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Curriculum Vitae of Yue Qi (she/her)

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Education:

June 2001	Ph.D. in Materials Science & minor in Computer Science California Institute of Technology (Caltech), Pasadena, CA Advisor: William A. Goddard, III
July 1996	B.S. in Materials Science and Engineering & B.S in Computer Science, Tsinghua University, Beijing, China

Employment:

2020 - present	**Brown University, Providence, RI**
2023 - present	Deputy Director of the Initiative for Sustainable Energy (ISE)
2020 - present	Joan Wernig Sorensen Professor of Engineering
2013-2020	**Michigan State University (MSU), East Lansing, MI**
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
2001-2013	**General Motors R&D, Warren, MI**
2006-2013	Staff Research Scientist, Chemical & Materials Systems Lab
2001-2006	Senior Research Scientist, Materials and Processing Lab
Summer 2000	Summer Intern, Materials and Processes Lab
	Adjunct Positions
2020-2021	Adjunct Professor, Department of Chemical Engineering and Materials Science, Michigan State University
2009-2013	Adjunct Professor, Department of Mechanical, Automotive & Materials Engineering, University of Windsor

Research Theme and Major Accomplishments (Computational material science):

- ***Multiscale Modeling of the Electro-Chemo-Mechanical Degradation Mechanisms in Batteries***

  o Developed a framework linking state-of-charge (SOC)–dependent mechanical properties to deformation and failure in battery electrodes, as demonstrated in a 2010 trilogy in JES and JPS (total citations >1300). It was first shown how lithium insertion stiffens graphite and softens silicon with DFT calculations [JES 157, A558 (2010); JPS 195, 6825 (2010)]. Then, the diffusion-induced strain and stress were predicted at the device scale with DFT inputs, followed by the first in situ strain maps of commercial graphite electrodes using digital image correlation to validate the model [JES 157, A741 (2010)]. The lithiation-induced softening in Si electrodes was confirmed by other experiments [e.g. Electrochem. Comm. 13, 818, (2011) by G. Yushin]. This work transformed lifetime modeling of batteries, adapted by GM and other battery life models in the literature [e.g., for "Battery Cycle Life Prediction with Coupled Chemical Degradation and Fatigue Mechanics", JES 159, A1730 (2012)].

  o The model continues to guide the development of next-generation electrode materials. It led to the predictions of critical particle size, which will tolerate internal cracking and avoid electrode fracture, enabling the design of single-crystalline high-Ni cathodes [Science 370, 1313 (2020), in collaboration

with Dr. J. Xiao]. This technology is now essential for high-energy lithium-ion batteries for electric vehicles.

- The work spurred studies of electro-chem-mechanics in other electrode materials, polymer separators, and solid-state batteries. For solid-state batteries, a DFT-informed phase field model was developed to reveal that electrons localized at internal planar defects (pores, grain boundaries, cracks) in solid electrolytes can nucleate Li metal and accelerate Li dendrite growth [Chem. Mat. 31, 7351 (2019); cited 245]. This prediction was later validated by various experimental techniques [e.g. Nat. Mat 20, 1485 (2021) via TEM; Nat. Comm 14, 1300 (2023) via KPFM; Nat. Mat. 24, 581 (2025) via NMR]. The discovery was used to guide the design of dendrite-free solid-state batteries via electro-chemo-mechanical coupling. [Joule 4, 2599 (2020) and JMPS 193, 105878 (2024)]
- Served as a thrust Leader for GM-Brown Collaborative Research Lab (CRL) and led the transformation from surface engineering thrust to battery electro-chemo-mechanical coupled degradation research within one year (2010)
- Initiated symposia across different research communities (ECS, MRS, Computational Mechanics) to promote the dialogue on mechano-electrochemical coupling, the first panel discussion on Multiscale Mechanics Issues for Li-ion Batteries at the 2011 International Computational Heterogeneous Materials Mechanics Conference (2011); the first Mechanical-Electrochemical Coupling symposium at ECS (2014); and first Symposium on "Multiscale modeling of battery materials" at the International Conference on Multiscale Materials modeling (2022).

