

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

- 2020 - present **Joan Wernig Sorensen Professor** of Engineering, Brown University
- 2018-2020 **Associate Dean** of Inclusion and Diversity, College of Engineering, Michigan State University
- 2018-2020 **Professor**, Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing, Michigan
- 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

IV. Publications (* students/postdocs in Qi's lab, underlines: (Co)-Corresponding Author)

Accepted Journal Papers

1. **Wu, Q.***, McDowell, M., **Qi, Y.**, "The effect of the electric double layer (EDL) in multi-component electrolyte reduction and solid electrolyte interphase (SEI) formation in lithium batteries", J. Am. Chem. Soc. (2023)
2. Zhang, D.; **Park J.***; **Xu, B.***; Liu, C.; Li, W.; Liu, X.; **Qi, Y.**; Luo, J., "Unusual aliovalent doping effects on oxygen non-stoichiometry in medium-entropy compositionally complex perovskite oxides", Dalton Transactions, (2023) DOI:10.1039/D2DT03759A

Published Journal Papers

1. **Jagad, H.D.***, SJ Harris, S.J., Sheldon, B.W., **Qi, Y.**, Tradeoff between the Ion Exchange-Induced Residual Stress and Ion Transport in Solid Electrolytes, Chem. Mater. 2022, 34, 19, 8694–8704
2. **Feng, M.***, **Yang, C.T.***, **Qi, Y.**, "The Critical Stack Pressure to Alter Void Generation at Li/Solid-Electrolyte Interfaces during Stripping" J. Electrochem. Soc., 2022, 169, 090526
3. **Swift MW***, **Jagad H***, **Park J.***, **Qie, Y***, **Wu, Y***, **Qi, Y.** Predicting low-impedance interfaces for solid-state batteries, Current Opinion in Solid State and Materials Science, 2022, 100990
4. Wu, M., Zhang, X., Zhao, Y. Yang. C., Jing, S., **Wu, Q.***, Brozena, A., Miller, J.T., Libretto, N.J., Wu, T., Bhattacharyya, S. Garaga, M.N., Zhang, Y., **Qi, Y.**, Greenbaum, S., Briber, R., Yan, Y., Hu, L., "A high-performance hydroxide exchange membrane enabled by Cu²⁺-crosslinked chitosan.", Nature Nanotechnology, 2022, 17, 629–636 (*Nature cover*)
5. **Lin, Y.X.***, Ticey, J., Oleshko, V., Zhu, Y., Zhao, X., Wang, C.S., Cumings, J., and **Qi, Y.**, "Carbon-Nanotube-Encapsulated-Sulfur Cathodes for Lithium-Sulfur Batteries: Integrated Computational Design and Experimental Validation", Nano Letters, 2022, 22, 1, 441–447
6. Yang, C., **Wu, Q.***, Xie, W., Zhang, X., Zhang. X., Brozena, A., Zheng, J., Garaga, M.N., Ko, B.H., Mao Y., He, H., Gao, Y., Wnag, P., Tyagi, M., Jiao, F., Briber, R., Albertus, P., Wang, C.S., Greenbaum, S., Hu, Y.Y., Winter, M., Xu, K., **Qi, Y.**, Hu, L. "Copper-Coordinated Cellulose Ion Conductors for Solid-State Batteries, Nature 2021, 598 (7882), 590-596 (*News by sciencedaily ..*)
7. Fuller E.J., Strelcov E., Jamie L. Weaver, J.L., **Swift, M.W.***, Sugar, J.D., Kolmakov, A., Zhitenev, N., McClelland, J.J., **Qi, Y.**, Dura, J., and Talin, A.A., Spatially Resolved Potential and Li-Ion Distributions Reveal Performance-Limiting Regions in Solid-State Batteries, ACS Energy Lett. 2021, 6, 3944–3951
8. **Feng, M.***; **Pan, J.***; **Qi, Y.**, The Impact of Electronic Properties of Grain Boundaries on the Solid-Electrolyte-Interphases (SEI) in Li-ion Batteries", JPCC 2021, 125 (29), 15821-15829
9. **Noel M. N.**, **Smiadak, D.M.**, **Pan, J.**; **Qi, Y.**, Zevalkink, A., Investigation of (001), (010), and (100) Surface Termination and Surface Energies of the Zintl Ca₅Ga₂Sb₆, Surface Science 2021, 714, 121918
10. Dai, Z.; Yadavalli, S.K; Chen, M.; **Abbaspourtamijani, A.***; **Qi, Y.**; Padture, N.P Interfacial toughening with self-assembled monolayers enhances perovskite solar cell reliability, Science 2021. 372, 618-622 (*Highlighted by Nature Energy "Get Tougher"*)
11. **Swift, M.W.***, **Swift, J.W.**, **Qi, Y.**, Modeling the electrical double layer at solid-state electrochemical interfaces, Nature Computational Science 2021, 1, 212-220 (*Highlighted by Nature News and Views*)
12. **Yang, C.T*** and **Qi, Y.**, Maintaining a flat Li surface during Li stripping process via interface design, Chemistry of Materials 2021, 33, 2814-2823
13. Zhang, M., Rao, Z., Kim, K.S., **Qi, Y.**, Feng, L., Sun, K., Chason, E., Molecular dynamics simulations of stress induced by energetic particle bombardment in Mo thin films, Materialia 2021, 16, 101043
14. Hu, G., Zhou, Q., Bhatlawande, A., **Park, J.***, Termuhlen, R., Ma, Y., Bieler, T.R., Yu, H.C., **Qi, Y.**, Hogan, T., Nicholas, J.D., Patterned Nickel Interlayers for Enhanced Silver Wetting, Spreading and Adhesion on Ceramic Substrates, Scripta Materialia 2021, 196, 113767
15. Nation, L., Wu, Y., Li, X., Chi, M.F., **Wu, Y.Q.***, **Qi, Y.**, Sheldon, B.W., Redox-Couple Investigations in Si-Doped Li-Rich Cathode Materials, Phys. Chem. Chem. Phys. 2021,23, 2780-2791

