014, Orlando, FL.
79. 8th U.S.-China Electric Vehicle and Battery Technology Workshop, September 20-22, 2013, Chengdu, China.
80. The Battery Show, September 17-19, 2013 Novi, Michigan.
81. 2nd ReLiable Li-Air Workshop, September 9-10, 2013 Copenhagen, Denmark
82. Denso Research Laboratories, August 23, 2013, Nisshin, Japan.
83. RIKEN Advanced Science Institute, August 22, 2013, Wako, Japan.
84. American Chemical Society National Meeting, "Chemical Mechanisms in Advanced Materials," September 8-12, 2013, Indianapolis.
85. Beyond Lithium Ion VI Conference, June 4-6, 2013, Boulder, Colorado.
86. U.S. National Academy of Sciences Indo-American Frontiers of Science Symposium, April 7-10, 2013, Agra, India.
87. Detroit Section of the Electrochemical Society, February 20, 2013, Southfield, MI.
88. U.S. Dept. of Energy, Adsorbent Hydrogen Storage Workshop, Nov. 27, 2012, Washington, D.C.
89. Denso International America Inc., Research and Engineering Division, June 29, 2012, Southfield, MI.
90. WHEC 2012, World Hydrogen Energy Conference, June 3-7, 2012, Toronto, Canada.
91. 5th US-China Electric Vehicle and Battery Technology Workshop, April 16-17, 2012,

Hangzhou, China.

92. U.S. National Academy of Engineering-Alexander von Humboldt German-American Frontiers of Engineering Symposium, March 28-31, 2012, Potsdam, Germany.
93. 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.
94. 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.
95. Electronic Materials & Applications Conference, symposium on "Energy Storage Materials and Systems," Jan. 18-20, 2012, Orlando.
96. 4th US-China Electric Vehicle and Battery Technology Workshop, August 4-5, 2011, Argonne, IL.
97. Frontiers of Energy Materials Workshop, Penn State, May 18, 2011.
98. General Motors R&D Center, Warren, MI, Aug. 10, 2011.
99. MS&T 2011, "7th Annual Symposium on Phase Stability, Diffusion, Kinetics, and Their Applications (PSDK)," October 2011, Columbus.
100. TMS 2011 Annual Meeting, 10th Symposium on "Computational Thermodynamics and Kinetics of Materials, " March 2011, San Diego
101. Chemistry Department Seminar, University of Detroit Mercy, Nov. 9, 2010.
102. MRS 2010 Spring Meeting, Symposium Y: "Computational Approaches to Materials for Energy," April 2010, San Francisco
103. School of Mechanical, Aerospace, Chemical, and Materials Engineering, Arizona State University, Nov. 13, 2009, Tempe, AZ
104. Physics Department Colloquium, Case Western Reserve University, Oct. 1, 2009, Cleveland, OH.
105. XVIII International Materials Research Congress 2009, August 16-21, Cancun, Mexico.
106. NIST Workshop on Atomistic Simulations for Industrial Needs, April 27-28, 2009, Gaithersburg, MD.
107. Japan Institute of Metals 2009 Spring Meeting, Session S1: "Hydrogen Storage Materials," March 28-30, Tokyo, Japan.
108. APS 2009 March Meeting, Invited Session: "Computational Design of Hydrogen Storage Materials," March 16-20, Pittsburgh, PA.
109. Chemical Engineering and Materials Science Dept. Colloquium, Michigan State University, March 5, 2009, East Lansing, MI.
110. MRS 2009 Spring Meeting "Symposium HH: Quantitative Characterization of Nanostructured Materials," April 13-17, San Francisco, CA.
111. MS&T'08 Conference "Discovery and Optimization of Materials through Computational Design," October 5-9, Pittsburgh, PA.
112. NIST Workshop "Atomistic Simulations for Industrial Needs," April 28-29, 2008, Gaithersburg, MD.

