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):

- ***Electro-Chemo-Mechanical Modeling of Electrode Degradation and Battery Failure***

  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 to show how lithium insertion stiffens or softens graphite and silicon with DFT calculations [JES 157, A558 (2010); JPS 195, 6825 (2010)] and induce strain and stress at the device scale, 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 [e.g., for "Battery Cycle Life Prediction with Coupled Chemical Degradation and Fatigue Mechanics", JES 159, A1730 (2012)] by M. Verbrugge and other GM researchers and many other electrode degradation models.

  o The model continues to guide the development of next-generation electrode materials; predictions of particle size tolerance to internal cracking enabled the design of single-crystalline high-Ni cathodes

[Science 370, 1313 (2020), in collaboration with Dr. J. Xiao]. This technology is now central to 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], guiding 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). (Zhang *et al.* 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 was created to predict the energy landscape for the electrochemical reaction, the combination of a solvated Li-ion with an electron on the electrode into a deposited Li-

atom (EES 12, 1286 (2019); citation=117) and obtain a Butler–Volmer type of kinetics equation. 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:

- 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
- 2011, Keynote Speaker at MIT Materials Day on "Computational Materials Science and Engineering"
- 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:

- 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 Chemistry 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; 1 Master student

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 Application*s",
  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, 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: (>19100 citations and H index=66 according to Google Scholar)

a) Peer-Reviewed Journal Papers

(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.

(170) Qi, Y.; Liu, J. L.; Feng, M.; Tantratian, K.; Chen, L.; Xiao, X. C.; Sachdev, A. K. From the Passivation Layer on Aluminum to Lithium Anode in Batteries. *Metallurgical and Materials Transactions a-Physical Metallurgy and Materials Science* **2025**, *56* (2), 429-438. DOI: 10.1007/s11661-024-07658-4.

(169) Dai, Z. H.; You, S.; Chakraborty, D.; Li, S. R.; Zhang, Y. D.; Ranka, A.; Barlow, S.; Berry, J. J.; Marder, S. R.; Guo, P. J.; et al. Connecting Interfacial Mechanical Adhesion, Efficiency, and Operational Stability in High Performance Inverted Perovskite Solar Cells. *Acs Energy Letters* **2024**, *9* (4), 1880-1887. DOI: 10.1021/acsenergylett.4c00510.

(168) Hsieh, I. T.; Wu, Y. Q.; Li, B.; Qi, Y. First-principles study of the structures and redox mechanisms of Ni-rich lithium nickel manganese cobalt oxides. *Solid State Ionics* **2024**, *411*. DOI: 10.1016/j.ssi.2024.116556.

(167) Xiao, J.; Adelstein, N.; Bi, Y. J.; Bian, W. J.; Cabana, J.; Cobb, C. L.; Cui, Y.; Dillon, S. J.; Doeff, M. M.; Islam, S. M.; et al. Assessing cathode-electrolyte interphases in batteries. *Nature Energy* **2024**. DOI: 10.1038/s41560-024-01639-y.

(166) Pechersky-Savich, T.; Xu, B. Y.; Varenik, M.; Li, J. Y.; Wachtel, E.; Ehre, D.; Routh, P. K.; Marcella, N.; Frenkel, A. I.; Qi, Y.; et al. Correlated Displacement of Dynamic Elastic Dipoles Produces Nonclassical Electrostriction in Zr-Doped Ceria. *Chemistry of Materials* **2024**, *36* (16), 7665-7675. DOI: 10.1021/acs.chemmater.4c00688.

(165) Liu, C. J.; Park, J.; De Santiago, H. A.; Xu, B. Y.; Li, W.; Zhang, D. W.; Zhou, L. F.; Qi, Y.; Luo, J.; Liu, X. B. Perovskite Oxide Materials for Solar Thermochemical Hydrogen Production from Water Splitting through Chemical Looping. *Acs Catalysis* **2024**, *14* (19), 14974-15013. DOI: 10.1021/acscatal.4c03357.

(164) Pustorino, G.; Jagad, H.; Li, W. Z.; Feng, M.; Poma, M.; Ko, J.; Johari, P.; Qi, Y. Mechanical and Electronic Properties of Bulk and Surface Li6PS5Cl Argyrodite: First-Principles Insights on Li-Filament Resistance. *Chemistry of Materials* **2024**, *37* (1), 313-321. DOI: 10.1021/acs.chemmater.4c02577.

(163) Jagad, H. D.; Fu, J. T.; Fullerton, W. R.; Li, C. Y.; Detsi, E.; Qi, Y. A Physics-based Model Assisted by Machine-Learning for Sodium-ion Batteries with both Liquid and Solid Electrolytes. *Journal of the Electrochemical Society* **2024**, *171* (6). DOI: 10.1149/1945-7111/ad4a11.

(162) Xu, B. Y.; Park, J.; Zhang, D. W.; De Santiago, H. A.; Li, W.; Liu, X. B.; Luo, J.; Lany, S.; Qi, Y. Local Ordering, Distortion, and Redox Activity in (La0.75Sr0.25)(Mn0.25Fe0.25Co0.25Al0.25)O3 Investigated by a Computational Workflow for Compositionally Complex Perovskite Oxides. *Chemistry of Materials* **2024**, *36* (10), 4990-5001. DOI: 10.1021/acs.chemmater.3c03038.

(161) Feng, M.; Liu, X.; Harris, S. J.; Sheldon, B. W.; Qi, Y. A multiscale model to understand the interface chemistry, contacts, and dynamics during lithium stripping. *Journal of the Mechanics and Physics of Solids* **2024**, *193*. DOI: 10.1016/j.jmps.2024.105878.

(160) Park, J.; Nicholas, J. D.; Qi, Y. Surface Gibbs free energy analyses of Sr segregation in lanthanum strontium iron oxide. *Surface Science* **2023**, *732*. DOI: 10.1016/j.susc.2023.122268.