16. Liu, Z., **Li, Y.S.***, Ji, Y., Zhang, Q.L., Xiao, X.C., Yao, Y., Chen, L.Q., **Qi, Y.**, Dendrite Free Li based on the Lesson Learned from the Li and Mg Electrodeposition Morphology Simulations, *Cell Reports Physical Science* 2021, 2(1), 100294
17. Bi, Y., Tao, J., **Wu, Y.Q.***, Li, L., Xu, Y., Hu, E., Wu, B., Hu., J., Wang, C.M, Zhang, J.G., **Qi, Y.**, Xiao, J., Reversible Planar Gliding and Microcracking in Single Crystalline Ni-rich Cathode for Advanced Li-ion Batteries, *Science* 2020, 370(6522), 1313-1317, *Science Cover article*
18. **Qi, Y.**, Ban, C.M., Harris, S., A Proposed New Paradigm for Preventing Li Metal Penetration Through Solid Electrolytes, *Joule* 2020, 4(2), 2599-2608
19. **Yang, C.T.***, **Lin, Y.X.***, Li, B., Xiao, X.C., **Qi, Y.**, The Bonding Nature and Adhesion of Polyacrylic Acid (PAA) Coating on Li-metal for Li Dendrite Prevention, *ACS Appl. Mater. Interfaces* 2020, 12(45), 51007–51015
20. **Park J.Y.***, **Phongpreecha, T***, Nicholas, J.D, and **Qi Y.**, Enhancing liquid metal wetting on oxide surfaces via patterned nanoparticles, *Acta Mat.* 2020, 199, 551-560
21. O'Hearn, K.A., **Swift, M.W.***, **Liu, J.L.***, Magoulas, I., Piecuch, P., van Duin, A.C.T., H. Metin Aktulga, H.M., **Qi, Y.**, Optimization of the Reax Force Field for Lithium Dioxide using a High Fidelity Charge Model, *J. of Chemical Physics, Special Topics: Classical Molecular Dynamics (MD) Simulations: Codes, Algorithms, Force Fields, and Applications* 2020, 153 (8), 084107
22. Sinz, P., **Swift, M.W.***, Brumwell, X., **Liu, J.L.***, **Kim, K.J.***, **Qi, Y.**, Hirn, M., Wavelet Scattering Networks for Atomistic Systems with Extrapolation of Material Properties”, *J. of Chemical Physics, Special Topics: Machine Learning Meets Chemical Physics* 2020, 153 (8), 084109
23. Thenuwara, A; Shetty, P; Kondekar, N; Sandoval, S; Cavallaro, K; May, R; **Yang, C.T.***; Marbella, L; **Qi, Y**; McDowell, M, Efficient Low-Temperature Cycling of Lithium Metal Anodes by Tailoring the Solid-Electrolyte Interphase, *ACS Energy Letters* 2020, 5(7), 2411-2420
24. **Lin, Y.X.***, Zheng, J., Wang, C.S., **Qi, Y.**, The origin of the two-plateaued or one-plateaued open circuit voltage in Li/S batteries, *Nano Energy* 2020, 75, 104915
25. **Tian, H.K.***, Chakraborty, A., Talin, A.A., Eisenlohr, P., **Qi, Y.**, Evaluation of the electrochemo-mechanically induced stress in all-solid-state Li-ion batteries, *J. Electrochem. Soc.* 2020, 167, 090541
26. **Das, T.***; Nicholas, J.D.; **Qi, Y.**, Composition, Crystallography, and Oxygen Vacancy Ordering Impacts on the Oxygen Ion Conductivity of Lanthanum Strontium Ferrite, *PCCP* 2020, 22, 9723-9733
27. Wang, L., **Lin, Y.***, DeCarlo, S., Wang, Y., Leung, K.; **Qi, Y.**, Xu, K., Wang, C., Eichhorn, B., Compositions and Formation Mechanisms of Solid-Electrolyte-Interphase (SEI) on Microporous Carbon/Sulfur Cathodes, *Chemistry of Materials*, 2020, 32, 9, 3765-3775
28. Harris, O, **Lin, Y.X.***, **Qi, Y.**, Leung, K., Tang, M. How transition metals enable electron transfer through the SEI: Part I. Experiments and Butler-Volmer modeling, *Journal of The Electrochemical Society* 2020, 167(1), 013502
29. Xu, J.G., **Tian, H.K.***, **Qi, J.***, Zhang, Q.L., **Qi, Y.**, Xiao, X.C., Mechanical and Electronic Stabilization of Solid Electrolyte Interphase with Sulfite Additive for Lithium Metal Batteries, *J. Electrochem. Soc.* 2019, 166 (14), A3201-A3206
30. Kang, N., **Lin, Y.X.***, Yang, L., Lu, D., Xiao, J., **Qi, Y.**, Cai, M., Understanding the electrochemical performance of lithium-sulfur batteries with different sulfur electrode, *Nature Communications* 2019, 10, Article number: 4597
31. **Tian, H.K.***, Liu, Z., Ji, Y., Chen, L.Q., **Qi, Y.**, Interfacial Electronic Properties Dictate Li Dendrite Growth in Solid Electrolytes, *Chemistry of Materials* 2019, 31(18) 7351-7359
32. **Swift, M.W.*** and **Qi, Y.**, First-principles prediction of potentials and space-charge layers in all-solid-state batteries, *Phys. Rev. Lett.* 2019, 122, 167702
33. **Li, Y.S.***, **Qi, Y.**, Energy Landscape of the Charge Transfer Reaction at the Complex Li/SEI/Electrolyte Interface, *Energy Environ. Sci.* 2019,12, 1286-1295 (*Highlighted by Nature Energy; Selected for 2019 EES hot Articles*)
34. Dong, X., **Lin, Y.X.***, Li, P., Ma, Y., Huang, J., Guo, Z., Bin, D., Wang, Z., Wang, Y.G., **Qi, Y.**, Xia, Y.Y., High Energy Rechargeable Metallic Lithium Battery At -70°C Enabled By A Co-Solvent Electrolyte, *Angew. Chem. Int. Ed.* 2019, 58(17) 5623-5627

