# Curriculum Vitae of Yue Qi, Ph.D


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## I. Education

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|---|---|
| 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

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| 2023 - present | Deputy Director of the Initiative for Sustainable Energy (ISE) |
| 2020 - present | **Joan Wernig Sorensen Professor** of Engineering<br>Brown University |
| 2018-2020 | **Associate Dean** of Inclusion and Diversity, College of Engineering |
| 2018-2020 | **Professor**, Department of Chemical Engineering and Materials Science, |
| 2013-2018 | **Associate Professor**, Department of Chemical Engineering and Materials Science, Michigan State University |
| 2001-2013 | **Staff Research Scientist**, Chemical & Materials Systems Lab, General Motors R&D |
| 2009-2013 | **Adjunct Professor**, Department of Mechanical, Automotive & Materials Engineering, University of Windsor |
| Summer 2000 | **Summer Intern**, Materials and Processes Lab, General Motors |

## III. Awards and Honors

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| 2023 | Dean's Award for Impact in Diversity, Equity, and Inclusion in Teaching and Advising |
| 2020 | ELATES Fellowship for the Executive Leadership in Academic Technology, Engineering, and Science training program. |
| 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 |
| 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) [including top journals of Science, Nature, Nature Materials, Nature Computational Science, Nature Communications, with >15000 citations on google scholar]

**Published Journal Papers**

1. **Qi, Y,** Swift, M.W; Fuller, E.J.; Talin, A.A; "Interface Potentials inside Solid-State Batteries: Origins and Implications, MRS Bulletin 2023, (accepted)
2. Varenik, M.; **Xu, B.***; Li, J.; Gaver, E.; Wachtel, E.; Here, D.; Routh, P.K.; Frenkel, A.I.; **Qi, Y.**; Lubomirsky, I.; Lead-free Zr-doped ceria ceramics with low permittivity displaying giant electrostriction, Nature Communication 2023, 14, 7371
3. Efaw, C.M.; **Wu, Q.***; Gao, N.; Zhang, Y.; Zhu H.M.; Gering, K.; Hurley, M.F.; Xiong, H.; Hu, E.; Xu, W.; Zhang, J.G.; Dufek, E.J.; Xiao, J.; Yang, X.Q.; Liu, J.; **Qi, Y.**; Li, B., "Localized High-Concentration Electrolytes Get More Localized through Micelle-Like Structures", Nature Materials, 2023, doi.org/10.1038/s41563-023-01700-3.) *(News by Tech Times, Materials Today ..)*
4. **Abbaspourtamijani, A.***; **Chakraborty, D.***; White H.S.; Newrock M.; **Qi, Y.**; "Tailoring Ag Electron-Donating Ability for Organohalide Reduction: A Bilayer Electrode Design", Langumuir 2023, 39, 15705–15715
5. **Qi, Y**., "Measuring is Believing", Nature Energy 2023, doi.org/10.1038/s41560-023-01371-z
6. **Hossain, M.J.***; **Wu, Q.*;** Bernardez, E.; Quilty, C.D.; Marschilok, A.C; Takeuchi, E.S.; Bock, D.; Takeuchi, K.J; and **Qi, Y.**; "Optimizing the Ionic Conductivity and Solvation Structures of Localized High Concentration Fluorinated Electrolytes for Lithium-Ion Batteries" , J. Phys. Chem. Lett. 2023, 14, 7718–7731
7. Zhang, W.; **Gu, C.***; Wang, Y.; Ware, S.; Lu, L.; Lin, S.; **Qi, Y.**; See, K.; "Improving the Mg Sacrificial Anode for Synthetic Electrochemistry by Tailoring Electrolyte Composition", JACS Au 2023, 3, 2280–2290
8. **Park, J.*;** Nicholas, J.D.**; Qi, Y.,** "Surface Gibbs Free Energy Analyses of Sr Segregation in Lanthanum Strontium Iron Oxide", Surface Sci. 2023, 732, 122268
9. **Park J.***; **Xu, B.***; Pan, J., Zhang, D., Lany, S., Liu, X.; Lou, J; **Qi, Y.**; "Accurate prediction of oxygen vacancy concentration with disordered A-site cations in high-entropy perovskite oxides: from binary to quaternary", npj Comp. Mat. 2023, 9, 29
10. Zhang, D; De Santiago, H.; **Xu, B.***; Liu, C.; Trindell, J.; Li, W.; **Park, J.***; Rodriguez, M.; Coker, E.; Sugar, J.; McDaniel, A.; Lany, S.; Ma, L.; Wang, Y.; Collins, G.; Tian, H.; Li, W.; **Qi, Y.**; Liu, X.; Luo, J., "Compositionally Complex Perovskite Oxides for Solar Thermochemical Water Splitting", Chemistry of Materials 2023, 35, 1901-1915
11. **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, 145, 4, 2473-2484
12. 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, 52, 1082-1088
13. **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
14. **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
15. **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
16. 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)*