(159) Zhang, W. Y.; Gu, C. X.; Wang, Y.; Ware, S. D.; Lu, L. X.; Lin, S.; Qi, Y.; See, K. A. Improving the Mg Sacrificial Anode in Tetrahydrofuran for Synthetic Electrochemistry by Tailoring Electrolyte Composition. *Jacs Au* **2023**. DOI: 10.1021/jacsau.3c00305.
(158) Varenik, M.; Xu, B. Y.; Li, J. Y.; Gaver, E.; Wachtel, E.; Ehre, D.; Routh, P. K.; Khodorov, S.; Frenkel, A. I.; Qi, Y.; et al. Lead-free Zr-doped ceria ceramics with low permittivity displaying giant electrostriction. *Nature Communications* **2023**, *14* (1). DOI: 10.1038/s41467-023-43032-5.
(157) Zhang, D. W.; Park, J.; Xu, B. Y.; Liu, C. J.; Li, W.; Liu, X. B.; Qi, Y.; Luo, J. Unusual aliovalent doping effects on oxygen non-stoichiometry in medium-entropy compositionally complex perovskite oxides. *Dalton Transactions* **2023**, *52* (4), 1082-1088. DOI: 10.1039/d2dt03759a.
(156) Qi, Y. Measuring is believing. *Nature Energy* **2023**, *8* (12), 1307-1308. DOI: 10.1038/s41560-023-01371-z.
(155) Zhang, D. W.; De Santiago, H. A.; Xu, B. Y.; Liu, C. J.; Trindell, J. A.; Li, W.; Park, J.; Rodriguez, M. A.; Coker, E. N.; Sugar, J. D.; et al. Compositionally Complex Perovskite Oxides for Solar Thermochemical Water Splitting. *Chemistry of Materials* **2023**, *35* (5), 1901-1915. DOI: 10.1021/acs.chemmater.2c03054.
(154) Efaw, C. M.; Wu, Q. S.; Gao, N. S. J.; Zhang, Y. G.; Zhu, H. Y.; Gering, K.; Hurley, M. F.; Xiong, H.; Hu, E. Y.; Cao, X.; et al. Localized high-concentration electrolytes get more localized through micelle-like structures. *Nature Materials* **2023**. DOI: 10.1038/s41563-023-01700-3.
(153) Wu, Q. S.; McDowell, M. T.; Qi, Y. Effect of the Electric Double Layer (EDL) in Multicomponent Electrolyte Reduction and Solid Electrolyte Interphase (SEI) Formation in Lithium Batteries. *Journal of the American Chemical Society* **2023**. DOI: 10.1021/jacs.2c11807.
(152) Abbaspourtamijani, A.; Chakraborty, D.; White, H. S.; Neurock, M.; Qi, Y. Tailoring Ag Electron Donating Ability for Organohalide Reduction: A Bilayer Electrode Design. *Langmuir* **2023**, *39* (44), 15705-15715. DOI: 10.1021/acs.langmuir.3c02260.
(151) Park, J.; Xu, B. Y.; Pan, J.; Zhang, D. W.; Lany, S.; Liu, X. B.; Luo, J.; Qi, Y. Accurate prediction of oxygen vacancy concentration with disordered A-site cations in high-entropy perovskite oxides. *Npj Computational Materials* **2023**, *9* (1). DOI: 10.1038/s41524-023-00981-1.
(150) Qi, Y.; Swift, M. W.; Fuller, E. J.; Talin, A. A. Interface potentials inside solid-state batteries: Origins and implications. *Mrs Bulletin* **2023**, *48* (12), 1239-1246. DOI: 10.1557/s43577-023-00625-1.
(149) Hossain, M. J.; Wu, Q. S.; Bernardez, E. J. M.; Quilty, C. D.; Marschilok, A. C.; Takeuchi, E. S.; Bock, D. C.; Takeuchi, K. J.; Qi, Y. The Relationship between Ionic Conductivity and Solvation Structures of Localized High-Concentration Fluorinated Electrolytes for Lithium-Ion Batteries. *Journal of Physical Chemistry Letters* **2023**, *14* (34), 7718-7731. DOI: 10.1021/acs.jpclett.3c01453.
(148) Feng, M.; Yang, C. T.; Qi, Y. The Critical Stack Pressure to Alter Void Generation at Li/Solid-Electrolyte Interfaces during Stripping. *Journal of the Electrochemical Society* **2022**, *169* (9). DOI: 10.1149/1945-7111/ac91aa.
(147) Lin, Y. X.; Ticey, J.; Oleshko, V.; Zhu, Y. J.; Zhao, X. S.; Wang, C. S.; Cumings, J.; Qi, Y. Carbon-Nanotube-Encapsulated-Sulfur Cathodes for Lithium-Sulfur Batteries: Integrated Computational Design and Experimental Validation. *Nano Letters* **2022**, *22* (1), 441-447. DOI: 10.1021/acs.nanolett.1c04247.
(146) Swift, M. W.; Jagad, H.; Park, J.; Qie, Y.; Wu, Y. Q.; Qi, Y. Predicting low-impedance interfaces for solid-state batteries. *Current Opinion in Solid State & Materials Science* **2022**, *26* (3). DOI: 10.1016/j.cossms.2022.100990.
(145) Wu, M. L.; Zhang, X.; Zhao, Y.; Yang, C. P.; Jing, S. S.; Wu, Q. S.; Brozena, A.; Miller, J. T.; Libretto, N. J.; Wu, T. P.; et al. A high-performance hydroxide exchange membrane enabled by Cu2+-crosslinked chitosan. *Nature Nanotechnology* **2022**, *17* (6), 629. DOI: 10.1038/s41565-022-01112-5.