35. Liu, J.L.*; Wang, Q.G.; **Qi, Y.**, Atomistic Simulation of the Formation and Fracture of Oxide Bilayers in Cast Aluminum, *Acta Materialia* 2019, 164, 673-682 (*Selected and featured by Advances in Engineering*)
36. **Phongprecha, T.***; Liu, J.*; Hodge, D.; **Qi, Y.**, Adsorption of Lignin β -O-4 Dimers on Metal Surfaces in Vacuum and Solvated Environments, *ACS Sustainable Chem. Eng.* 2019, 7(2), 2667-2678 (*Selected by the Virtual Special Issue - Catalytic Byproduct Valorization in Future Biorefineries*)
37. Nation, L.; Wu, Y.; **James, C.***; **Qi, Y.**; Powell, B.; Sheldon, B.W. Si-Doped High-Energy Li_{1.2}Mn_{0.54}Ni_{0.13}Co_{0.13}O₂ Cathode with Improved Capacity for Lithium-Ion Batteries, *Journal of Materials Science* 2018, 33(24), 4182-4191
38. Liu, Z.; Lu, P.; Zhang, Q.L.; Xiao, X.C.; **Qi, Y.**; Chen, L.Q.; A Bottom-up Formation Mechanism of Solid Electrolyte Interphase (SEI) Revealed by Isotope-Assisted Time-of-Flight Secondary Ion Mass Spectrometry (TOF SIMS), *Physical Chemistry Letters* 2018, 9 (18), 5508-5514
39. **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
40. **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
41. **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)
42. **Phongprecha, 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 Ytria-Stabilized-Zirconia, *Acta Materialia* 2018, 152, 229-238
43. 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; Web of Science Highly Cited Paper and Hot Paper*)
44. 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
45. 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*)
46. **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
47. 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
48. **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
49. 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
50. Pan, J.; Lany, S.; **Qi, Y.**, Computationally Driven Two-Dimensional Materials Design: What Is Next?, *ACS Nano* 2017, 11, 7560-7564 (*Invited Perspective*)
51. **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
52. **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
53. **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

