Curriculum Vitae of Yue Qi, Ph.D

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I. Education

June 2001	**Ph.D. in Materials Science & minor in Computer Science, Caltech**, Pasadena, CA Dissertation: Molecular dynamics (MD) studies on phase transformation and deformation behaviors in FCC metals and alloys, Advisor: William A. Goddard, III
July 1996	**B.S. in Materials Science & Computer Science**, **Tsinghua University**, Beijing, China

II. Employment

2018-present	**Professor**, Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing, Michigan
2018-present	**Associate Dean** of Inclusion and Diversity, College of Engineering, Michigan State University
2013-2018	**Associate Professor**, Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing, Michigan
2001-2013	**Staff Research Scientist**, Chemical & Materials Systems Lab, General Motors R&D, Warren, Michigan
2009-2013	**Adjunct Professor**, Department of Mechanical, Automotive & Materials Engineering, University of Windsor, Windsor, Ontario
Summer 2000	**Summer Intern**, Materials and Processes Lab, General Motors, Warren, Michigan

III. Awards and Honors

2017	The Minerals, Metals & Materials (TMS) Society **Brimacombe Medalist (mid-career award)**, *for her contributions in multidisciplinary computational materials science, from groundbreaking work on chemical-mechanical coupling to breakthroughs in understanding Li-ion battery failure*.
2013	TMS EMPMD **Young Leader Professional Development Award**
2011	Invited speaker at MIT Materials Day on "Computational Materials Science and Engineering"
2009	GM **Campbell Award** for Fundamentals of Interfacial Tribology
2009	GM **Campbell Award** for Multi-scale Modeling of High-temperature Deformation in Aluminum
2009	Reported in APS Profiles in Versatility — The Auto Industry's a Deal for Physicists
2006	GM **Campbell Award** for Advances in Nano-scale Plasticity
1999	**Feynman Prize** in Nanotechnology for Theoretical Work
1995	Tsinghua Excellent Student Fellowship
2017	Best Poster Award at the 49th Annual Midwest Theoretical Chemistry Conference (MWTCC)
2014	Best Poster award at 225th Electrochemical Society (ECS) Meetings
2013	Invited Cover Article, Journal of Physical Chemistry C 2013, 117 (17), 8579-8593
2012	Journal of Physics-Condensed Matter 2012 Highlights, JPCM 2012, 24 (22), 225003
2009	MRS "outstanding symposium paper", Journal of Materials Research 24 (8), 2461-2470

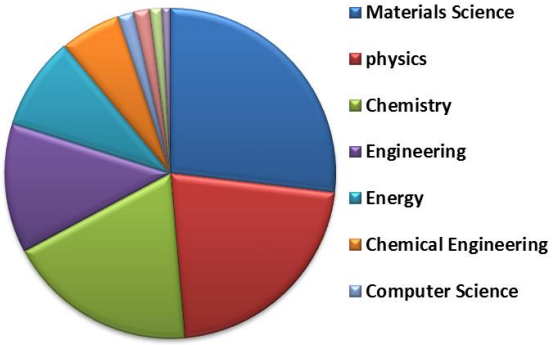
Publications

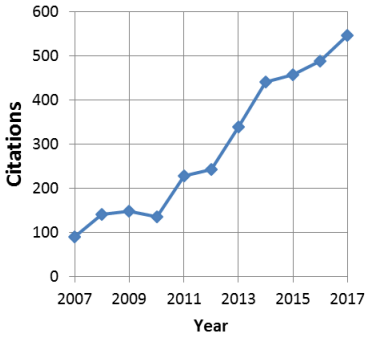
Total 104 Journal Publications credited to Yue Qi (at Caltech, General Motors, and MSU).

Citations:

Web of Science:	total citation 3798	H-index=32
Scopus:	total citation 3880	H-index=34
Google Scholar:	total citation 5183	H-index=39

Subject matter statistics and citations from Scopus:





* Graduate student or postdoc advised by Qi

_ Underlined as the corresponding author

Papers under Review

1. Balachandran, S., **Liu, J.***, Seal, J., **Qi, Y.**, Crimp, M.A., The Role of Incoherent Twin (9R) Boundaries on Slip Resistance in High Purity Nickel: Electron Channeling Contrast Imaging and Molecular Dynamics Simulations, Acta Materialia (2018)

Published Journal Papers

1. **Das, T.***; Nicholas, J.D.; Sheldon, B.W., **Qi, Y.**, Anisotropic Chemical Strain in Cubic Ceria due to Oxygen-Vacancy-Induced Elastic Dipoles, Phys. Chem. Chem. Phys. 2018, 20 (22), 15293-15299
2. **Tian, H.K.***, Xu, B., **Qi, Y.**, Computational Study of Lithium Nucleation Tendency in LLZO and Rational Design of Interlayer Materials to Prevent Lithium Dendrites, Journal of Power Source 2018, 392, 79-86
3. **Li, Y.S.***, **Qi, Y.**, Transferable SCC-DFTB Parameters for Li-Metal and Li-Ions in Inorganic Compounds and Organic Solvents, Journal of Physical Chemistry C (2018)
4. **Phongpreecha, T.***; Nicholas, J.D.; Bieler, T.R.; **Qi, Y.**, Computational Design of Metal Oxides to Enhance the Wetting and Adhesion of Silver-based Brazes on Yttria-Stabilized-Zirconia, Acta Materialia 2018, 152, 229-238
5. Wang, A.P., **Kadam, S.***, Li, H., Shi, S.Q., **Qi, Y.**, Review on Modeling of the Solid Electrolyte Interphase (SEI) for Lithium-Ion Batteries, npj Computational Materials 2018, 4, 15 (Invited Review), *(Highlighted as one of the 10 Ionizing Papers in March 2018 by Research Interfaces)*
6. Yulaev, A.; Oleshko, V.; Haney, P.; **Liu, J.***; **Qi, Y.**; Talin, A.A.; Leite, M; Kolmakov, A., From Microparticles to Nanowires and Back: Radical Transformations in Plated Li Metal Morphology Revealed via in situ Scanning Electron Microscopy, Nano Letter 2018, 18, 1644–1650
7. Lin, C.F., **Qi, Y.**, Gregorczyk, K., Lee, S.B., Rubloff, G., Nanoscale Protection Layers to Mitigate Degradation in High Energy Electrochemical Energy Storage Systems, Accounts of Chemical Research 2018, 51, 97-106 *(Invited Article)*