(144) Jagad, H. D.; Harris, S. J.; Sheldon, B. W.; Qi, Y. Tradeoff between the Ion Exchange-Induced Residual Stress and Ion Transport in Solid Electrolytes. *Chemistry of Materials* **2022**. DOI: 10.1021/acs.chemmater.2c01806.
(143) Liu, Z.; Li, Y. S.; Ji, Y. Z.; Zhang, Q. L.; Xiao, X. C.; Yao, Y.; Chen, L. Q.; Qi, Y. Dendrite-free Lithium Based on Lessons Learned from Lithium and Magnesium Electrodeposition Morphology Simulations. *Cell Reports Physical Science* **2021**, *2* (1). DOI: 10.1016/j.xcrp.2020.100294.
(142) Hu, G. Z.; Zhou, Q.; Bhatlawande, A.; Park, J.; Termuhlen, R.; Ma, Y. X.; Bieler, T. R.; Yu, H. C.; Qi, Y.; Hogan, T.; et al. Patterned nickel interlayers for enhanced silver wetting, spreading and adhesion on ceramic substrates. *Scripta Materialia* **2021**, *196*. DOI: 10.1016/j.scriptamat.2021.113767.
(141) Zhang, M.; Rao, Z. X.; Kim, K. S.; Qi, Y.; Fang, L.; Sun, K.; Chason, E. Molecular dynamics simulation of stress induced by energetic particle bombardment in Mo thin films. *Materialia* **2021**, *16*. DOI: 10.1016/j.mtla.2021.101043.
(140) Dai, Z. H.; 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* (6542), 618. DOI: 10.1126/science.abf5602.
(139) Fuller, E. J.; Strelcov, E.; Weaver, J. L.; Swift, M. W.; Sugar, J. D.; Kolmakov, A.; Zhitenev, N.; McClelland, J. J.; Qi, Y.; Dura, J. A.; et al. Spatially Resolved Potential and Li-Ion Distributions Reveal Performance-Limiting Regions in Solid-State Batteries. *Acs Energy Letters* **2021**, *6* (11), 3944-3951. DOI: 10.1021/acsenergylett.1c01960.
(138) Yang, C. P.; Wu, Q. S.; Xie, W. Q.; Zhang, X.; Brozena, A.; Zheng, J.; Garaga, M. N.; Ko, B. H.; Mao, Y. M.; He, S. M.; et al. Copper-coordinated cellulose ion conductors for solid-state batteries. *Nature* **2021**, *598* (7882), 590-+. DOI: 10.1038/s41586-021-03885-6.
(137) Feng, M.; Pan, J.; Qi, Y. Impact of Electronic Properties of Grain Boundaries on the Solid Electrolyte Interphases (SEIs) in Li-ion Batteries. *Journal of Physical Chemistry C* **2021**, *125* (29), 15821-15829. DOI: 10.1021/acs.jpcc.1c03186.
(136) Nation, L.; Wu, Y.; Liu, X. M.; Chi, M. F.; Wu, Y. Q.; Qi, Y.; Sheldon, B. W. Redox-couple investigations in Si-doped Li-rich cathode materials. *Physical Chemistry Chemical Physics* **2021**, *23* (4), 2780-2791. DOI: 10.1039/d0cp05737a.
(135) Yang, C. T.; Qi, Y. Maintaining a Flat Li Surface during the Li Stripping Process via Interface Design. *Chemistry of Materials* **2021**, *33* (8), 2814-2823. DOI: 10.1021/acs.chemmater.0c04814.
(134) Swift, M. W.; Swift, J. W.; Qi, Y. Modeling the electrical double layer at solid-state electrochemical interfaces. *Nature Computational Science* **2021**, *1* (3), 212-220. DOI: 10.1038/s43588-021-00041-y.
(133) 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*. DOI: 10.1016/j.susc.2021.121918.
(132) Das, T.; Nicholas, J. D.; Qi, Y. Composition, crystallography, and oxygen vacancy ordering impacts on the oxygen ion conductivity of lanthanum strontium ferrite. *Physical Chemistry Chemical Physics* **2020**, *22* (17), 9723-9733. DOI: 10.1039/d0cp00206b.
(131) Wang, L. N.; Lin, Y. X.; Decarlo, S.; Wang, Y.; Leung, K.; Qi, Y.; Xu, K.; Wang, C. S.; Eichhorn, B. W. Compositions and Formation Mechanisms of Solid-Electrolyte Interphase on Microporous Carbon/Sulfur Cathodes. *Chemistry of Materials* **2020**, *32* (9), 3765-3775. DOI: 10.1021/acs.chemmater.9b05027.
(130) Bi, Y. J.; Tao, J. H.; Wu, Y. Q.; Li, L. Z.; Xu, Y. B.; Hu, E. Y.; Wu, B. B.; Hu, J. T.; Wang, C. M.; Zhan, J. G.; et al. Reversible planar gliding and microcracking in a single-crystalline Ni-rich cathode. *Science* **2020**, *370* (6522), 1313. DOI: 10.1126/science.abc3167.
(129) Thenuwara, A. C.; Shetty, P. P.; Kondekar, N.; Sandoval, S. E.; Cavallaro, K.; May, R.; Yang, C. T.; Marbella, L. E.; Qi, Y.; McDowell, M. T. Efficient Low-Temperature Cycling of Lithium Metal Anodes by Tailoring the Solid-Electrolyte Interphase. *Acs Energy Letters* **2020**, *5* (7), 2411-2420. DOI: 10.1021/acsenergylett.0c01209.