17. **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
18. 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 ..)*
19. 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
20. **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
21. **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 $Ca_5Ga_2Sb_6$, Surface Science 2021, 714, 121918
22. 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")*
23. **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)*
24. **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
25. 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
26. 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
27. 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
28. 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
29. 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)*
30. **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
31. **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
32. **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
33. 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
34. 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

35. 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
36. **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
37. **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
38. **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
39. 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
40. 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
41. 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
42. 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
43. **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
44. **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
45. **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)*
46. 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
47. **Liu, J.L.***, Wang, Q.G., **Qi, Y.**, Atomistic Simulation of the Formation and Fracture of Oxide Bifilms in Cast Aluminum, Acta Materialia 2019, 164, 673-682 *(Selected and featured by Advances in Engineering)*
48. **Phongpreecha, 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)*
49. Nation, L., Wu, Y, **James, C.***, **Qi, Y.**, Powell, B., Sheldon, B.W. Si-Doped High-Energy Li1.2Mn0.54Ni0.13Co0.13O2 Cathode with Improved Capacity for Lithium-Ion Batteries, Journal of Materials Science 2018, 33(24), 4182-4191
50. 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
51. **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
52. **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
53. **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)

54. **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
55. 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)*
56. 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
57. 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)*
58. **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
59. 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
60. **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
61. 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
62. Pan, J., Lany, S., **Qi, Y.**, Computationally Driven Two-Dimensional Materials Design: What Is Next?, ACS Nano 2017, 11, 7560-7564 *(Invited Perspective)*
63. **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
64. **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
65. **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
66. **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
67. 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
68. **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)*
69. **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)*
70. **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
71. **James, C.***; Wu, Y.; Sheldon, B. W.; **Qi, Y.**. The Impact of oxygen vacancies on lithium vacancy formation and diffusion in $Li_{2-x}MnO_{3-\delta}$., Solid State Ionics 2016, 289, 87-94
72. **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

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74. 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
75. 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
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159. **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. **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 $Li_{2-x}MnO_{3-\delta}$., 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. 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. “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 ~ 01-31-2024 (Collaborators: B. Sheldon at Brown University; X.C. Xiao at General Motors)

7. “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)

8. “Controllable Oxygen Vacancy in Artificial Cathode-Electrolyte Interface (CEI) to Stabilize NMC811”, US Department of Energy (DOE)/EERE/VTO/Idahol National Lab, $270,000 toward Qi, 1/1/2023 ~ 12/30/2025

9. "Blocking Li Metal Dendrites in Solid Electrolytes with Ion-Exchange Induced Residual Stresses”, US Department of Energy (DOE)/EERE/VTO/Pacific North National Laboratory, ($300,000 toward Qi, 1/1/2023 ~ 12/30/2025, PI: Brian Sheldon at Brown)

### Finished:

10. “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)

11. “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)

12. “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)

13. “Electrolyte and SEI Modeling”, General Motors, $85,000, 1/1/2021 ~ 12/30/2022 (PI: Qi)

14. “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)

15. “Dendrite Growth Morphology Modeling in Liquid and Solid Electrolytes”, US Department of Energy (DOE), $1,135125 (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)

16. “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)

17. “*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)

18. “Understanding the role of oxides in aluminum alloy casting via atomistic simulations”, General Motors Corporation, $69,288, 09-16-2015 ~ 11-15-2016

19. “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)

20. “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)

21. “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)

22. “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)

23. “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)

## VI. 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 2021,2022,2023 |
| **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 Udine, Italy | 2021, 2023 |
| 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 |

## VII. Service and Leadership

### Inclusion and Diversity

- Sep 2021 – 2023, 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 won 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

| | |
|---|---|
| 2023 | Yue Qi, Secretary of the ASME Materials Division Executive Committee |
| 2023~present | Associate Editor for ECS Journal of Solid State Science and Technology |
| 2023~present | Associate Editorial Board of Materials Letters |
| 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 228$^{th}$ 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

## 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)