2. Multiscale and Mechanistic Modeling of Solid Electrolyte Interphase (SEI) in Li-Ion Batteries

- Before Dr. Qi's contributions, solid electrolyte interphases (SEI) and other battery interfaces were treated as empirically observed but poorly understood "black boxes." Her work of using *first-principles-informed multiscale modeling* to uncover the structure-property relationship of SEI turned electrochemical interfaces into designable elements.
- Led a multidisciplinary team at GM and developed the first mechanistic model for Li^+ transport through SEI, combining DFT-based defect thermodynamics and mesoscale diffusion models; introduced a new "knock-off" diffusion mechanism and quantitatively interpreted TOF-SIMS experiments (JACS 134, 15476 (2012), citation=690). R. Kostecki commented that "*A link between the composition of the SEI and Li transport across the hybrid interlayer has further been established by (this model)*" [Nature Review Materials 6, 1036 (2021)].
- Developed a general voltage-dependent defect thermodynamics model for ionic conduction in SEI and coatings on electrodes (JPC 117, 8579 (2013) and PRB 91, 134116 (2015); total citation> 500); the model predicted defect-mediated electron leakage as a function of SOC, later validated by direct experiments (Xu et al., Nat. Energy 8, 1345, 2023) and battery life models (Köbbing et al., J. Power Sources 561, 232651, 2023). A. Latz commented that "*For the first time, it proposes diffusion of neutral lithium interstitials as SEI growth mechanism.*" [Current Opinion in Electrochemistry 13, 61 (2019)].
- Constructed a DFT-informed space charge layer model and explained why LiF enhances transport when paired with other species, despite its poor standalone Li-ion conductivity. The model led to a multicomponent design of SEI layers (in collaboration with X.C. Xiao). (Nano Lett. 16, 2011 (2016), citation=416). C.S. Wang commented that "*This paradox might be better understood in the light of the work by Zhang et al., …*" [JES 166, A5184 (2019)]. This work stimulated the pursuit of forming LiF-rich SEI via high F-containing electrolytes (from anions, solvents, and additives) in the field and a new theory of micelle-like localized high concentration electrolyte design strategy. [Nat. Mater. 22, 1531 (2023)].
- Connected quantum-level simulations with phase-field models (in collaboration with L.Q. Chen) to enable the first fully predictive, multiscale description of charge transfer kinetics at reactive metal interface. First, a half-cell model at DFT and DFTB level was created to predict the energy landscape for the electrochemical reaction, the combination of a solvated Li-ion with an electron on the electrode

to form a deposited Li-atom, then the Butler–Volmer kinetics equation was obtained. (EES 12, 1286 (2019); citation=117). This work represents the first charge-transfer kinetics model for lithium deposition derived entirely from first-principles calculations, rather than being fitted to experimental data. Nature Energy highlighted this model with "*The most fundamental charge-transfer reactions at a Li metal anode …. Despite their importance, fundamental understanding of these processes is difficult to acquire from experiments. There are also challenges for computational approaches,…. Now, Yunsong Li and Yue Qi at Michigan State University have developed a Li/SEI/electrolyte half-cell model, and using combined density functional theory and tight-binding methods they are able to obtain the charge-transfer and energy profile across the interface*." [Nat. Energy 4, 257 (2019)] These predictions were formulated in the phase field model, which predicted the mossy Li and faceted Mg morphologies during electrodeposition, consistent with experimental observations. (Cell Rep Phys Sci 2, 100294 (2021)].

- Authored a widely cited review on SEI modeling in *npj Computational Materials*, establishing a foundational reference for researchers in solid-state electrochemistry and interface design.