(128) Qi, Y.; Ban, C. M.; Harris, S. J. A New General Paradigm for Understanding and Preventing Li Metal Penetration through Solid Electrolytes. *Joule* **2020**, *4* (12), 2599-2608. DOI: 10.1016/j.joule.2020.10.009.
(127) Yang, C. T.; Lin, Y. X.; Li, B. S.; Xiao, X. C.; Qi, Y. The Bonding Nature and Adhesion of Polyacrylic Acid Coating on Li-Metal for Li Dendrite Prevention. *Acs Applied Materials & Interfaces* **2020**, *12* (45), 51007-51015. DOI: 10.1021/acsami.0c14050.
(126) 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. *Journal of Chemical Physics* **2020**, *153* (8). DOI: 10.1063/5.0016020.
(125) Park, J.; Phongpreecha, T.; Nicholas, J. D.; Qi, Y. Enhanced liquid metal wetting on oxide surfaces via patterned particles. *Acta Materialia* **2020**, *199*, 551-560. DOI: 10.1016/j.actamat.2020.08.037.
(124) O'Hearn, K. A.; Swift, M. W.; Liu, J. L.; Magoulas, I.; Piecuch, P.; van Duin, A. C. T.; Aktulga, H. M.; Qi, Y. Optimization of the Reax force field for the lithium-oxygen system using a high fidelity charge model. *Journal of Chemical Physics* **2020**, *153* (8). DOI: 10.1063/5.0014406.
(123) 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. *Journal of the Electrochemical Society* **2020**, *167* (9). DOI: 10.1149/1945-7111/ab8f5b.
(122) 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*. DOI: 10.1016/j.nanoen.2020.104915.
(121) Phongpreecha, T.; Liu, J.; Hodge, D. B.; Qi, Y. Adsorption of Lignin β-O-4 Dimers on Metal Surfaces in Vacuum and Solvated Environments. *Acs Sustainable Chemistry & Engineering* **2019**, *7* (2), 2667-2678. DOI: 10.1021/acssuschemeng.8b05736.
(120) 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. DOI: 10.1016/j.actamat.2018.11.008.
(119) Li, Y. S.; Qi, Y. Energy landscape of the charge transfer reaction at the complex Li/SEI/electrolyte interface. *Energy & Environmental Science* **2019**, *12* (4), 1286-1295. DOI: 10.1039/c8ee03586e.
(118) Dong, X. L.; Lin, Y. X.; Li, P. L.; Ma, Y. Y.; Huang, J. H.; Bin, D.; Wang, Y. G.; Qi, Y.; Xia, Y. Y. High-Energy Rechargeable Metallic Lithium Battery at-70°C Enabled by a Cosolvent Electrolyte. *Angewandte Chemie-International Edition* **2019**, *58* (17), 5623-5627. DOI: 10.1002/anie.201900266.
(117) Swift, M. W.; Qi, Y. First-Principles Prediction of Potentials and Space-Charge Layers in All-Solid-State Batteries. *Physical Review Letters* **2019**, *122* (16). DOI: 10.1103/PhysRevLett.122.167701.
(116) Harris, O. C.; Lin, Y. X.; Qi, Y.; Leung, K.; Tang, M. H. How Transition Metals Enable Electron Transfer through the SEI: Part I. Experiments and Butler-Volmer Modeling. *Journal of the Electrochemical Society* **2019**, *167* (1). DOI: 10.1149/2.0022001jes.
(115) Xu, J. G.; Tian, H. K.; Qi, J.; Qi, Y.; Zhang, Q. L.; Xiao, X. C. Mechanical and Electronic Stabilization of Solid Electrolyte Interphase with Sulfite Additive for Lithium Metal Batteries. *Journal of the Electrochemical Society* **2019**, *166* (14), A3201-A3206. DOI: 10.1149/2.0331914jes.
(114) Tian, H. K.; Liu, Z.; Ji, Y. Z.; Chen, L. Q.; Qi, Y. Interfacial Electronic Properties Dictate Li Dendrite Growth in Solid Electrolytes. *Chemistry of Materials* **2019**, *31* (18), 7351-7359. DOI: 10.1021/acs.chemmater.9b01967.
(113) Kang, N.; Lin, Y. X.; Yang, L.; Lu, D. P.; Xiao, J.; Qi, Y.; Cai, M. Cathode porosity is a missing key parameter to optimize lithium-sulfur battery energy density. *Nature Communications* **2019**, *10*. DOI: 10.1038/s41467-019-12542-6.

(112) Lin, C. F.; Qi, Y.; Gregorczyk, K.; Lee, S. B.; Rubloff, G. W. Nanoscale Protection Layers To Mitigate Degradation in High-Energy Electrochemical Energy Storage Systems. *Accounts of Chemical Research* **2018**, *51* (1), 97-106. DOI: 10.1021/acs.accounts.7b00524.
(111) Yulaev, A.; Oleshko, V.; Haney, P.; Liu, J. L.; Qi, Y.; Talin, A. A.; Leite, M. S.; Kolmakov, A. From Microparticles to Nanowires and Back: Radical Transformations in Plated Li Metal Morphology Revealed via *in Situ* Scanning Electron Microscopy. *Nano Letters* **2018**, *18* (3), 1644-1650. DOI: 10.1021/acs.nanolett.7b04518.
(110) Wang, A. P.; Kadam, S.; Li, H.; Shi, S. Q.; Qi, Y. Review on modeling of the anode solid electrolyte interphase (SEI) for lithium-ion batteries. *Npj Computational Materials* **2018**, *4*. DOI: 10.1038/s41524-018-0064-0.
(109) Li, Y. S.; Qi, Y. Transferable Self-Consistent Charge Density Functional Tight-Binding Parameters for Li-Metal and Li-Ions in Inorganic Compounds and Organic Solvents. *Journal of Physical Chemistry C* **2018**, *122* (20), 10755-10764. DOI: 10.1021/acs.jpcc.8b01839.
(108) Das, T.; Nicholas, J. D.; Sheldon, B. W.; Qi, Y. Anisotropic chemical strain in cubic ceria due to oxygen-vacancy-induced elastic dipoles. *Physical Chemistry Chemical Physics* **2018**, *20* (22), 15293-15299. DOI: 10.1039/c8cp01219a.
(107) 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. DOI: 10.1016/j.actamat.2018.04.024.
(106) Tian, H. K.; Xu, B.; Qi, Y. Computational study of lithium nucleation tendency in $Li_7La_3Zr_2O_{12}$ (LLZO) and rational design of interlayer materials to prevent lithium dendrites. *Journal of Power Sources* **2018**, *392*, 79-86. DOI: 10.1016/j.jpowsour.2018.04.098.
(105) Liu, Z.; Lu, P.; Zhang, Q. L.; Xiao, X. C.; Qi, Y.; Chen, L. Q. A Bottom-Up Formation Mechanism of Solid Electrolyte Interphase Revealed by Isotope-Assisted Time-of-Flight Secondary Ion Mass Spectrometry. *Journal of Physical Chemistry Letters* **2018**, *9* (18), 5508-5514. DOI: 10.1021/acs.jpclett.8b02350.
(104) Nation, L.; Wu, Y.; James, C.; Qi, Y.; Powell, B. R.; Sheldon, B. W. Si-doped high-energy $Li_{1.2}Mn_{0.54}Ni_{0.13}Co_{0.13}O_2$ cathode with improved capacity for lithium-ion batteries. *Journal of Materials Research* **2018**, *33* (24), 4182-4191. DOI: 10.1557/jmr.2018.378.
(103) Tian, H. K.; Qi, Y. Simulation of the Effect of Contact Area Loss in All-Solid-State Li-Ion Batteries. *Journal of the Electrochemical Society* **2017**, *164* (11), E3512-E3521. DOI: 10.1149/2.0481711jes.
(102) Das, T.; Nicholas, J. D.; Qi, Y. Long-range charge transfer and oxygen vacancy interactions in strontium ferrite. *Journal of Materials Chemistry A* **2017**, *5* (9), 4493-4506. DOI: 10.1039/c6ta10357j.
(101) Liu, J. L.; Huang, Z. W.; Pan, Z. L.; Wei, Q. M.; Li, X. D.; Qi, Y. Atomistic Origin of Deformation Twinning in Biomineral Aragonite. *Physical Review Letters* **2017**, *118* (10). DOI: 10.1103/PhysRevLett.118.105501.
(100) 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* (7), 4330-4338. DOI: 10.1021/acs.nanolett.7b01389.
(99) Pan, J.; Lany, S.; Qi, Y. Computationally Driven Two-Dimensional Materials Design: What Is Next? *Acs Nano* **2017**, *11* (8), 7560-7564. DOI: 10.1021/acsnano.7b04327.
(98) 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. DOI: 10.1016/j.jpowsour.2017.08.006.
(97) Xiong, S.; Li, Y. S.; Sun, J. L.; Qi, Y. Integrated Computation and Experimental Investigation on the Adsorption Mechanisms of Anti-Wear and Anti-Corrosion Additives on Copper. *Journal of Physical Chemistry C* **2017**, *121* (40), 21995-22003. DOI: 10.1021/acs.jpcc.7b04460.