54. **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
55. 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 LiCoO₂ cathode in aqueous electrolyte with interphase-forming additive, *Energy and Environmental Science* 2016, 9, 3666-3673
56. **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*)
57. **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*)
58. **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
59. **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-δ}. *Journal: Solid State Ionics* 2016, 289, 87-94
60. **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
61. 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
62. 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
63. 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
64. **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
65. **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
66. 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
67. **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;
68. Sun, S.; **Qi, Y.**; Zhang, T. Y., Dissecting graphene capacitance in electrochemical cell. *Electrochimica Acta* 2015, 163, 296-302;
69. 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;
70. 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;
71. 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;
72. **Kim, S. Y.***; **Qi, Y.**, Property Evolution of Al₂O₃ Coated and Uncoated Si Electrodes: A First Principles Investigation. *Journal of the Electrochemical Society* 2014, 161 (11), F3137-F3143;
73. 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;

74. 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;
75. **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;
76. **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.
77. **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*)
78. **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.
79. 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;
80. 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;
81. 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;
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83. **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), 051912
84. **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*)
85. **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;
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87. Zhang, H.; Liu, X.; **Qi, Y.**; Liu, V., On the $\text{La}_{2/3-x}\text{Li}_x\text{TiO}_3/\text{Al}_2\text{O}_3$ composite solid-electrolyte for Li-ion conduction. *Journal of Alloys and Compounds* 2013, 577, 57-63.
88. 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;
89. 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*)
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Reviewed Conference Papers

1. **Liu, J.L.***, Wang, Q.G., **Qi, Y.**, Connecting Oxide Bifilms' Properties from Atomistic Simulations with Virtual Casting of Aluminum, Shape Casting, In: Tiryakioğlu M., Griffiths W., Jolly M. (eds) Shape Casting. The Minerals, Metals & Materials Series. Springer, Cham. https://doi.org/10.1007/978-3-030-06034-3_4
2. Brumwell, X., Sinz, P., **Kim, K.J.***, **Qi, Y.**, Hirn, M., Steerable Wavelet Scattering for 3D Atomic Systems with Application to Li-Si Energy Prediction, The Neural Information Processing Systems (NIPS) workshop on “Machine Learning for Molecules and Materials.” (2018)
3. **James, C.***; Wu, Y.; Sheldon, B. W.; **Qi, Y.**. Computational Analysis of Coupled Anisotropic Chemical Expansion in Li_{2-x}MnO_{3- δ} , *MRS Advances* 2016, 1 (15) 1037-1042.
4. **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