113. MRS 2008 Spring Meeting "DOE Theory Focus Session on Hydrogen Storage Materials," March 24, San Francisco.
114. TMS Annual Meeting: "Career Forum," March 2008, New Orleans.
115. University of Michigan, Guest Lecture for MSE 250, Materials for Energy, Nov. 2007.
116. Erwin Schrodinger Institute–University of Vienna, Theory Meets Industry Workshop, 12 June 2007
117. University of Michigan, Materials Science and Engineering Colloquium, 2 February 2007
118. Lawrence Livermore National Laboratory, Metals and Alloys Group, 14 April 2005
119. University of Texas at El Paso, Department of Physics Colloquium, 6 April 2005
120. Ford Research Laboratory, Physical and Environmental Sciences Department, 4 April 2005
121. Pacific Northwest National Laboratory, Energy Science and Technology Directorate, Jan. 2005
122. University of Tennessee, Department of Materials Science and Engineering, October 2004
123. Oak Ridge National Laboratory, Joint Institute for Computational Sciences, October 2004
124. CECAM Workshop on Oxide-Metal Interfaces: Progress and Challenges, October 2001, Lyon, France
125. Advances in Surface Engineering—Fundamentals and Applications, Materials Research Society Meeting, November 2001, Boston, MA
126. 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-$O_2$ 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 $Li_7La_3Zr_2O_{12}$." Chair
8. Haesun Park (Mech. Eng.), December 2018. "Atomistic Modelling Approaches to the Challenges in Lithium – Sulfur Batteries." Chair
9. Jeff Lowe (Chem. Eng.), December 2018. "First-principles Modeling of Anode/Electrolyte Interfaces in Beyond Li-ion Batteries." Chair
10. Kwangnam Kim (Mech. Eng.), April 2020. "Computational Discovery of Solid Electrolytes for Batteries: Interfacial Phenomena and Ion Mobility." Chair

11. Kyle Nagy (Mech. Eng.), August 2020. "Atomic Scale Modeling of Fundamental Characteristics of Metal Anodes and Solid Electrolytes: Overpotentials, Elastic Properties, and Grain Boundary Transport." Chair
12. Mallory Fuhst (Applied Physics), expected September 2022. Chair
13. Everardo Olide (Applied Physics), expected September 2022. Chair
14. Steven Kiyabu (Mechanical Engineering), expected September 2022. Chair.
15. Chisang Park (Mechanical Engineering), expected September 2023. Chair.
16. Jeong Seop Yoon (Mechanical Engineering), expected September 2023. Chair.
17. Hafeez Sulaimon (Mechanical Engineering), expected December 2024. Chair.

**Postdoctoral Researchers Advised/Co-advised**

1. Dr. Justin Purewal (April 2010 – April 2012)
2. Dr. Malay Rana Kumar (May 2011 – August 2014)
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)
8. Dr. Jeff Smith (2018 – 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.
7. Hafeez Suilamon, 2018-2020, Materials Science & Engineering.
8. Daewoong Kim, 2019-2020, Mechanical Engineering.

**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 $CO_2$ 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 Steinhauser, 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 – 2019
14. SURE: Atomistic Simulation of Materials for Energy Storage, Jackson Teener, 5/2018 – 2019
15. SURE: Atomistic Simulation of Materials for Energy Storage, Justin Stobart, 5/2018 – 2019
16. UROP: System-Level Modeling of Thermal Energy Storage Devices, Patrick Girard, 2020

**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*: Telluride Science Research Center Summer School: "School on Fundamentals for Electrochemical Energy Conversion and Storage," June 22-26, 2021, Telluride, CO; APS April 2nd 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, 2021; NSF Division of Chemical, Bioengineering, Environmental, and Transport Systems (CBET), 2014, 2015, 2016, 2017, 2020, 2021; 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. *Discussion Leader-Simulations Across Scales:* Gordon Research Conference: 'Batteries: Understanding Coupled Behaviors of Energy Storage Beyond Energy and Power,' February 16-20, 2020, Ventura, CA
9. *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 599-007 | Professional Skills for Graduate Student Success | Joint Instructor | F20 | 43 |
| ME 433/533 | Advanced Energy Solutions | Joint Instructor | F20 | 112 |
| ME 599-007 | Professional Skills for Graduate Student Success | Joint Instructor | F19 | 34 |
| ME 507 | Atomistic Computer Modeling of Materials | Sole Instructor | F19 | 14 |
| 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 |

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|---|---|---|---|---|
| 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 599-007: Professional Skills for Graduate Student Success.*** Re-introduced and re-scoped this (previously abandoned) course for incoming graduate students. The course is team-taught by more than 2 dozen ME faculty. The course objective is to broadly describe best practices for research, and to introduce policies and procedures for successful completion of graduate studies in the UM ME Department. Specific topics covered include: steps in the PhD process; mentoring; the research process; identifying research opportunities and formulating hypotheses; research methodologies; time management; improving one's writing and presentations; diversity, equity, and inclusion; career planning.
2. **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 $CO_2$ 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*
3. **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/L1VVo
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.