8. **Das, T.***; Nicholas, J.D.; **Qi, Y.**, Polaron Size and Shape Effects on Oxygen Vacancy Interactions in Lanthanum Strontium Ferrite, J. Mater. Chem. A 2017, 5, 25031-25043
9. Suo, L., Oh. D., **Lin, Y.X.***, Zhou, Z., Borodin, O., Gao, T., Kushima, A., Wang, Z., Kim, H.C., **Qi, Y.**, Yang, W.L., Pan, F., Li, J., Xu, K., Wang, C.S., How Solid-Electrolyte-Interphase Forms in Aqueous Electrolytes, Journal of American Chemical Society 2017, 139, 18670-18680
10. **Xiong, S.***, **Li, Y.S.***, Sun, J.L., **Qi, Y.**, An integrated computation and experiment investigation on the adsorption mechanisms of anti-wear and anti-corrosion additives on copper, The Journal of Physical Chemistry C 2017, 121, 21995–22003
11. Nation, L., Li, J.C., **James, C.***, **Qi, Y.**, Dudney, N., Sheldon, B.W., In situ Stress Measurements during Electrochemical Cycling of Lithium-Rich Cathodes, Journal of Power Sources 2017, 364, 383-391
12. Pan, J., Lany, S., **Qi, Y.**, Computationally Driven Two-Dimensional Materials Design: What Is Next?, ACS Nano 2017, 11, 7560-7564 *(Invited Perspective)*
13. **Kim, K.J.*; Wortman, J.*; Kim, S.Y.*; Qi, Y.,** Atomistic Simulation Derived Insight on the Irreversible Structural Changes of Si Electrode during Fast and Slow Delithiation, Nano Letters. 2017, 17, 4330–4338
14. **Tian, H.K.*; Qi, Y.,** Simulation of the Effect of Contact Area Loss in All-Solid-State Batteries", Journal of the Electrochemical Society, J. Electrochem. Soc. 2017 164, E3512-E3521
15. **Liu, J.L.***; Huang, Z.; Pan, Z.; Wei, Q.M.; Li, X.D.; **Qi, Y.**, Atomistic origin of deformation twinning in biomineral aragonite, Phys. Rev. Lett. 2016, 118, 105501
16. **Das, T.***; Nicholas, J.D.; **Qi, Y.**, Long-range charge transfer and oxygen vacancy interactions in strontium ferrite, J. Mater. Chem. A 2017, 5, 4493-4506
17. Wang, F.; **Lin, Y.X.***; Suo L.; Fan X.; Gao, T.; Yang C.; Han, F.; **Qi, Y.**; Xu, K.; Wang, C.S., Stabilizing high-voltage $LiCoO_2$ cathode in aqueous electrolyte with interphase-forming additive, Energy and Environmental Science 2016, 9, 3666-3673
18. **Li, Y.S.***; Leung, K.; **Qi, Y.**, Computational exploration of the Li-electrode | electrolyte interface in the presence of a nanometer thick solid-electrolyte interphase (SEI) layer, Acc. Chem. Res. 2016, 49, 2363–2370 *(Invited Article)*
19. **Lin, Y. X.***; Liu, Z.; Leung, K.; Chen, L. Q.; Lu, P.; **Qi, Y.**. Connecting the irreversible capacity loss in Li ion batteries with the electronic insulating properties of solid electrolyte interphase (SEI) components, Journal of Power Sources 2016, 309, 221-230 *(Selected and Featured by Advances in Engineering)*
20. **Stournara, M.E.***; Kumar, R.; **Qi, Y**.; Sheldon, B.W., Ab initio diffuse-interface model for lithiated electrode interface evolution, Phys. Rev. E 2016, 94, 012802
21. **James, C.***; Wu, Y.; Sheldon, B. W.; **Qi, Y.**. The Impact of oxygen vacancies on lithium vacancy formation and diffusion in $Li_{2-x}MnO_{3-\delta}$. Journal: Solid State Ionics 2016, 289, 87-94
22. **Pan, J.***; Zhang, Q.; Xiao, X. C.; Cheng, Y. T.; **Qi, Y.**. Design of nano-structured heterogeneous solid ionic coatings through a multi-scale defect model. Applied Materials & Interfaces 2016, 8, 5687-5693
23. Ostadhossein, A., **Kim, S.Y.***, Cubuk, E.D., **Qi, Y.**, and van Duin, A.C.T., Atomic Insight into the Lithium Storage and Diffusion Mechanism of SiO2/Al2O3 Electrodes of Lithium Ion Batteries: ReaxFF Reactive Force Field Modeling, The Journal of Physical Chemistry A 2016, 120 (13), 2114-2127
24. Zhang, Q.; **Pan, J.***; Lu, P.; Liu, Z.; Verbrugge, M. W.; Sheldon, B. W.; Cheng, Y. T.; **Qi, Y.**; Xiao, X. C.. Synergetic Effects of Inorganic Components in Solid Electrolyte Interphase on High Cycle Efficiency of Lithium Ion Batteries. Nano Letters 2016, 16, 2011-2016
25. Liu, Z.; **Qi, Y.**; **Lin, Y. X.***; Chen, L.; Lu, P.; Chen, L. Q.. Interfacial Study on Solid Electrolyte Interphase at Li metal Anode: Implication for Li Dendrite Growth, Journal of the Electrochemical Society 2016, 163, A592-598
26. **Kim, S. Y.***; Ostadhossein, A.; Adri van Duin, A.; Xiao, X.; Gao, H.; **Qi, Y.**. Self-generated concentration and modulus gradients coating design to protect Si nano-wire electrodes during lithiation. Physical Chemistry Chemical Physics 2016, 18, 3706-3715
27. **Kim, K. J.***; **Qi, Y.**, Vacancies in Si Can Improve the Concentration Dependent Lithiation Rate – Molecular Dynamics Studies of Lithiation Dynamics of Si Electrodes. Journal of Physical Chemistry C 2015, 119 (43), 24265–24275