3. Interfacial chemo-mechanical coupling in other applications for Energy and Sustainability

- Introduced chemistry into mechanics in tribology in the early 2000s as part of a broader initiative to enable near-frictionless surfaces and environmentally friendly machining processes. Developed a tensile test simulation protocol for interfaces with DFT [PRB 69, 235401 (2004); citation=150] and predicted that hydrogen-terminated diamond-like carbon (DLC) coatings minimize aluminum adhesion transfer, a finding later confirmed experimentally by GM colleagues [Surf. Coat. Technol. 200, 2970, 2006]. Further integrated DFT with thermodynamics to map environment-dependent frictional behaviors [Surf. Sci. 600, 2955 (2006); citation=191]. E. Erdemir commented on the simulations that "*computer simulations have shown the existence of such repulsive forces among fully hydrogenated DLC surfaces.*" [Physics Today 71, 40 (2018)]. This fundamental work informed the design of carbon coatings (U.S. Patent 8057133) and led to her receiving the GM Campbell Award in 2011. This work further led to the implementation of DLC coatings on piston rings to enhance fuel efficiency and durability. (The first implementation was on Chevrolet Ecotec 1.4L turbo engines around 2011~2012). "Through years of lab research, *we've acquired an understanding of how to work with DLC at the atomic level*," said M. Lukitsch, GM senior researcher, in a news release. At least one million 1.4L Ecotec engines have been assembled since then, based on an automotive Fleet report.
- Developed reactive molecular dynamics (MD) simulations using ReaxFF to investigate chemo-mechanical coupling in oxidation-sensitive metals (e.g., Al, Mg, Ta, Li), revealing that ambient gas environments profoundly alter deformation mechanisms at nano- to meso-scales (Sen et al., Nat. Comm. 5, 3595 (2014); citation=94). Proposed a strain rate vs oxidation rate competition framework and developed semi-analytical criteria that define loading regimes for oxide "self-healing" versus fracture, extending the understanding from atomic to macro scales. The nanometer aluminum wire simulations were directly related to the surface flaws during the hot forming of meter-long car liftgates. J. Li et al. later experimentally confirmed that "*The strain-rate sensitivity discovered here agrees well with MD modeling results by Sen et al...*" [*Nano Lett.* 18, 2492, (2018)]. The reactive MD model was further developed to predict the oxide bifilm formation and fracture during aluminum casting, linked to virtual casting simulations by Q.G. Wang at GM [Acta Mater. 164, 673 (2019)]. This work earned her student the Acta Student Award of the Year.
- Developed a DFT-based mechanistic understanding and predictive descriptor for metal–oxide adhesion in Ag–CuO reactive air brazing. Identified $CuAlO_2$, as a new and superior interlayer than CuO for enhancing Ag/YSZ wetting and sealing in solid oxide fuel cells [Acta Mat 152, 229 (2018)], confirmed by experiments later [Ceramics Inter. 47, 31413 (2021)]].
- Clarified halogen bonding with DFT calculations for the design of self-assembled monolayers to toughen the interfaces and enhance perovskite solar cell reliability (in collaboration with N. Padture) [Science, 372, 618 (2021)].

Awards and Honors:

- **2026, Fellow of MRS (Materials Research Society),** Citation*: For developing predictive multiscale multiphysics simulation methods to uncover the electro-chemical-mechanical coupled mechanisms at interfaces/interphases in critical energy storage and sustainability technologies and for dedication to multidisciplinary education and services*
- **2025, the American Ceramic Society (ACerS)'s Ross Coffin Purdy Awards,** "*given to the author or authors who made the most valuable contribution to ceramic technical literature*", for the paper of "Lead-free Zr-doped ceria ceramics with low permittivity displaying giant electrostriction" published in Nature Communications, 14, 7371, 2023.
- Dean's Award for Impact in Diversity, Equity, and Inclusion in Teaching and Advising at Brown University (2023)
- Inaugural Joan Wernig Sorensen Professor of Engineering (2023-present) at Brown University
- ELATES Fellowship for the Executive Leadership in Academic Technology, Engineering, and Science training program (Class of 2020~2022)
- **2017, The Minerals, Metals & Materials (TMS) Society Brimacombe Medalist** (mid-career award), for her contributions to *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**
- 2009, General Motors Campbell Award for *Fundamentals of Interfacial Tribology*
- 2009, GM Campbell Award for *Fundamental research on Multi-scale Modeling of High-temperature Deformation in Aluminum*
- 2006, GM Campbell Award for *Advances in Nano-scale Plasticity*
- 1999, Co-recipient of the Feynman Prize in Nanotechnology for Theoretical Work in *Modeling of molecular machines*