(96) Das, T.; Nicholas, J. D.; Qi, Y. Polaron size and shape effects on oxygen vacancy interactions in lanthanum strontium ferrite. *Journal of Materials Chemistry A* **2017**, *5* (47), 25031-25043. DOI: 10.1039/c7ta06948k.
(95) Suo, L. M.; Oh, D.; Lin, Y. X.; Zhuo, Z. Q.; Borodin, O.; Gao, T.; Wang, F.; Kushima, A.; Wang, Z. Q.; Kim, H. C.; et al. How Solid-Electrolyte Interphase Forms in Aqueous Electrolytes. *Journal of the American Chemical Society* **2017**, *139* (51), 18670-18680. DOI: 10.1021/jacs.7b10688.
(94) Wang, F.; Lin, Y. X.; Suo, L. M.; Fan, X. L.; Gao, T.; Yang, C. Y.; Han, F. D.; Qi, Y.; Xu, K.; Wang, C. S. Stabilizing high voltage $LiCoO_2$ cathode in aqueous electrolyte with interphase-forming additive. *Energy & Environmental Science* **2016**, *9* (12), 3666-3673. DOI: 10.1039/c6ee02604d.
(93) 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* (3), A592-A598. DOI: 10.1149/2.0151605jes.
(92) Kim, S. Y.; Ostadhossein, A.; van Duin, A. C. T.; Xiao, X. C.; Gao, H. J.; Qi, Y. Self-generated concentration and modulus gradient coating design to protect Si nano-wire electrodes during lithiation. *Physical Chemistry Chemical Physics* **2016**, *18* (5), 3706-3715. DOI: 10.1039/c5cp07219k.
(91) Zhang, Q. L.; Pan, J.; Lu, P.; Liu, Z. Y.; 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* (3), 2011-2016. DOI: 10.1021/acs.nanolett.5b05283.
(90) Pan, J.; Zhang, Q. L.; Xiao, X. C.; Cheng, Y. T.; Qi, Y. Design of Nanostructured Heterogeneous Solid Ionic Coatings through a Multiscale Defect Model. *Acs Applied Materials & Interfaces* **2016**, *8* (8), 5687-5693. DOI: 10.1021/acsami.5b12030.
(89) 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. DOI: 10.1016/j.jpowsour.2016.01.078.
(88) Ostadhossein, A.; Kim, S. Y.; Cubuk, E. D.; Qi, Y.; van Duin, A. C. T. Atomic Insight into the Lithium Storage and Diffusion Mechanism of SiO_2/Al_2O_3 Electrodes of Lithium Ion Batteries: ReaxFF Reactive Force Field Modeling. *Journal of Physical Chemistry A* **2016**, *120* (13), 2114-2127. DOI: 10.1021/acs.jpca.5b11908.
(87) 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. DOI: 10.1016/j.ssi.2016.02.019.
(86) Stournara, M. E.; Kumar, R.; Qi, Y.; Sheldon, B. W. *Ab initio* diffuse-interface model for lithiated electrode interface evolution. *Physical Review E* **2016**, *94* (1). DOI: 10.1103/PhysRevE.94.012802.
(85) Li, Y. S.; Leung, K.; Qi, Y. Computational Exploration of the Li-ElectrodelElectrolyte Interface in the Presence of a Nanometer Thick Solid-Electrolyte Interphase Layer. *Accounts of Chemical Research* **2016**, *49* (10), 2363-2370. DOI: 10.1021/acs.accounts.6b00363.
(84) 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). DOI: 10.1103/PhysRevB.91.134116.
(83) Sun, S.; Qi, Y.; Zhang, T. Y. Dissecting graphene capacitance in electrochemical cell. *Electrochimica Acta* **2015**, *163*, 296-302. DOI: 10.1016/j.electacta.2015.02.049.
(82) 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. DOI: 10.1021/acs.jpcc.5b06953.