28. Chen, L., Zhang, HW., Liang, LY, Liu, Z., **Qi, Y.**, Lu, P., Chen, J., Chen, LQ, Modulation of dendritic patterns during electrodeposition: A nonlinear phase-field model, Journal of Power Sources 2015, 300 (30), 376-385
29. **Pan, J.***; Cheng, Y. T.; **Qi, Y**., General method to predict voltage-dependent ionic conduction in a solid electrolyte coating on electrodes. Physical Review B 2015, 91 (13), 134116;
30. Sun, S.; **Qi, Y.**; Zhang, T. Y., Dissecting graphene capacitance in electrochemical cell. Electrochimica Acta 2015, 163, 296-302;
31. Chen, J.; Sun, T.; **Qi, Y.**; Li, X., A Coupled Penetration-Tension Method for Evaluating the Reliability of Battery Separators. ECS Electrochemistry Letters 2014, 3 (6), A41-A44;
32. Chen, J.; Yan, Y.; Sun, T.; **Qi, Y.**; Li, X., Deformation and fracture behaviors of microporous polymer separators for lithium ion batteries. RSC Advances 2014, 4 (29), 14904-14914;
33. Chen, J.; Yan, Y.; Sun, T.; **Qi, Y.**; Li, X., Probing the Roles of Polymeric Separators in Lithium-Ion Battery Capacity Fade at Elevated Temperatures. Journal of the Electrochemical Society 2014, 161 (9), A1241-A1246;
34. **Kim, S. Y.***; **Qi, Y.**, Property Evolution of Al_2O_3 Coated and Uncoated Si Electrodes: A First Principles Investigation. Journal of the Electrochemical Society 2014, 161 (11), F3137-F3143;
35. Nicholas, J. D.; **Qi, Y.**; Bishop, S. R.; Mukherjee, P. P., Introduction to Mechano-Electro-Chemical Coupling in Energy Related Materials and Devices. Journal of the Electrochemical Society 2014, 161 (11), Y11-Y12;
36. Oliver, D. J.; Paul, W.; El Ouali, M.; Hagedorn, T.; Miyahara, Y.; **Qi, Y.**; Gruetter, P. H., One-to-one spatially matched experiment and atomistic simulations of nanometre-scale indentation. Nanotechnology 2014, 25 (2), 025701;
37. **Qi, Y.**; Hector, L. G.; **James, C.***; **Kim, K. J.***, Lithium Concentration Dependent Elastic Properties of Battery Electrode Materials from First Principles Calculations. Journal of the Electrochemical Society 2014, 161 (11), F3010-F3018;
38. **Sen, F. G.***; Alpas, A. T.; van Duin, A. C. T.; **Qi, Y.**, Oxidation-assisted ductility of aluminium nanowires. Nature Communications 2014, 5; art. no. 3959.
39. **Stournara, M. E.***; **Qi, Y.**; Shenoy, V. B., From Ab Initio Calculations to Multiscale Design of Si/C Core-Shell Particles for Li-Ion Anodes. Nano Letters 2014, 14 (4), 2140-2149; *(Reported by Green Car Congress)*
40. **Yan, S. T.***; Xiao, X. R.; Huang, X. S.; Li, X. D.; **Qi, Y.**, Unveiling the environment-dependent mechanical properties of porous polypropylene separators. Polymer 2014, 55 (24), 6282-6292.
41. Chen, J.; Liu, J.; **Qi, Y.**; Sun, T.; Li, X., Unveiling the Roles of Binder in the Mechanical Integrity of Electrodes for Lithium-Ion Batteries. Journal of the Electrochemical Society 2013, 160 (9), A1502-A1509;
42. Howe, J. Y.; Burton, D. J.; **Qi, Y.**; Meyer, H. M., III; Nazri, M.; Nazri, G. A.; Palmer, A. C.; Lake, P. D., Improving microstructure of silicon/carbon nanofiber composites as a Li battery anode. Journal of Power Sources 2013, 221, 455-461;
43. Sen, F. G.; Meng-Burany, X.; Lukitsch, M. J.; **Qi, Y.**; Alpas, A. T., Low friction and environmentally stable diamond-like carbon (DLC) coatings incorporating silicon, oxygen and fluorine sliding against aluminum. Surface & Coatings Technology 2013, 215, 340-349;
44. **Sen, F. G.***; **Qi, Y.**; Alpas, A. T., Tribology of fluorinated diamond-like carbon coatings: first principles calculations and sliding experiments. Lubrication Science 2013, 25 (2), 111-121;
45. **Sen, F. G.***; **Qi, Y.**; van Duin, A. C. T.; Alpas, A. T., Oxidation induced softening in Al nanowires. Applied Physics Letters 2013, 102 (5);
46. **Shi, S.***; **Qi, Y.**; Li, H.; Hector, L. G., Jr., Defect Thermodynamics and Diffusion Mechanisms in Li_2CO_3 and Implications for the Solid Electrolyte Interphase in Li-Ion Batteries. Journal of Physical Chemistry C 2013, 117 (17), 8579-8593; *(Invited Cover Article)*
47. **Stournara, M. E.**; Xiao, X.; **Qi, Y.**; Johari, P.; Lu, P.; Sheldon, B. W.; Gao, H.; Shenoy, V. B., Li Segregation Induces Structure and Strength Changes at the Amorphous Si/Cu Interface. Nano Letters 2013, 13 (10), 4759-4768;