Institutional Service and Leadership:

- Engineering Executive Committee member for the Materials Science Program, coordinating teaching and recruiting, representing Brown at the University Materials Council (Aug 2024 ~ present). The ranking of the Materials Program increased by 12 from 2024~2025.
- Deputy Director of the Initiative for Sustainable Energy (ISE), research and initiatives lead (2023~present)
- Governance committee for the School of Professional Studies (2022-2023)
- Sustainability in Education Working Group at Brown (2023)
- Thrust Leader for GM-Brown Collaborative Research Lab (CRL) (2006 -2013) and supervised the transformation of the GM-Brown Collaborative Research Program from surface engineering to battery research within one year (2010)
- Sep 2021 – 2023, Inaugural DEI committee chair at the School of Engineering, Brown University. 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, served as the first Associate Dean for Inclusion and Diversity in the College of Engineering at Michigan State University. 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 Service and Leadership:

a) Editorships:

- Editor for *Solid State Ionics* (2025 ~ present)
- Associate Editor for *ECS Journal of Solid-State Science and Technology (JSS) (*2023~present)
- Associate Editorial Board of *Materials Letters (*2023~present*)*
- Editorial Board of *npj Computational Materials* (2022~present)
- Key Reader for *Metallurgical and Materials Transactions* (2014~2020)
- Topic Editor for "*Women in Battery Science and Technology*", a special issue by Frontiers, Switzerland (2023-2024)
- Associate editor for the *special issue of JES* on the topic of "mechano-electro-chemical coupling in energy-related materials and devices" (2014)

b) Membership in Professional Committees:

- ASME Materials Division Executive Committee (2022-2024)
- Panel Lead for DOE BES workshop on Basic Research Needs for Next Generation Electrical Energy Storage (2017)
- Vice-chair, Chair-Elect, and Chair of the Energy Subdivision of Physical Chemistry division of the American Chemical Society (2014~2016)
- Chair of American Vacuum Society Michigan Chapter (2015~2017)
- 2016 TMS, AIME Henry DeWitt Smith Scholarship Committee
- 2013 TMS Young Leaders Committee

c) Organizer of Professional Conferences:

- 2026, Co-Chair (one of the five) for the MRS 2026 Fall Meeting in Boston, MA (https://www.mrs.org/meetings-events/annual-meetings/2026-mrs-fall-meeting)
- 2025, Organizer for Symposium "Computational Electrochemistry" at ECS fall meeting
- 2024, Organizer for Symposium "Computational Electrochemistry" at ECS spring meeting
- 2024, Organizer for Symposium of "Next-Generation EV Battery Materials—Bridging Academic, Government and Industry Research" at MRS Spring Meeting
- 2024, Organizer for the special Symposium of "An Atoms to Autos Approach for Materials Innovations for Lightweighting" at TMS Annual Meeting
- 2022, Organizer for Symposium "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" at the ECS Spring Meeting
- 2018, Organizer for Symposium "Solid-Solid Interfaces in Batteries, Energy Storage and Conversion - Diagnostic and Modeling" at 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
- 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 the ECS 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 Spring meeting

- 2011, Organizer for Focus Session Computational Design of New Materials for APS March meeting
- 2009, Organizer for Focus Session Interface Science and Engineering for APS March meeting
- 2008, Organizer for Computational Material Design via Multiscale Modeling for MRS Fall meeting
- 2008, Organizer for Focus Session Engineering interfaces for new materials: Modeling and Experiments for APS March meting
- 2006, Organizer for Focus Session Friction, Fracture and Deformation for APS March meetings

Teaching and Outreach:

(Developed courses on energy storage and materials modeling at all levels, led international multiscale battery modeling education, and created hands-on STEM outreach programs)