(81) Chen, L.; Zhang, H. W.; Liang, L. Y.; Liu, Z.; Qi, Y.; Lu, P.; Chen, J.; Chen, L. Q. Modulation of dendritic patterns during electrodeposition: A nonlinear phase-field model. *Journal of Power Sources* **2015**, *300*, 376-385. DOI: 10.1016/j.jpowsour.2015.09.055.
(80) 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. DOI: 10.1149/2.0031411jes.
(79) 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. DOI: 10.1149/2.0231411jes.
(78) Kim, S. Y.; Qi, Y. Property Evolution of Al_2O_3 Coated and Uncoated Si Electrodes: A First Principles Investigation. *Journal of the Electrochemical Society* **2014**, *161* (11), F3137-F3143. DOI: 10.1149/2.0301414jes.
(77) Chen, J. C.; Yan, Y. D.; Sun, T.; Qi, Y.; Li, X. D. Deformation and fracture behaviors of microporous polymer separators for lithium ion batteries. *Rsc Advances* **2014**, *4* (29), 14904-14914. DOI: 10.1039/c4ra00983e.
(76) Chen, J. C.; Yan, Y. D.; Sun, T.; Qi, Y.; Li, X. D. 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. DOI: 10.1149/2.0351409jes.
(75) Chen, J. C.; Sun, T.; Qi, Y.; Li, X. D. A Coupled Penetration-Tension Method for Evaluating the Reliability of Battery Separators. *Ecs Electrochemistry Letters* **2014**, *3* (6), A41-A44. DOI: 10.1149/2.012405eel.
(74) Oliver, D. J.; Paul, W.; El Ouali, M.; Hagedorn, T.; Miyahara, Y.; Qi, Y.; Grütter, P. H. One-to-one spatially matched experiment and atomistic simulations of nanometre-scale indentation. *Nanotechnology* **2014**, *25* (2). DOI: 10.1088/0957-4484/25/2/025701.
(73) 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. DOI: 10.1021/nl500410g.
(72) Sen, F. G.; Alpas, A. T.; van Duin, A. C. T.; Qi, Y. Oxidation-assisted ductility of aluminium nanowires. *Nature Communications* **2014**, *5*. DOI: 10.1038/ncomms4959.
(71) Yan, S. T.; Xiao, X. R.; Huang, X. S.; Li, X. D.; Qi, Y. Unveiling the environment-dependent mechanical properties of porous polypropylene separatorsle. *Polymer* **2014**, *55* (24), 6282-6292. DOI: 10.1016/j.polymer.2014.09.067.
(70) Howe, J. Y.; Burton, D. J.; Qi, Y.; Meyer, H. M.; 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. DOI: 10.1016/j.jpowsour.2012.08.026.
(69) Chen, J. C.; Liu, J. Y.; Qi, Y.; Sun, T.; Li, X. D. 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. DOI: 10.1149/2.088309jes.
(68) 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. DOI: 10.1016/j.surfcoat.2012.08.092.
(67) 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). DOI: 10.1063/1.4790181.
(66) Sun, C. F.; Karki, K.; Jia, Z.; Liao, H. W.; Zhang, Y.; Li, T.; Qi, Y.; Cumings, J.; Rubloff, G. W.; Wang, Y. H. A Beaded-String Silicon Anode. *Acs Nano* **2013**, *7* (3), 2717-2724. DOI: 10.1021/nn4001512.
(65) Sen, F. G.; Qi, Y.; Alpas, A. T. Tribology of fluorinated diamond-like carbon coatings: first principles calculations and sliding experiments. *Lubrication Science* **2013**, *25* (2), 111-121. DOI: 10.1002/ls.1166.

(64) Shi, S. Q.; Qi, Y.; Li, H.; Hector, L. G. Defect Thermodynamics and Diffusion Mechanisms in Li₂CO₃ and Implications for the Solid Electrolyte Interphase in Li-Ion Batteries. *Journal of Physical Chemistry C* **2013**, *117* (17), 8579-8593. DOI: 10.1021/jp310591u.
(63) Stournara, M. E.; Xiao, X. C.; Qi, Y.; Johari, P.; Lu, P.; Sheldon, B. W.; Gao, H. J.; Shenoy, V. B. Li Segregation Induces Structure and Strength Changes at the Amorphous Si/Cu Interface. *Nano Letters* **2013**, *13* (10), 4759-4768. DOI: 10.1021/nl402353k.
(62) Zhang, H.; Liu, X. B.; Qi, Y.; Liu, V. On the $La_{2/3-x}Li_{3x}TiO_3/Al_2O_3$ composite solid-electrolyte for Li-ion conduction. *Journal of Alloys and Compounds* **2013**, *577*, 57-63. DOI: 10.1016/j.jallcom.2013.04.195.
(61) Sheldon, B. W.; Soni, S. K.; Xiao, X. C.; Qi, Y. Stress Contributions to Solution Thermodynamics in Li-Si Alloys (vol 15, pg A9, 2012). *Electrochemical and Solid State Letters* **2012**, *15* (4), S3-S3. DOI: 10.1149/2.030204esl.
(60) Sheldon, B. W.; Soni, S. K.; Xiao, X. C.; Qi, Y. Stress Contributions to Solution Thermodynamics in Li-Si Alloys. *Electrochemical and Solid State Letters* **2012**, *15* (1), A9-A11. DOI: 10.1149/2.016201esl.
(59) Qi, Y.; Xu, Q. C.; Van der Ven, A. Chemically Induced Crack Instability When Electrodes Fracture. *Journal of the Electrochemical Society* **2012**, *159* (11), A1838-A1843. DOI: 10.1149/2.026211jes.
(58) Sen, F. G.; Qi, Y.; Alpas, A. T. Anchoring platinum on graphene using metallic adatoms: a first principles investigation. *Journal of Physics-Condensed Matter* **2012**, *24* (22). DOI: 10.1088/0953-8984/24/22/225003.
(57) Shang, S. L.; Hector, L. G.; Shi, S. Q.; Qi, Y.; Wang, Y.; Liu, Z. K. Lattice dynamics, thermodynamics and elastic properties of monoclinic Li₂CO₃ from density functional theory. *Acta Materialia* **2012**, *60* (13-14), 5204-5216. DOI: 10.1016/j.actamat.2012.06.006.
(56) Shi, S. Q.; Lu, P.; Liu, Z. Y.; Qi, Y.; Hector, L. G.; Li, H.; Harris, S. J. Direct Calculation of Li-Ion Transport in the Solid Electrolyte Interphase. *Journal of the American Chemical Society* **2012**, *134* (37), 15476-15487. DOI: 10.1021/ja305366r.
(55) Wang, X. L.; An, K.; Cai, L.; Feng, Z. L.; Nagler, S. E.; Daniel, C.; Rhodes, K. J.; Stoica, A. D.; Skorpenske, H. D.; Liang, C. D.; et al. Visualizing the chemistry and structure dynamics in lithium-ion batteries by *in-situ* neutron diffraction. *Scientific Reports* **2012**, *2*. DOI: 10.1038/srep00747.
(54) Oliver, D. J.; Maassen, J.; El Ouali, M.; Paul, W.; Hagedorn, T.; Miyahara, Y.; Qi, Y.; Guo, H.; Grütter, 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. DOI: 10.1073/pnas.1208699109.
(53) Liang, L. Y.; 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). DOI: 10.1103/PhysRevE.86.051609.
(52) Qi, Y.; Lai, Y. H. Mesoscale modeling of the influence of morphology on the mechanical properties of proton exchange membranes. *Polymer* **2011**, *52* (1), 201-210. DOI: 10.1016/j.polymer.2010.11.013.
(51) Milas, I.; Qi, Y.; Sheldon, B. W.; Shenoy, V. B. First-principles study of void induced stresses at a diamond (100) grain boundary. *Journal of Applied Physics* **2011**, *109* (3). DOI: 10.1063/1.3544366.
(50) Du, N. N.; Qi, Y.; Krajewski, P. E.; Bower, A. F. The Effect of Solute Atoms on Aluminum Grain Boundary Sliding at Elevated Temperature. *Metallurgical and Materials Transactions a-Physical Metallurgy and Materials Science* **2011**, *42A* (3), 651-659. DOI: 10.1007/s11661-010-0326-z.
(49) Sen, F. G.; Qi, Y.; Alpas, A. T. Material transfer mechanisms between aluminum and fluorinated carbon interfaces. *Acta Materialia* **2011**, *59* (7), 2601-2614. DOI: 10.1016/j.actamat.2010.12.045.