48. Sun, C.-F.; Karki, K.; Jia, Z.; Liao, H.; Zhang, Y.; Li, T.; **Qi, Y.**; Cumings, J.; Rubloff, G. W.; Wang, Y., A Beaded-String Silicon Anode. ACS Nano 2013, 7 (3), 2717-2724;
49. Zhang, H.; Liu, X.; **Qi, Y.**; Liu, V., On the $La_{2/3-x}Li_{3x}TiO_3/Al_2O_3$ composite solid-electrolyte for Li-ion conduction. Journal of Alloys and Compounds 2013, 577, 57-63.
50. Liang, L.; **Qi, Y.**; Xue, F.; Bhattacharya, S.; Harris, S. J.; Chen, L.-Q., Nonlinear phase-field model for electrode-electrolyte interface evolution. Physical Review E 2012, 86 (5), 051609;
51. Oliver, D. J.; Maassen, J.; El Ouali, M.; Paul, W.; Hagedorn, T.; Miyahara, Y.; **Qi, Y.**; Guo, H.; Gruetter, P., Conductivity of an atomically defined metallic interface. Proceedings of the National Academy of Sciences of the United States of America 2012, 109 (47), 19097-19102; *(Reported by Phys.org, ZeitNews, redOrbit as research news)*
52. **Qi, Y.**; Xu, Q. C.; Van der Ven, A., Chemically induced crack instability when electrodes fracture. Journal of the Electrochemical Society 2012, 159 (11), A1838-A1843;
53. **Sen, F. G.***; **Qi, Y.**; Alpas, A. T., Anchoring platinum on graphene using metallic adatoms: a first principles investigation. Journal of Physics-Condensed Matter 2012, 24 (22), 225003; *(IOP Selected, Lab Talk report: http://iopscience.iop.org/0953-8984/labtalk-article/49544, JPCM 2012 Highlight)*
54. Shang, S.-L.; Hector, L. G., Jr.; **Shi, S.***; **Qi, Y.**; Wang, Y.; Liu, Z.-K., Lattice dynamics, thermodynamics and elastic properties of monoclinic Li_2CO_3 from density functional theory. Acta Materialia 2012, 60 (13-14), 5204-5216;
55. **Shi, S.***; Lu, P.; Liu, Z.; **Qi, Y.**; Hector, L. G.; Li, H.; Harris, S. J., Direct calculation of Li-Ion transport in the solid electrolyte interphase. Journal of the American Chemical Society 2012, 134 (37), 15476-15487;
56. Wang, X.-L.; An, K.; Cai, L.; Feng, Z.; Nagler, S. E.; Daniel, C.; Rhodes, K. J.; Stoica, A. D.; Skorpenske, H. D.; Liang, C.; Zhang, W.; Kim, J.; **Qi, Y.**; Harris, S. J., Visualizing the chemistry and structure dynamics in lithium-ion batteries by in-situ neutron diffraction. Scientific Reports 2012, 2. art. no. 747
57. Sheldon, B. W.; Soni, S. K.; Xiao, X.; **Qi, Y.**, Stress contributions to solution thermodynamics in Li-Si alloys. Electrochemical and Solid State Letters 2012, 15 (1), A9-A11;
58. Abou Gharam, A.; Lukitsch, M. J.; **Qi, Y.**; Alpas, A. T., Role of oxygen and humidity on the tribo-chemical behavior of non-hydrogenated diamond-like carbon coatings. Wear 2011, 271 (9-10), 2157-2163;
59. **Du, N.***; **Qi, Y.**; Krajewski, P. E.; Bower, A. F., The effect of solute atoms on aluminum grain boundary sliding at elevated temperature. Metallurgical and Materials Transactions A 2011, 42A (3), 651-659;
60. Johari, P.; **Qi, Y.**; Shenoy, V. B., The mixing mechanism during lithiation of Si negative electrode in Li-ion batteries: An ab initio molecular dynamics study. Nano Letters 2011, 11 (12), 5494-5500;
61. Krajewski, P. E.; Hector, L. G.; **Qi, Y.**; Mishra, R. K.; Sachdev, A. K.; Bower, A. F.; Curtin, W. A., Atoms to autos: A multi-scale approach to modeling aluminum deformation. JOM 2011, 63 (11), 24-32; *(Invited Article)*
62. Leung, K.; **Qi, Y.**; Zavadil, K. R.; Jung, Y. S.; Dillon, A. C.; Cavanagh, A. S.; Lee, S. H.; George, S. M., Using atomic layer deposition to hinder solvent decomposition in lithium ion batteries: first-principles modeling and experimental studies. Journal of the American Chemical Society 2011, 133 (37), 14741-14754;
63. Milas, I.; **Qi, Y.**; Sheldon, B. W.; Shenoy, V. B., First-principles study of void induced stresses at a diamond (100) grain boundary. Journal of Applied Physics 2011, 109 (3), 033518; *(Selected for Virtual Journal of Nanoscale Science & Technology)*
64. **Qi, Y.**; Lai, Y., Mesoscale modeling of the influence of morphology on the mechanical properties of proton exchange membranes. Polymer 2011, 52 (1), 201-210;
65. **Sen, F. G.***; **Qi, Y.**; Alpas, A. T., Material transfer mechanisms between aluminum and fluorinated carbon interfaces. Acta Materialia 2011, 59 (7), 2601-2614.
66. Deshpande, R.; **Qi, Y.**; Cheng, Y. T., Effects of concentration-dependent elastic modulus on diffusion-induced stresses for battery applications. Journal of the Electrochemical Society 2010, 157 (8), A967-A971; *(Selected for Virtual Journal of Nanoscale Science & Technology)*