Courses Taught at Brown

- ENGN 2920H, Materials and Interfaces for Energy Storage Devices (developed since Fall 2021)
- ENGN 0030, Introduction to Engineering (created a 5-week Batteries Inside Out module in Fall 2024)
- ENGN 0040, Dynamics and Vibrations (Spring 2021,2022,2023)

Courses Taught at MSU

- MSE991, Special topics – Computational Materials Science (developed in Spring 2014, 2015)
- MSE991, Atomistic Simulations for Materials Science (became permanent course Spring 2016, 2018)
- MSE881, Computational Materials Science (redesigned into a series of courses in Spring 2020)
- MSE310, Phase Equilibria in Materials (Fall 2014~2018)
- MSE250, Introduction to Materials Science (Lab) (Spring 2015)
- MSE465, Design and Application of Engineering Materials (Spring 2017)

Other Teaching Activities

- Lecturer for an ICMS advanced course on "Batteries – Basic Principles, Experimental Investigations and Modeling across Scales", International Centre for Mechanical Sciences (ICMS), 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

Volunteering for Educational Outreach (especially girls in STEM)

- Organized a STEMAP event with RI 4-H. Conduct a workshop about batteries and electrochemistry, which will include a 20-minute lecture part and two hands-on demos. (2023, 2024)
- Developed and led hands-on sessions on "Making Materials on Computers" for the Girls Get Math Summer Camp at Brown (2023, 2024)
- 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 of 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)

Public Engagement

- Expert interviewed for an article in New York Times, "Relax, Electric Vehicles really are the best choice for the climate" by S. Porder (2023)
- 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

Students Mentored

Current Group: 1 postdocs; 7 PhD students;

Previously advised: 13 postdocs; 11 PhD students; 10 visiting PhD students; 5 Master students; 6 undergraduate students; 2 high school students

PhD Theses and Dissertations Directed:

- Harsh Jagad (PhD), Materials Science, Brown University, 2025,
  "*Atomistically Informed Multiscale Modelling of Electro-chemo-mechanically Coupled Phenomenon in Sodium and Solid State Batteries*"
  Subsequent position: Battery Startup
- Boyuan Xu (PhD), Physics, Brown University, 2024,
  "*Computational Study of Point Defects' Formation, Interaction, Local Distortion, and Strain in Complex Metal Oxides for Hydrogen Generation and Electrostriction Applications*",
  Subsequent position: Suzhou Laboratory
- Min (Frank) Feng (PhD), Materials Science, Brown University, 2024,
  "*Multiscale Modeling Assisted Design of Stable Li/Solid Electrolyte Interfaces/Interphases*",
  Subsequent position: GM
- Jiyun Park (PhD), Materials Science, Brown University, 2023,
  "*Modeling of oxygen vacancies, surfaces, and interfaces in oxides for alternative energy applications",*
  Subsequent position: Ford
- Hong-Kang Tian (PhD), Chemical Engineering, Michigan State University, 2022
  "*Interfacial Challenges of All-Solid-State Li-ion Batteries: Multis-scale Computational Approach",*
  Current Position: Associate Professor at National Cheng Kung University, Taiwan.
- Yuxiao Lin (PhD), Materials Science and Engineering, Michigan State University, 2019
  "*Interfacial Mechanisms Understanding and Material Design for Li-S batteries via Integrated Computational Approache*s"
  Subsequent position: Postdoc Fellow at Idaho National Lab
- Jialin Liu (PhD), Materials Science and Engineering, Michigan State University, 2019
  "Atomic Simulations on Chemical-Mechanical Coupled Deformation in Complex Nano Structures"
  Subsequent position: 3M
- Joe, T. Phongpreecha (PhD), Chemical Engineering, Michigan State University, 2018
  "Understanding the Solid/Solid and Liquid/Solid interface phenomena for alternative energy applications"
  Subsequent position: Postdoc Fellow at Stanford University