5. 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
2. 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

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

V. Invited Presentations at Conferences

- The Role of SEI Heterogeneity on Charge Transfer Reactions at Li/SEI/electrolyte Interfaces, Distinguished Invited Speaker, Dec 2022, Boston, MA, MRS 2021 Fall Meeting & Exhibit
- The impact of the Interface layer on Li Plating and Stripping morphology, Oct 2022, College Station, TX, Keynote talk at the SES Conference
- When electrons meet ions, multiscale modeling of interfaces in Li-ion Batteries, Aug 2022, Lake of Garda, Italy, European Mechanics Society Colloquium, Multiscale Mechanics, Multiphysics Modeling and Simulations for Energy Storage
- Modeling of the potential distribution and the electrical double layer in solid-state batteries, July 2022, Boston, MA, Keynote Talk at the 23rd International Conference on Solid State Ionics (SSI-23)
- The impact of Interface layer on Lithium Plating and Stripping Morphology, May 2022, Vancouver, Canada, 241st ECS meeting,
- Differentiate the Intrinsic and Extrinsic interface resistance in all-solid-state Li-ion Batteries, May 2022, Online MRS 2022 Spring Meeting.
- Understanding the role of electronic and interfacial properties during Li plating and stripping, Dec 2021, Boston, MA, MRS 2021 Fall Meeting & Exhibit
- Modeling of the potential distribution and the electrical double layer in solid-state batteries, Dec 2021, Boston, MA, MRS 2021 Fall Meeting & Exhibit
- Ion and Electron Transport at Li/SEI/electrolyte Interfaces, Nov, 2021, UT Austin Energy Institute, Workshop on Batteries for Sustainable Future (virtual)
- The Electrochem-Mechanics of Interfaces in All-solid-state Li-ion Batteries, April 2021 Virtual MRS Spring Meeting & Exhibit
- Connecting Atomistic Simulations with Continuum Model for the Charge Transfer Reaction at the Electrode/Electrolyte Interface, April 2021, Oxford Battery Modelling Symposium (Virtual)
- Modeling of the Transfer Transfer Reactions at Li/SEI/electrolyte Interface and Dendrite Free Morphology, April 2021, ACS Spring 2021 (Virtual)
- Modeling of the Charge Transfer Reactions at Li/SEI/electrolyte Interface and Dendrite Free Morphology, Dec 2020, 2020 Virtual MRS Spring/Fall Meeting
- Simulating Materials in Devices --- Considering the electronic and ionic freedom at the Solid-Electrolyte and Electrode Interfaces, Oct 2020, 4th Forum of Materials Genome Engineering (China, online)
- Solvation and De-solvation vs. Electrolyte Design in Li-ion Batteries, Sep 2020, BIOVIA Customer Conference (Virtual)
- Modeling of Interfaces in All-Solid-State Li-ion Batteries, Jan 2020, The 47th Conference on the Physics and Chemistry of Surfaces and Interfaces, (PCSI-47), Boulder, Co
- Modeling of the interfacial Electrochemo-mechanical effects in All-solid-state Li-ion Batteries, Dec 2019, MRS Fall Meeting, Boston, MA
- The Electronic Reasons for Li Dendrite Growth in Solid Electrolytes, Dec 2019, MRS Fall Meeting, Boston, MA
- Modeling of the Space-Charge Layers from First-Principles Calculations, Nov 2019, 1st Workshop "Theory meets experiment", Helmholtz Institute Ulm, Ulm, Germany
- Modeling of Space-Charge Layers via First-Principles Calculations, Oct 2019, 236th ECS Meeting, Atlanta, GA
- Modeling the origin of the interface resistance in Solid-State Batteries, Oct 2019, MS&T 2019, Portland, OR
- Atomically-informed phase-field modeling of Li and Mg electrodeposition morphologies, Aug 2019, ACS National Meeting, San Diego, CA