67. **Du, N.***; **Qi, Y.**; Krajewski, P. E.; Bower, A. F., Aluminum Σ3 grain boundary sliding enhanced by vacancy diffusion. Acta Materialia 2010, 58 (12), 4245-4252;
68. **Guo, H.***; **Qi, Y.**, Environmental conditions to achieve low adhesion and low friction on diamond surfaces. Modelling and Simulation in Materials Science and Engineering 2010, 18 (3), 034008; *(Invited Article)*
69. **Guo, H.***; **Qi, Y.**; Li, X., Adhesion at diamond/metal interfaces: A density functional theory study. Journal of Applied Physics 2010, 107 (3), 033722;
70. Harris, S. J.; Deshpande, R. D.; **Qi, Y.**; Dutta, I.; Cheng, Y. T., Mesopores inside electrode particles can change the Li-ion transport mechanism and diffusion-induced stress. Journal of Materials Research 2010, 25 (8), 1433-1440;
71. **Qi, Y.**; **Guo, H.***; Hector, L. G.; Timmons, A., Threefold increase in the Young's modulus of graphite negative electrode during lithium intercalation. Journal of the Electrochemical Society 2010, 157 (5), A558-A566;
72. **Qi, Y.**; Harris, S. J., In situ observation of strains during lithiation of a graphite electrode. Journal of the Electrochemical Society 2010, 157 (6), A741-A747;
73. Shenoy, V.; Johari, P.; **Qi, Y.**, Elastic softening of amorphous and crystalline Li-Si Phases with increasing Li concentration: A first-principles study. Journal of Power Sources 2010, 195 (19), 6825-6830.
74. Ward, D. K., Farkas, D., J Lian, J., Curtin, W. A. Wang, J., Kim, K. S., **Qi, Y.**, Engineering size-scaling of plastic deformation in nanoscale asperities, Proceedings of the National Academy of Sciences 2009, 106 (24) 9580-9585;
75. Brunello, G.; Lee, S. G.; Jang, S. S.; **Qi, Y.**, A molecular dynamics simulation study of hydrated sulfonated poly(ether ether ketone) for application to polymer electrolyte membrane fuel cells: Effect of water content. Journal of Renewable and Sustainable Energy 2009, 1 (3) 033101; *(Cover Article)*
76. Cipoletti, D. E.; Bower, A. F.; **Qi, Y.**; Krajewski, P. E., The influence of heterogeneity in grain boundary sliding resistance on the constitutive behavior of AA5083 during high-temperature deformation. Materials Science and Engineering A 2009, 504 (1-2), 175-182;
77. **Guo, H.***; Xiao, X.; **Qi, Y.**; Xu, Z. H.; Li, X., Enhance diamond coating adhesion by oriented interlayer microcracking. Journal of Applied Physics 2009, 106 (12), 123514;
78. Kong, L. T.; Denniston, C.; Muser, M. H.; **Qi, Y.**, Non-bonded force field for the interaction between metals and organic molecules: a case study of olefins on aluminum. Physical Chemistry Chemical Physics 2009, 11 (43), 10195-10203;
79. **Qi, Y.**; Sheldon, B. W.; **Guo, H.***; Xiao, X., Kothari, A. K., Impact of surface chemistry on grain boundary induced intrinsic stress evolution during polycrystalline thin film growth. Physical Review Letters 2009, 102 (5), 056101;
80. **Sen, F. G.***; **Qi, Y.**; Alapas, A. T., Surface stability and electronic structure of hydrogen- and fluorine-terminated diamond surfaces: A first principles investigation. Journal of Materials Research 2009, 24 (8), 2461-2470; *(MRS "outstanding symposium paper")*
81. Soldera, A.; **Qi, Y.**; Capehart, W. T., Phase transition and morphology of polydispersed ABA(') triblock copolymers determined by continuous and discrete simulations. Journal of Chemical Physics 2009, 130 (6), 064902;
82. Xia, S.; **Qi, Y.**; Perry, T. A.; Kim, K. S., Strength characterization of Al/Si interfaces: A hybrid method of nanoindentation and finite element analysis. Acta Materialia 2009, 57 (3), 695-707;
83. Yasi, J. A.; Nogaret, T.; Trinkle, D. R.; **Qi, Y.**; Hector, L. G.; Curtin, W. A., Basal and prism dislocation cores in magnesium: comparison of first-principles and embedded-atom-potential methods predictions. Modelling and Simulation in Materials Science and Engineering 2009, 17 (5), 055012;
84. **Guo, H.***; **Qi, Y.**; Li, X., Predicting the hydrogen pressure to achieve ultralow friction at diamond and diamondlike carbon surfaces from first principles. Applied Physics Letters 2008, 92 (24), 241921;
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89. **Qi, Y.**; Krajewski, P. E., Molecular dynamics simulations of grain boundary sliding: The effect of stress and boundary misorientation. Acta Materialia 2007, 55 (5), 1555-1563;
90. **Qi, Y.**; Mishra, R. K., Ab initio study of the effect of solute atoms on the stacking fault energy in aluminum. Physical Review B 2007, 75 (22), 224105;
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92. Zhang, Q.; **Qi, Y.**; Hector, L.G., Cagin, T., Goddard, W. A., Origin of static friction and its relationship to adhesion at the atomic scale. Physical Review B 2007, 75 (14), 144114;
93. **Qi, Y.**; Konca, E.; Alpas, A. T., Atmospheric effects on the adhesion and friction between non-hydrogenated diamond-like carbon (DLC) coating and aluminum - A first principles investigation. Surface Science 2006, 600 (15), 2955-2965;
94. **Ward, D. K.***; Curtin, W. A.; **Qi, Y.**, Aluminum-silicon interfaces and nanocomposites: A molecular dynamics study. Composites Science and Technology 2006, 66 (9), 1151-1161;
95. **Ward, D. K.***; Curtin, W. A.; **Qi, Y.**, Mechanical behavior of aluminum-silicon nanocomposites: A molecular dynamics study. Acta Materialia 2006, 54 (17), 4441-4451;
96. Wescott, J. T.; **Qi, Y.**; Subramanian, L.; Capehart, T. W., Mesoscale simulation of morphology in hydrated perfluorosulfonic acid membranes. Journal of Chemical Physics 2006, 124 (13), 134702;
97. **Qi, Y.**; Hector, L. G.; Ooi, N.; Adams, J. B., A first principles study of adhesion and adhesive transfer at Al(111)/graphite(0001). Surface Science 2005, 581 (2-3), 155-168;
98. Zhang, Q.; **Qi, Y.**; Hector, L. G.; Çağın, T.; Goddard, W. A; Atomic simulations of kinetic friction and its velocity dependence at Al/Al and α -Al_2O_3/ α -Al_2O_3 interfaces. Physical Review B 2005, 72 (4), 045406;
99. **Qi, Y.**; Hector, L. G., Adhesion and adhesive transfer at aluminum/diamond interfaces: A first-principles study. Physical Review B 2004, 69 (23), 235401;
100. Zhang, Q., Çağın, T., van Duin, A., Goddard, W. A., **Qi, Y.**, Hector, L. G., Adhesion and nonwetting-wetting transition in the Al/α− Al_2O_3 interface, Physical Review B 2004, 69 (4), 045423;
101. **Qi, Y.**; Hector, L. G., Hydrogen effect on adhesion and adhesive transfer at aluminum/diamond interfaces. Physical Review B 2003, 68 (20), 201403.
102. **Qi, Y.**; Cheng, Y. T.; Çağın, T.; Goddard, W. A., Friction anisotropy at Ni(100)/(100) interfaces: Molecular dynamics studies. Physical Review B 2002, 66 (8), 085420;
103. Goddard, W. A.; Çağın, T.; **Qi, Y.**; Zhou, Y.; Che, J.. First Principles Multiscale Modeling of Physico-Chemical Aspects of Tribology, Tribology Series 2001, 39, 15-33
104. **Qi, Y.**; Çağın, T.; Goddard, W.A, MPiSIM: Massively parallel simulation tool for metallic system. Journal of Computer-Aided Materials Design 2001, 8 (2-3), 185-192;
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106. **Qi, Y.**; Çağın, T.; Johnson, W. L.; Goddard, W. A., Melting and crystallization in Ni nanoclusters: The mesoscale regime. Journal of Chemical Physics 2001, 115 (1), 385-394;
107. **Qi, Y.**; Strachan, A.; Çağın, T.; Goddard, W. A., Large scale atomistic simulations of screw dislocation structure, annihilation and cross-slip in FCC Ni. Materials Science and Engineering A 2001, 309, 156-159.
108. Çağın, T. Che, J., **Qi, Y.**, Zhou, J., Demiralp, E., Gao, G., Goddard, W. A., Computational materials chemistry at the nanoscale", Journal of Nanoparticle Research 1999, 1 (1) 51-69

109. Ikeda, H.; **Qi, Y.**; Çağın, T.; Samwer, K., Johnson, W. L., Goddard, W. A., Strain rate induced amorphization in metallic nanowires. Physical Review Letters 1999, 82 (14), 2900-2903;

110. **Qi, Y.**; Çağın, T.; Kimura, Y.; Goddard, W. A., Molecular-dynamics simulations of glass formation and crystallization in binary liquid metals: Cu-Ag and Cu-Ni. Physical Review B 1999, 59 (5), 3527-3533.

Reviewed Conference Papers

1. **James, C.***; Wu, Y.; Sheldon, B. W.; **Qi, Y.**. Computational Analysis of Coupled Anisotropic Chemical Expansion in $Li_{2-x}MnO_{3-\delta}$., MRS Advances 2016, 1 (15) 1037-1042.
2. **Liu J.***; Li, X. D.; **Qi, Y.**. Computational Insights into High Strain Rate Self-stiffening Mechanism in Nacre, Proceedings of the American Society for Composites 2015 - Thirtieth Technical Conference on Composite Materials, Ed:.Xiao X., Loos. A., Liu, D., DEStech Publications, Inc, 2015 Pg. 2040-2050
3. Çağın, T.; Kimura, Y., **Qi, Y.**; Li, H., Ikeda, H., Johnson, W. L.; Goddard, W. A., Calculation of mechanical, thermodynamic and transport properties of metallic glass formers, Materials Research Society Symposium Proceedings 1999, 554, 43-50;