- Kwang-Jin Kim (PhD), Materials Science and Engineering, Michigan State University, 2018
  "Reactive Force Field Based Atomistic Simulations of Silicon Anode upon Lithiation and Delithiation in Lithium-ion Batteries"
  Subsequent position: Research Engineer at Dongjin Semichem, Korea;
- Christine James (PhD), Chemical Engineering, Michigan State University, 2018
  "Correlation of Point Defects in Lithium-rich-layered Cathode Materials for Lithium-ion Battery"
  Subsequent position: Princeton Theological Seminary
- Tridip Das (PhD) Chemical Engineering, Michigan State University (2017)
  "Understanding Oxygen Vacancy Formation, Interaction, Transport, and Strain in SOFC Components via Combined Thermodynamics and First Principles Calculations".
  Subsequent position: Intel
- Jie Pan (PhD), Chemical and Materials Engineering, University of Kentucky (2016) (Co-advised with Y.T. Cheng)
  "Understanding Electrical Conduction in Lithium Ion Batteries through Multi-scale Modeling"
  Subsequent position: Postdoc fellow at National Renewal Energy Lab
- Maria E. Stournara (PhD), Materials Science, Brown University. (2014) (Co-advised with V. Shenoy)
  "Computational Studies of Bulk and Interface Properties in Li-ion Battery Anodes"
  Subsequent position: Postdoc fellow at Fritz Haber Institute of the Max Planck Society
- Fatih G. Sen (PhD), Engineering Materials, University of Windsor, 2013 (Co-advised with A. Alpas)
  "Atomistic simulations to micro-mechanisms of adhesion in automotive applications",
  Subsequent position: Postdoc fellow at Argonne National Lab
- Ningning Du (PhD), Solid Mechanics, Brown University. (2010) (Co-advised with A. Bower)
  "Multi-scale Modeling of Deformation and Failure Mechanisms of Al Alloys at Elevated Temperature."
- Subsequent position: Principal Engineer at Medtronic

Selected Awards and Honors to Group Members

- 2025, Gregory Pustorino, NASA Graduate Student Research Fellowship
- 2025, Harsh Jagad, *William N. Findley Award* for the best paper on the mechanical behavior of materials at Brown
- 2024, Lincoln Mtemeri, *Presidential Postdoctoral Fellowship at Brown*
- 2022, Wenzao Li, *Hibbitt Postdoctoral Research Fellow at Brown*
- 2019, Jialin Liu, *Acta Student Award*
- 2017, Christine James, *U.S. DOE Graduate Student Research Award*
- 2017, Jialin Liu, *Best Poster Award at the 49th Annual Midwest Theoretical Chemistry Conference*
- 2014, Tridip Das, *Best Poster award at 225th Electrochemical Society (ECS) Meetings*
- 2012, Fatih Sen, *Journal of Physics-Condensed Matter 2012 Highlights (10 out of all the papers published in JPCM in 2012) for his paper JPCM 24 (22), 225003*

Publications List: (~21300 citations and H index=69 according to Google Scholar)

a) Peer-Reviewed Journal Papers

(183) Mtemeri, L.; Qi, Y. Structural descriptors controlling pore-filling mechanism in hard carbon electrode during sodiation. *EES Batteries* **2026**, DOI: 10.1039/D5EB00210A.

(182) Raj, V.; Wang, Y.; Feng, M.; Naik, K. G.; Jain, M.; Vishnugopi, B. S.; Deng, S.; Schorr, N. B.; Salazar, M.; Heusser, A. M.; et al. Grain boundary zirconia-modified garnet solid-state electrolyte. *Nature Materials* **2025**. DOI: 10.1038/s41563-025-02374-9.

(181) Mal, D. D.; Redkar, N.; Liu, K.; Park, H.; Kennedy, E. R.; Kim, S.; Li, W.; Yang, Y.; Qi, Y.; Neurock, M.; et al. Electrosynthesis of Agrochemicals via Alternating-Current-Driven Selective, Continuous Dehalogenation. *Journal of the American Chemical Society* **2025**, *147* (41), 37611-37621. DOI: 10.1021/jacs.5c12620.