- Atomic prediction of energy landscape of the charge transfer reaction at the complex Li/SEI/electrolyte interface Aug 2019, ACS National Meeting, San Diego, CA
- Static and Dynamics View of the Solid Electrolyte Interphase during Charge Transfer Reactions --- modeling and experiments, July 2019, ECEE 2019, Glasgow, Scotland
- Atomically-Informed Phase-field Modeling of Li and Mg Electrodeposition Morphologies, May 2019, 235th ECS Meeting, Dallas, TX
- Modeling the origin of the interface resistance in Solid-State batteries MRS Spring Meeting, April 2019, Phoenix, AZ
- Understanding the electrolyte concentration and the effect of solvation for Li-S batteries, March 2019, ACS National Meeting, Orlando, FL
- Connecting Oxide Bifilms' Properties from Atomistic Simulations with Virtual Casting of Aluminum, TMS 2019, Mar 2019, San Antonio, TX
- Computing the Anisotropic Chemical Strain in Non-Stoichiometric Oxides for Solid Oxide Fuel Cell and Li-ion Battery Applications, Electronic Materials and Applications (EMA 2019), Jan 2019, Orlando, FL
- Polaron Size and Shape Effects on Oxygen Vacancy Interactions in Lanthanum Strontium Ferrite, MS&T 2018, Oct 2018, Columbus OH
- Comparison of the interfacial reaction kinetics and plating morphology of lithium and magnesium anodes, 256th ACS National Meeting, Aug 2018, Boston, MA
- Computing the Anisotropic Chemical Strain in Non-Stoichiometric Oxides for Solid Oxide Fuel Cell and Li-ion Battery Applications, 233rd ECS Meeting, May 2018, Seattle, WA
- Simulation of lithium ion transport through the complex electrode/SEI/electrolyte interface, May 2018, 233rd ECS Meeting, Seattle, WA
- Quantify the irreversible structural and chemical changes in nanostructured Si and SiO electrodes, MRS Spring Meeting, April 2018, Phoenix, AZ
- Simulation of lithium ion transport through the complex electrode/SEI/electrolyte interface, 255th ACS National Meeting, March, 2018, New Orleans, LA
- 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 $\text{La}_{1-x}\text{Sr}_x\text{FeO}_{3-\delta}$, 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

- When ions meet electrons --- Modeling the interfaces in Solid-State Batteries, Purdue ECS Chapter Fall 2021 Webinar
- When ions meet electrons --- Modeling the interfaces in Solid-State Batteries, University of Houston, Electrical and Computer Engineering, April 2021 (virtual)
- When ions meet electrons --- Modeling the interfaces in Solid-State Batteries, University of Virginia, Mechanical and Aerospace Engineering Department, April 2021 (virtual)
- When ions meet electrons --- Modeling the interfaces in Solid-State Batteries, University of Pennsylvania, Materials Science and Engineering Department, March 2021 (virtual)
- When ions meet electrons --- Modeling the interfaces in Solid-State Batteries, Stony Brook University seminar, Department of Chemistry, Feb 2021 (virtual)
- When ions meet electrons --- Modeling the interfaces in Solid-State Batteries, Georgia Tech, School of Materials Science and Engineering, Feb 2021 (virtual)
- Simulations of the Thin Passivation Layers - for Aluminum Forming and Lithium-Ion Battery Durability, Department of Materials Science and Engineering, University of Michigan, Dec, Nov 2018

- Simulations of the Thin Passivation Layers - for Aluminum Forming and Lithium-Ion Battery Durability, Department of Materials Science and Engineering, Cornell, Nov 2018
- 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

VI. Awarded Research Funding

Current:

1. "Predicting Charge Transfer Reactions and Morphology Evolution at Complex Electrode/Electrolyte Interfaces Starting from First-Principles", NASA, \$740,000, 2/11/201 ~ 2/10/2024 (PI: Qi)
2. "Collaborative Research: Functionalities of solids enabled by labile elastic dipoles", US-Israel Binational Science Foundation (BSF), \$135,000, 11/1/2021 ~ 10/31/2025 (in collaboration with I. Lubomirsky at Weizmann Institute of Science)
3. "FMRG: Sustainable Route to 3D solid-state Sodium-ion battery by direct ink writing and capillary rise infiltration", National Science Foundation (NSF), \$280,000 toward Qi, 9/1/2021 ~ 8/31/2025 (Lead PI: Eric Detsi at U. Penn)
4. "Fluorinated Ester Local High Concentration Electrolytes for Operation of Li-ion Batteries Under Extreme Conditions", US Department of Energy (DOE), \$450,000 toward Qi, 10/1/2021~12/31/2024 (Lead PI: E.S. Takeuchi at SUNY)
5. "Center for Synthetic Organic Electrochemistry", National Science Foundation (NSF), \$954,500 toward Qi, 9/1/2020~8/30/2025 (Lead PI: Shelley Minteer at U. of Utah)
6. "New High-Entropy Perovskite Oxides with Increased Reducibility and Stability for Thermochemical Hydrogen Generation", US Department of Energy (DOE), \$283,750 toward Qi, 10/1/2019 ~ 1/30/2023 (PI: J. Luo at UC San Diego and Co-PI: X.B. Liu at University of West Virginia)
7. "Fundamental Understanding of Dynamic Interfacial Phenomena in Solid State Batteries", US Department of Energy (DOE), \$ 200,000 toward Qi, 7-1-2020 ~ 5-30-2023 (PI: X.C. Xiao at General Motors; Co-PIs: B. Sheldon at Brown University; Y.T. Cheng at U. of Kentucky)
8. "GOALI - Collaborative Research: Chemically Induced Stresses and Degradation Mechanisms in Ceramic Materials for Li Ion Batteries" National Science Foundation (NSF), \$274,000, 08-01-2018 ~ 07-31-2023 (Collaborators: B. Sheldon at Brown University; X.C. Xiao at General Motors)
9. "Fast Charging, Solid-State, Roll to Roll Processed Li Metal Batteries Enabled by Intercalated Ions in Cellulose Molecular Channels" US Department of Energy (DOE)/EERE, \$292,500 toward Qi, 6/24/2022 ~ 6/23/2025 (PI: Liangbing Hu at University of Maryland)

Finished:

10. "Collaborative Research: Promoting or Suppressing Solid-State Phase Transformation via Interface Control", National Science Foundation (NSF), \$79,769 02-15-2020 ~ 01-31-2022 (PI: Qi; Collaborator: G. Rubloff at U. of Maryland)
11. "Electrolyte and SEI Modeling", General Motors, \$85,000, 1/1/2021 ~ 12/30/2022 (PI: Qi)
12. "High Performance Circuit Pastes for Solid Oxide Fuel Cell Applications", US Department of Energy (DOE), \$50,000 toward Qi, 08-16-2018 ~ 08-15-2020 (PI: J.D. Nicholas, Co-PI: T. Hogan, T.R. Bieler, H.C. Yu)
13. "Dendrite Growth Morphology Modeling in Liquid and Solid Electrolytes", US Department of Energy (DOE), \$1,135,125 (total), \$487,535 toward Qi, 01-01-2017 ~ 12-31-2019 (Lead PI: Qi; Co-PIs: L.Q. Chen at Penn State; X.C. Xiao at General Motors)
14. "In-situ Diagnostics of Coupled Electrochemical-Mechanical Properties of Solid Electrolyte Interphases on Lithium Metal for Rechargeable Batteries", US Department of Energy (DOE)/General Motors (prime), \$274,776, 10-01-2016 ~ 12-31-2019 (Lead PI: X.C. Xiao at General Motors, Co-PIs: Y.T. Cheng at University of Kentucky; B. Sheldon & H.J. Gao at Brown University)