Book Chapters

1. Verbrugge, M. W.; **Qi, Y.**; Baker, D. R.; Cheng, Y. T.. Diffusion-induced stress within core-shell structures and implications for robust electrode design and materials selection, **Electrochemical Engineering Across Scales: From Molecules to Processes, Advances in Electrochemical Sciences and Engineering**, Edited by R.C. Alkire and J. Lipkowski, John Wiley & Sons, 2015, p193-225

Awarded Patents

1. Coated Seal For Sealing Parts In A Vehicle Engine, **Qi, Y.** and Yuen P. K., US7968167
2. Machining of Aluminum Surfaces, **Qi, Y,** US 8057133
3. Battery module for mitigating gas accumulation and methods thereof, **Qi, Y.,** Moote, J., Lin, Q., Harris, S.J., US 9281548, US9601732

Invited Presentations at Conferences

- Modeling the Lithiation and Delithiation Process at a Passivated Lithium Electrode Surface, GRC Electrochemistry, January 2018, Ventura, CA
- Quantify the Fundamental Irreversible Structural and Chemical Changes for Nanostructure Designs in Battery Applications, Joint ECS-SCE meeting, December, 2017, Shanghai, China
- Computational Insights to Charge Transfer Reactions at the Complex Electrode/SEI/Electrolyte Interface, 254th ACS National Meeting, August 2017, Washington DC
- DFT and DFTB simulations of lithium ion transport through the complex electrode/SEI/electrolyte interface. 21st International Conference on Solid State Ionics (SSI-21), June 2017, Padua, Italy
- Computational Studies of Charge Transfer, Oxygen vacancy Formation and Interaction in $La_{1-x}SrxFeO_{3-\delta}$, 21st International Conference on Solid State Ionics (SSI-21), June 2017, Padua, Italy
- Multi-component and Multi-functional Protection coating for high capacity anodes (Li and Si), MRS Spring meeting, April 2017, Phoenix, AZ
- Computational Design of the Nanostructure of CNT-encapsulated-S Cathodes, 2017 TMS Annual Meeting, March 2017, San Diego, CA
- Computational Design of Coatings, Interfaces, and nano-structures for Si based electrodes, 2016 CINT Users Meeting, Sep 2016, Santa Fe, NM
- Computational Design of Coatings, Interfaces, and nano-structures for Si based electrodes, 229th ECS Meeting, May. 2016, San Diego, CA
- Mechano-Electro-Chemical (MEC) Coupling in Lithium Intercalation Compounds, Materials Challenges in Alternative & Renewable Energy (MCARE 2016), April 2016, Tempa, FL
- The role of Fe-O complex in determining Oxygen nonstoichiometry in the Lanthanum Strontium Ferrite (LSF) System, TMS 2016, Feb 2016, Nashville, TN
- Mechano-Electro-Chemical (MEC) Coupling in Lithium Intercalation Compounds, 228th ECS Meeting, Oct. 2015, Phoenix, AZ
- From Material Modeling to Li-ion Battery Life Prediction --- a Closer Look at the Degradation Mechanisms, Battery Congress (Keynote presentation), June 2015, Troy, MI
- Predicting Lithium Transport in Solid Electrolyte Interphases (SEI), 20th International Conference on Solid State Ionics (SSI-20), June 2015, Keystone, CO
- Integrating SOC dependent material properties into Li-ion battery failure modeling toward the design of Si composite electrode, MRS Spring Meeting, April 2015, San Francisco, CA
- Predicting Lithium Transport in Solid Electrolyte Interphases, 144th TMS Annual Meeting & Exhibition, March 2015, Orlando, FL
- Predict and Design Interface Properties for Si based Electrode in Li-Ion Batteries, 144th TMS Annual Meeting & Exhibition, March 2015, Orlando, FL
- Predicting Transport Properties in Solid Electrolyte Interphases (SEI), 227th ECS Meeting, May 2015, Chicago, IL
- Predicting the transport properties of the solid electrolyte interphase (SEI) in Li-ion batteries MRS Fall Meeting, Nov 2014, Boston, MA.
- Integrating State of Charge (SOC) Dependent Material Properties into Li-ion Battery Failure Modeling. Shanghai University, MGI Research Forum on Energy Storage and Conversion, Dec 2014, Shanghai, China
- Predicting interface properties in Li-ion batteries. 1st International Symposium on Energy Challenges and Mechanics (Keynote presentation), July 2014, Aberdeen, Scotland, UK.
- Defect facilitated electron leakage through the solid electrolyte interphase in Li-ion batteries. 248th ACS National Meeting, Aug 2014, San Francisco, CA
- Integrating state of charge (SOC) dependent material properties into Li-ion battery failure modeling. 248th ACS National Meeting, Aug 2014, San Francisco, CA

- Predicting the transport and mechanical properties of the solid electrolyte interphase in Li-ion batteries. Society of Engineering Science 50th Annual technical Meeting, June 2013, Providence, RI.
- Direct Calculation of Li-ion Transport in the Solid Electrolyte Interphase (SEI), 246th ACS National Meeting, Sep 2013, Indianapolis, IN
- Integrating State of Charge (SOC) Dependent Material Properties Into Li-Ion Battery Failure Modeling, 224th ECS Meeting, Oct 2013, San Francisco, CA
- Mesoscale Modeling of the Morphology and the Mechanical Properties of Proton Exchange Membranes, 142nd TMS Annual Meeting & Exhibition, March 2013, San Antonio, TX
- Understanding and predicting Li transport through SEI, PRiME & ECS Fall Meeting, Oct 2012, Honolulu, HI
- How Li transports through the solid electrolyte interphase, Batteries Gordon Conference, Mar. 2012, Ventura, CA
- How Li ions transport through SEI -- Insights Gained From Experiments and Predictive Modeling Battery Congress, Apr. 2012, Ann Arbor, MI
- Designing Interfaces for Nano Crystalline Diamond Coatings, MRS Fall Meeting, Dec 2011, Boston, MA
- Coupling chemistry and mechanics to understand the influence of environments on material properties, MRS Fall Meeting, Dec 2011, Boston, MA
- Computational Materials Design - From Hard Coatings to Soft Membranes, MIT Materials Day, Oct 2011, Cambridge, MA
- Integrating SOC Dependent Material Properties into Li-ion Battery Failure Modeling, MS&T, Oct 2011, Columbus, OH
- Atomistic Predictions on Chemical Effects at Grain Boundaries, MS&T, Oct 2011, Columbus, OH
- Multiscale mechanics issues for Li-ion batteries, The Third International Conference of Heterogeneous Materials Mechanics (ICHMM), May 2011, Shanghai, China
- Modeling and Visualization of Anode Materials' Deformation during Li Insertion, ECS Detroit Section Meeting, Oct 2010, Southfield, MI
- Designing Interfaces for Nano Crystalline Diamond Coatings, MS&T, Oct 2010, Houston, TX
- Integrating material properties and Microstructures into Li-ion battery failure modeling, DOE Computational Materials Science Network meeting at NIST, Sep 2010, Gaithersburg, MD
- Integrating Atomic Potentials Across Interfaces, Workshop on Industrial Needs for Atomic Potentials at NIST, July 2010, Gaithersburg, MD
- Atomistic Predictions for Grain Boundary Sliding in Aluminum and The Effect of Solute Additions, MS&T, Oct 2009, Pittsburgh, PA
- Modeling, Measuring and Scale Bridging of the mechanical properties at Al/Si interface, Workshop on Industrial Needs for Atomic Potentials at NIST, Apr. 2009, Gaithersburg, MD
- Multiscale modeling for metal forming & a wish list of alloying elements, Workshop on Industrial Needs for Atomic Potentials at NIST, Apr. 2008, Gaithersburg, MD
- Can one atomic layer change adhesion, adhesive transfer and friction MRS Spring Meeting, March 2008, San Francisco, CA
- Computational Materials Design for Automobiles, Accelrys Science Forum, Oct 2007, Princeton, NJ
- Mechanical behavior of aluminum-silicon interfaces, MS&T, Sep 2007, Detroit, MI
- Multiscale modeling in automobile materials research: For engines, door panels and fuel cells,234th ACS National Meeting, Aug 2007, Boston, MA
- Atomic Modeling of Adhesion, Adhesive Transfer and Friction, Workshop on Mechanical Behaviour of Systems at Small Length Scales, Feb 2007, Bangalore, India,
- Atomic Modeling of Adhesion, Adhesive Transfer and Friction at Aluminum/Carbon Interfaces, 232nd ACS National Meeting, Sep 2006, San Francisco, CA