(48) Abou Gharam, A.; Lukitsch, M. J.; Qi, Y.; Alpas, A. T. Role of oxygen and humidity on the tribo-chemical behaviour of non-hydrogenated diamond-like carbon coatings. *Wear* **2011**, *271* (9-10), 2157-2163. DOI: 10.1016/j.wear.2010.12.083.
(47) Leung, K.; Qi, Y.; Zavadil, K. R.; Jung, Y. S.; Dillon, A. C.; Cavanagh, A. S.; Lee, S. H.; George, S. M. Using Atomic Layer Deposition to Hinder Solvent Decomposition in Lithium Ion Batteries: First-Principles Modeling and Experimental Studies. *Journal of the American Chemical Society* **2011**, *133* (37), 14741-14754. DOI: 10.1021/ja205119g.
(46) Krajewski, P. E.; Hector, L. G.; Qi, Y.; Mishra, R. K.; Sachdev, A. K.; Bower, A. F.; Curtin, W. A. Atoms to Autos: A Multi-scale Approach to Modeling Aluminum Deformation. *Jom* **2011**, *63* (11), 24-32. DOI: 10.1007/s11837-011-0187-y.
(45) Johari, P.; Qi, Y.; Shenoy, V. B. The Mixing Mechanism during Lithiation of Si Negative Electrode in Li-Ion Batteries: An Ab Initio Molecular Dynamics Study. *Nano Letters* **2011**, *11* (12), 5494-5500. DOI: 10.1021/nl203302d.
(44) Qi, Y.; Harris, S. J. In Situ Observation of Strains during Lithiation of a Graphite Electrode. *Journal of the Electrochemical Society* **2010**, *157* (6), A741-A747. DOI: 10.1149/1.3377130.
(43) Qi, Y.; Guo, H. B.; Hector, L. G.; Timmons, A. Threefold Increase in the Young's Modulus of Graphite Negative Electrode during Lithium Intercalation. *Journal of the Electrochemical Society* **2010**, *157* (5), A558-A566. DOI: 10.1149/1.3327913.
(42) Deshpande, R.; Qi, Y.; Cheng, Y. T. Effects of Concentration-Dependent Elastic Modulus on Diffusion-Induced Stresses for Battery Applications. *Journal of the Electrochemical Society* **2010**, *157* (8), A967-A971. DOI: 10.1149/1.3454762.
(41) Guo, H. B.; Qi, Y.; Li, X. D. Adhesion at diamond/metal interfaces: A density functional theory study. *Journal of Applied Physics* **2010**, *107* (3). DOI: 10.1063/1.3277013.
(40) Guo, H. B.; Qi, Y. Environmental conditions to achieve low adhesion and low friction on diamond surfaces. *Modelling and Simulation in Materials Science and Engineering* **2010**, *18* (3). DOI: 10.1088/0965-0393/18/3/034008.
(39) Du, N. N.; Qi, Y.; Krajewski, P. E.; Bower, A. F. Aluminum Σ3 grain boundary sliding enhanced by vacancy diffusion. *Acta Materialia* **2010**, *58* (12), 4245-4252. DOI: 10.1016/j.actamat.2010.04.016.
(38) Harris, S. J.; Deshpande, R. D.; Qi, Y.; Dutta, I.; Cheng, Y. T. Mesopores inside electrode particles can change the Li-ion transport mechanism and diffusion-induced stress. *Journal of Materials Research* **2010**, *25* (8), 1433-1440. DOI: 10.1557/jmr.2010.0183.
(37) Shenoy, V. B.; Johari, P.; Qi, Y. Elastic softening of amorphous and crystalline Li-Si Phases with increasing Li concentration: A first-principles study. *Journal of Power Sources* **2010**, *195* (19), 6825-6830. DOI: 10.1016/j.jpowsour.2010.04.044.
(36) Kong, L. T.; Denniston, C.; Müser, M. H.; Qi, Y. Non-bonded force field for the interaction between metals and organic molecules: a case study of olefins on aluminum. *Physical Chemistry Chemical Physics* **2009**, *11* (43), 10195-10203. DOI: 10.1039/b906874k.
(35) Xia, S. M.; Qi, Y.; Perry, T.; Kim, K. S. Strength characterization of Al/Si interfaces: A hybrid method of nanoindentation and finite element analysis. *Acta Materialia* **2009**, *57* (3), 695-707. DOI: 10.1016/j.actamat.2008.10.011.
(34) Qi, Y.; Sheldon, B. W.; Guo, H.; Xiao, X.; Kothari, A. K. Impact of Surface Chemistry on Grain Boundary Induced Intrinsic Stress Evolution during Polycrystalline Thin Film Growth. *Physical Review Letters* **2009**, *102* (5). DOI: 10.1103/PhysRevLett.102.056101.
(33) Soldera, A.; Qi, Y.; Capehart, W. T. Phase transition and morphology of polydispersed ABA' triblock copolymers determined by continuous and discrete simulations. *Journal of Chemical Physics* **2009**, *130* (6). DOI: 10.1063/1.3071194.
(32) Cipoletti, D. E.; Bower, A. F.; Qi, Y.; Krajewski, P. E. The influence of heterogeneity in grain boundary sliding resistance on the constitutive behavior of AA5083 during high-temperature deformation. *Materials Science and Engineering a-Structural Materials Properties Microstructure and Processing* **2009**, *504* (1-2), 175-182. DOI: 10.1016/j.msea.2008.10.037.