15. “*de Novo* Computational Methods for Simulating Energy Materials”, MSU Foundation - Strategic Partnership Grants, \$399,503 (total), \$120,000 toward Qi, 07-01-2016 ~ 06-30-2019 (Lead PI Qi; Co-PIs: P. Piecuch, H. M. Aktulga, W. Lai)
16. “Understanding the role of oxides in aluminum alloy casting via atomistic simulations”, General Motors Corporation, \$69,288, 09-16-2015 ~ 11-15-2016
17. “Nanostructures for Electrical Energy Storage – Energy Frontier Center”, US Department of Energy (DOE)/University of Maryland (prime), \$640,000, 08-01-2014 - 07-31-2020 (Lead PI: Gary Rubloff at University of Maryland)
18. “Durable, Impermeable Brazes for Solid Oxide Fuel Cells”, US Department of Energy (DOE), \$242,909 toward Qi, 08-16-2014 ~ 08-15-2018 (PI: J.D. Nicholas, Co-PI: T.R. Bieler)
19. “GOALI - Collaborative Research: The Impact of Chemically Induced Stresses on Kinetic Processes and Degradation Mechanisms in Non-Stoichiometric Oxides”, National Science Foundation (NSF), \$275,000, 08-01-2014 ~ 07-31-2018 (Collaborators: B. Sheldon at Brown University; Y. Wu at General Motors)
20. “GOALI: Understanding and Predicting Li Dendrite Formation in Li-Ion Batteries”, National Science Foundation (NSF) / Penn State University (Prime), \$120,126, 04-01-2014 ~ 9-30-2016 (PI: L.Q. Chen at Penn State; Co-PI: P. Lu at General Motors)
21. “A Combined Experimental and Modeling Approach for the Design of High Current Efficiency Si Electrodes”, US Department of Energy (DOE)/General Motors (prime), \$317,868, 01-31-2014 ~ 12-31-2016, (PI: X.C. Xiao at General Motors, Co-PIs: Y.T. Cheng at University of Kentucky; B. Sheldon & H.J. Gao at Brown University)

VII. Teaching Experience

| Courses Taught at Brown | Students | Year |
|--|----------|-----------------------------------|
| ENGN 2920H, Materials and Interfaces for Energy Storage Devices, | 8 | Fall 2021, 2022 |
| ENGN 0040, Dynamics and Vibrations | 125 | Spring 2021, 2022 |
| Courses Taught at MSU | | |
| MSE991, Special topics – Computational Materials Science | 10~23 | Spring 2014, 2015 |
| MSE881, Computational Materials Science | 10 | Spring 2020 |
| MSE991, Atomistic Simulations for Materials Science | 10 | Spring 2016, 2018 |
| MSE310, Phase Equilibria in Materials | 35~40 | Fall 2014, 2015, 2016, 2017, 2018 |
| MSE250, Introduction to Materials Science (Lab) | 179 | Spring 2015 |
| MSE465, Design and Application of Engineering Materials | 35 | Spring 2017 |

| Other Teaching Activities | Location | Year |
|--|---|---------------|
| Lecturer for an ICMS advanced course on “Batteries – Basic Principles, Experimental Investigations and Modeling across Scales” | International Centre for Mechanical Sciences Hybrid online and at Udine, Italy | Sep20-24 2021 |
| 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 Tank Automotive Research, Development and Engineering Center | 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 |

VIII. Service and Leadership

Inclusion and Diversity

- 2020-2022 ELATES Fellowship to attend the Executive Leadership in Academic Technology, Engineering, and Science training program.
- Sep 2021 –present, Inaugural DEI committee chair at the School of Engineering, Brown University. Qi started the DEI committee, dramatically expanded faculty engagement on DEI activities, tripled URM Ph.D. applicants, developed and shared best practices for faculty and postdoc searching/hiring, and co-organized the first Ivy Collective’s Inclusivity in Engineering Doctoral Symposium in 2022.
- Aug 2018~June 2020, Qi served as the first Associate Dean for Inclusion and Diversity in the College of Engineering at Michigan State University. She immediately established two Diversity Awards in the college; initiated Dean’s Faculty Pathway Program to develop the pipeline for faculty from diverse backgrounds; dramatically increased the ratio of women faculty (50% in 2019 new hires), and led the college to win a Bronze Award by the American Society for Engineering Education (ASEE) – the highest level of recognition presented by the ASEE Diversity Recognition Program.

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 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 the 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

2022 Organizer for Symposium for “Solid-State Batteries—Life, Safety and Scalability” at MRS Fall Meeting
 2022 Lead Organizer for the first Symposium on “Multiscale modeling of battery materials” at the 10th International Conference on Multiscale Materials
 2022 Organizer for the “Mechano-Chemical Coupling Symposium” Symposium at the ECS Spring Meeting
 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 meeting
 2006 Organizer for Focus Session Friction, Fracture and Deformation for APS 2006 March meetings

Volunteering for Educational Outreach

- Spoke at the first in-person 2022 “URI Plugged into Energy Research (PIER) Series” on “It’s Electric! Rhode Island’s New Transportation System” for the general public
- 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)