- Atomic Simulation of Adhesion, Adhesive Transfer, and Friction at Al/Carbon interfaces, MRS Fall meeting, Nov 2005, Boston MA
- Deformation and Phase Transformation in Nano Single Crystals - When will Nano Crystals Start to Behave Strangely?, APS March Meeting, Mar 2002, Indianapolis, IN

Seminars at Universities and National Labs

- The thin passivation layer on aluminum and lithium metals, UNC Charlotte, NC, October 2017
- Understanding Oxygen Vacancy for Solid Oxide Fuel Cell and Battery Materials --- Charge Transfer, Polaron Shape, Strain, and Interactions, Department of Mechanical and Aerospace Engineering, West Virginia University, April 2017
- Modeling of the Interface and Interphases in Li-ion batteries, Department of Chemical & Biological Engineering, Drexel University, Dec 2016
- Modeling of the Interface and Interphases in Li-ion batteries, Physics Department, Wake Forest University, Oct 2016
- From material modeling to Li-ion Battery life prediction --- a closer look at the degradation mechanisms, Yanshan University, Jul 2016
- From material modeling to Li-ion Battery life prediction --- a closer look at the degradation mechanisms, Shanghai Jiaotong University, Jul 2016
- Modeling of the Interface and Interphases in Li-ion batteries, Department of Chemical and Materials Engineering, University of Kentucky, April 2016
- Predicting the transport and mechanical properties of the solid electrolyte interphase (SEI) in Li-ion batteries. Chemical and Biomolecular Eng. Department, University of Tennessee, Nov 2014
- Predicting the transport and mechanical properties of the solid electrolyte interphase (SEI) in Li-ion batteries. Georgia Institute of Technology, June 2014
- Coupling chemistry and mechanics to understand the influence of environment on material properties. The University of Science and Technology Beijing, China. Nov 2013
- Designing Interfaces for Diamond-like carbon (DLC) & Nano-crystalline Diamond (NCD) Coatings. Mechanical Engineering, Tsinghua University. Nov 2013
- Understanding and designing interfaces & interphases in Li-ion batteries. Institute of Physics, Beijing, China. Nov 2013
- The interconnection between modeling and experiments toward understanding Li-ion battery failures. The Hong Kong University of Science & Technology. Nov 2013
- Computational Materials Design - From Hard Coatings to Soft Membranes, Chemistry Department, Oakland University, Nov 2013
- The interconnection between modeling and experiments toward understanding Li-ion battery failures, PRISM Seminar, Princeton, Dec 2012
- Computational Material Design – From Hard Coatings to Soft Membranes, Transforming Energy Lecture Series, University of Maryland, July 2012
- The interconnection between modeling and experiments toward understanding Li-ion battery failures, Army Research Lab, July 2012
- Modeling and Visualization of Anode Materials' Deformation during Li Insertion, National Renewable National Lab, Nov 2011
- The interconnection between modeling and experiments toward understanding Li-ion battery failures, ECE Seminar, Wayne State University, Sep, 2011
- Computational Material Design – from hard coatings to soft membranes Michigan State University, Oct, 2010
- Modeling and Visualization of Anode Materials' Deformation during Li Insertion, Department of Materials Science & Engineering, Penn State University, April, 2010

- Modeling and Visualization of Anode Materials' Deformation during Li Insertion, Sandia National Lab, March, 2010
- Modeling and Visualization of Anode Materials' Deformation during Li Insertion, Department of Mechanical Engineering, Michigan State University, Feb, 2010
- Modeling and Visualization of Anode Materials' Deformation during Li Insertion, Oak Ridge Nation Lab, Nov, 2009
- Computational Material Design – from hard coatings to soft membranes, Materials Science and Engineering Department, Georgia Tech, Apr, 2009
- Enable NCD coating through experiments and modeling - bonding chemistry with mechanical properties , Department of Mechanical Engineering, IUPUI, Nov, 2008
- Computational Materials Design for Aluminum Dry Machining and Quick Plastic Forming, Solid State Seminar, Physics Department, McGill University, Oct, 2008
- Computational Material Design --- from hard coating to soft membrane Seminar in Chemistry Department, University of Sherbrooke, Oct, 2008
- Multi-scale Modeling in Tribology and Material Design, Seminar in the Mechanical Engineering Department, University of South Carolina, Nov, 2006
- Multiscale Modeling of Proton Exchange Membrane (PEM) for Fuel Cell Cars, Joint Materials/Solid Mechanics Seminar Series, Brown University, Oct, 2006
- Multi-scale Modeling in Tribology and Material Design, Mechanical Properties Seminar in the Materials Science and Engineering Department, Ohio State University, May, 2006
- Atomistic Simulations of Material Deformation, Joint Materials/Solid Mechanics Seminar Series, Brown University, July 2002

IV. Teaching and Supervisory Experience

Courses Taught at MSU	Students	Year
MSE991, Special topics – Computational Materials Science	10-~23	Spring 2014, 2015
MSE991, Atomistic Simulations for Materials Science	10	Spring 2016, 2018
MSE310, Phase Equilibria in Materials	35~40	Fall 2014, 2015, 2016, 2017
MSE250, Introduction to Materials Science (Lab)	179	Spring 2015
MSE465, Design and Application of Engineering Materials	35	Spring 2017