(180) Jagad, H. D.; Harris, S. J.; Sheldon, B. W.; Qi, Y. Ion Size Effects on the Thermodynamic, Kinetic, and Mechanical Properties during Ion Exchange in Solid-State Electrolytes. *Chemistry of Materials* **2025**, *37* (20), 8165-8177. DOI: 10.1021/acs.chemmater.5c01147.

(179) Gu, C.; Liu, K.; Pendergast, A.; Kawamata, Y.; Baran, P. S.; Neurock, M.; Qi, Y. Ion-Driven Dynamics of Charge-Neutral Species in the Electrical Double Layer: Insights from Alternating and Constant Polarity Simulations. *ACS Electrochemistry* **2025**, 1 (12), 2749-2760. DOI: 10.1021/acselectrochem.5c00344.

(178) Arzumanyan V, Liu C, Zhang D, Li W, Luo J, Liu X, Qi Y. Structural effects on oxygen vacancies and redox behavior in Mn-based perovskite oxides. *Solid State Ionics.* **2025,** 432, 117067. DOI: 10.1016/j.ssi.2025.117067.

(177) Lavie, A.; Xu, B.; Khodorov, S.; Singh, H.; Liu, J.; Hajbi, T.-E.; Wachtel, E.; Feldman, Y.; Ehre, D.; Donetsky, D.; Frenkel, A. I.; Qi, Y.; Lubomirsky, I. Elastic dipole alignment is the origin of anelasticity and electrostriction in aliovalent-doped ceria. *Acta Materialia* **2025**, *297*, 121327. DOI: 10.1016/j.actamat.2025.121327.

(176) Zhao, L.; Feng, M.; Wu, C.; Guo, L.; Chen, Z.; Risal, S.; Ai, Q.; Lou, J.; Fan, Z.; Qi, Y.; Yao, Y. Imaging the evolution of lithium-solid electrolyte interface using operando scanning electron microscopy. *Nature Communications* **2025**, *16* (1), 4283. DOI: 10.1038/s41467-025-59567-8

(175) Goodwin, Z. A. H.; Markiewitz, D. M.; Wu, Q.; Qi, Y.; Bazant, M. Z. Theory of Cation Solvation in the Helmholtz Layer of Li-Ion Battery Electrolytes. *ACS Applied Energy Materials* **2025**, *8* (12), 8376-8387. DOI: 10.1021/acsaem.5c00883.

(174) Zhang, K.; Ji, Y.; Wu, Q.; Nabavizadeh, S. A.; Qi, Y.; Chen, L.-Q. Simulating solid electrolyte interphase formation spanning 10^8 time scales with an atomically informed phase-field model. *Energy & Environmental Science* **2025**, *18* (15), 7541-7554, DOI: 10.1039/D5EE01030F.

(173) Mao, K.; Liu, C.; Wang, Y.; Gu, C.; Putziger, J. M.; Cemalovic, N. I.; Muniz, C.; Qi, Y.; Lin, S. Dynamic kinetic resolution of phosphines with chiral supporting electrolytes. *Nature* **2025**, *643* (8074), 1288-1296. DOI: 10.1038/s41586-025-09238-x.

(172) Wu, Q. S.; Qi, Y. Revealing heterogeneous electric double layer (EDL) structures of localized high-concentration electrolytes (LHCEs) and their impact on solid-electrolyte interphase (SEI) formation in lithium batteries. *Energy & Environmental Science* **2025**, *18* (6), 3036-3046. DOI: 10.1039/d5ee00206k.

(171) Li, W. Z.; Cain, J. D.; Pieczonka, N. P. W.; Liu, Z. Y.; Sayed, S. Y.; Qi, Y. A Hybrid Intercalation and Conversion Mechanism for Reversible Lithium Storage in Layered Silicane (SiH) with Low Molar Volume Change. *ACS Energy Letters* **2025**, *10* (3), 1099-1106. DOI: 10.1021/acsenergylett.4c03063.

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~180 Invited and Keynote Presentations at Other Conferences, Workshops, University and National Labs

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