Other Teaching Activities	Location	Year
One day tutorial on “Materials for Li-Ion Batteries: Structures, Performance, and Durability”	Electrochemical Society meeting	Spring, 2011
Training course on “Basics of Electrochemical Cells and Li-ion Batteries”	U.S. Army TARDEC	Spring 2010
Guest lecture on “Practical density function theory” for the “Quantum, Statistical, and Continuum Mechanics” Course	Brown University	Fall 2006
A series of lectures on “fundamentals of atomic simulations”	Materials and Processing Lab, GM R&D	Summer 2001

K-12 Outreach and Recruiting	Year
Led a fruit battery station on MSU STEM Demo Day for Girl Scouts	Feb 2014, 2015
Designed and led a station on “Predicting Atomic Structure with Computers" at the "Introduce a Girl to Engineering Day".	Feb 2016, 2017
Designed and taught a module on “computer and materials” for 6-8th grade girls in the Spartan Girls in Engineering summer camp	July, 2015, 2016
Lectured and designed hands-on laboratory activities for 40-50 high school students in the High School Engineering Institute (HSEI) Program.	July 2015
Presented Materials Science program on Preview Day and ADS to high school students. *At least two students emailed me after the preview day, saying that they will select MSE as their major*.	2013, 2014
Hosted high school student in my lab via the Michigan State University High School Honors Science/Mathematics/Engineering Program (HSHSP)	2014

PhD Students Advised
Christine James, Kwang-Jin Kim, Yuxiao Lin, Jialin Liu, Hong-Kang Tian, Joe, T. Phongpreecha, Tridip Das

Postdoc Researchers Advised
Dr. Michael Swift, Dr. Bo Xu, Dr. Yun-song Li, Dr. Sung-Yup Kim, Dr. Siqi Shi, Dr. Haibo Guo

Other PhD Students Co-Advised through Collaborations
Jie Pan, Maria E. Stournara, Fatih Sen, Ningning Du, Sang Xiong, Shutian Yan, Shuman Xia, Donald Ward,

Master Student, Undergraduate and High School Student Researchers Advised
PhucThanh Tran, James Wortman, Young Kim, Nupur Banerjee

V. Service

Professional Society Membership

MRS, Materials Research Society (2001-present)
TMS, The Minerals, Metals and Materials Society (2004 – present)
ECS, The Electrochemical Society (2009 – present)
ACS, American Chemical Society (2012 – present)
AVS, American Vacuum Society (2012 – present)
APS, American Physical Society (2001 – 2011)

Leadership role

2017	Discussion Panel Lead for DOE BES workshop on Basic Research Needs for Next Generation Electrical Energy Storage
2014~2016	Vice-chair, Chair-Elect, and Chair of the Energy Subdivision of Physical Chemistry division of American Chemistry Society
2015~2017	Chair of American Vacuum Society Michigan Chapter
2014~present	Key Reader for Metallurgical and Materials Transactions
2016	TMS, AIME Henry DeWitt Smith Scholarship Committee
2013	TMS Young Leaders Committee

Conference and Symposia Organizer

2018	Organizer for Symposium “Solid-Solid Interfaces in Batteries, Energy Storage and Conversion - Diagnostic and Modeling” at the 2018 MRS Spring Meeting.
2016	Organizer for Symposium “Battery Modeling and Computation” at the 229th ECS Meeting.
2016	Organizer for Symposium “Electrochemistry at Solid/Liquid Interfaces” at the 251st ACS National Meeting & Exposition
2015	Lead Organizer for Symposium “Batteries - Theory, Modeling, and Simulation” at 228th ECS meeting
2014	Chair for 40th Annual Symposium American Vacuum Society – Michigan Chapter
2014	Organizer for Symposium Mechanical-Electrochemical Coupling in Energy Related Materials and Devices for ECS 2014 Spring meeting
2013	Program Chair for 2013 Battery Congress
2011	Panel Leader on Multiscale Mechanics Issues for Li-ion Batteries at the 2011 International Computational Heterogeneous Materials Mechanics meeting conference
2011	Organizer for Symposium Microstructure, Mechanisms, and Modeling of Battery Materials for ECS 2011 Spring meeting
2011	Organizer for Focus Session Computational Design of New Materials for APS 2011 March meeting
2009	Organizer for Focus Session Interface Science and Engineering for APS 2009 March meeting
2008	Organizer for Computational Material Design via Multiscale Modeling for MRS 2008 Fall meeting
2008	Organizer for Focus Session Engineering interfaces for new materials: Modeling and Experiments for APS 2008 March meting
2006	Organizer for Focus Session Friction, Fracture and Deformation for APS 2006 March meetings

Department / School / University Service:

- Graduate Coordinator for MSE program (recruitment, admission, and advising) (2016~present)
- Chaired 2015 and 2016 CHEMS Forum (2015, 2016)
- University Committee for the Library (2014~present)
- CHEMS Curriculum Committee

- CHEMS Chair Search Committee (2016~2017)
- Multiple faculty search committees for CHEMS, ME, and CMSE (2014~present)
- Presented Materials Science program on Preview Day and ADS to high school students.
- Advisor for SWE (Society of Women Engineering).

Volunteering for Educational Outreach

- Led a station on "Building Atomic Structure with Computers" at the "Michigan State Introduce a Girl to Engineering Day". (2016, 2017)
- Taught at Spartan Girls in Engineering summer camp (2015, 2016)
- Led a fruit battery station on MSU STEM Demo Day for Girl Scouts.(2014, 2015)
- Judge for Women in Engineering Poster Presentation Competition, University Pennsylvania (2008).
- Volunteer for MS&T 2007 Student Camp (2007)
- Presenter at the Sally Ride Science Festivals for girls (2006)
- Presenter at the GM R&D open house for high school students (2004)

Reviewing activity (journals and research agencies)

Regular Journal Reviewer (average 15~20 annually):

The Journal of Physical Chemistry
Nano Letter
Chemistry of Materials
ACS Applied Materials & Interfaces
Physical Chemistry Chemical Physics
Nano Horizon (RCS Publishing)
Chemistry of Materials
Journal of Materials Chemistry A
Journal of Electrochemical Society
Electrochimica Acta
Metallurgical and Materials Transactions
Journal of Materials Research
Journal of Materials Science
Journal of Applied Physics
Computational Materials Science
Surface Science
Corrosion Science
Journal of Electronic Materials
Solid State Ionics
Extreme Mechanics Letters

Proposal Reviewer:

National Science Foundation
U.S. Department of Energy - Basic Energy Sciences
U.S. Department of Energy - Office of Energy Efficiency & Renewable Energy
ACS – Petroleum Research Fund