(31) Brunello, G.; Lee, S. G.; Jang, S. S.; Qi, Y. A molecular dynamics simulation study of hydrated sulfonated poly(ether ether ketone) for application to polymer electrolyte membrane fuel cells: Effect of water content. *Journal of Renewable and Sustainable Energy* **2009**, *1* (3). DOI: 10.1063/1.3138922.
(30) Ward, D. K.; Farkas, D.; Lian, J.; Curtin, W. A.; Wang, J.; Kim, K. S.; Qi, Y. Engineering size-scaling of plastic deformation in nanoscale asperities. *Proceedings of the National Academy of Sciences of the United States of America* **2009**, *106* (24), 9580-9585. DOI: 10.1073/pnas.0900804106.
(29) Yasi, J. A.; Nogaret, T.; Trinkle, D. R.; Qi, Y.; Hector, L. G.; Curtin, W. A. Basal and prism dislocation cores in magnesium: comparison of first-principles and embedded-atom-potential methods predictions. *Modelling and Simulation in Materials Science and Engineering* **2009**, *17* (5). DOI: 10.1088/0965-0393/17/5/055012.
(28) Sen, F. G.; Qi, Y.; Alpas, A. T. Surface stability and electronic structure of hydrogen- and fluorine-terminated diamond surfaces: A first principles investigation. *Journal of Materials Research* **2009**, *24* (8), 2461-2470. DOI: 10.1557/jmr.2009.0309.
(27) Guo, H. B.; Xiao, X. C.; Qi, Y.; Xu, Z. H.; Li, X. D. Enhance diamond coating adhesion by oriented interlayer microcracking. *Journal of Applied Physics* **2009**, *106* (12). DOI: 10.1063/1.3267162.
(26) Xiao, X.; Sheldon, B. W.; Qi, Y.; Kothari, A. K. Intrinsic stress evolution in nanocrystalline diamond thin films with deposition temperature. *Applied Physics Letters* **2008**, *92* (13). DOI: 10.1063/1.2906903.
(25) Guo, H. B.; Qi, Y.; Li, X. D. Predicting the hydrogen pressure to achieve ultralow friction at diamond and diamondlike carbon surfaces from first principles. *Applied Physics Letters* **2008**, *92* (24). DOI: 10.1063/1.2946661.
(24) Noreyan, A.; Qi, Y.; Stoilov, V. Critical shear stresses at aluminum-silicon interfaces. *Acta Materialia* **2008**, *56* (14), 3461-3469. DOI: 10.1016/j.actamat.2008.03.037.
(23) Qi, Y.; Hector, L. G. Planar stacking effect on elastic stability of hexagonal boron nitride. *Applied Physics Letters* **2007**, *90* (8). DOI: 10.1063/1.2679007.
(22) Qi, Y.; Krajewski, P. E. Molecular dynamics simulations of grain boundary sliding: The effect of stress and boundary misorientation. *Acta Materialia* **2007**, *55* (5), 1555-1563. DOI: 10.1016/j.actamat.2006.10.016.
(21) Zhang, Q.; Qi, Y.; Hector, L. G.; Cagin, T.; Goddard, W. A. Origin of static friction and its relationship to adhesion at the atomic scale. *Physical Review B* **2007**, *75* (14). DOI: 10.1103/PhysRevB.75.144114.
(20) Wu, X. L.; Qi, Y.; Zhu, Y. T. Partial-mediated slips in nanocrystalline Ni at high strain rate. *Applied Physics Letters* **2007**, *90* (22). DOI: 10.1063/1.2745250.
(19) Qi, Y.; Mishra, R. K. Ab initio study of the effect of solute atoms on the stacking fault energy in aluminum. *Physical Review B* **2007**, *75* (22). DOI: 10.1103/PhysRevB.75.224105.
(18) Campañá, C.; Müser, M. H.; Denniston, C.; Qi, Y.; Perry, T. A. Elucidating the contact mechanics of aluminum silicon surfaces with Green's function molecular dynamics. *Journal of Applied Physics* **2007**, *102* (11). DOI: 10.1063/1.2815640.
(17) Wescott, J. T.; Qi, Y.; Subramanian, L.; Capehart, T. W. Mesoscale simulation of morphology in hydrated perfluorosulfonic acid membranes. *Journal of Chemical Physics* **2006**, *124* (13). DOI: 10.1063/1.2177649.
(16) Ward, D. K.; Curtin, W. A.; Qi, Y. Aluminum-silicon interfaces and nanocomposites: A molecular dynamics study. *Composites Science and Technology* **2006**, *66* (9), 1151-1161. DOI: 10.1016/j.compscitech.2005.10.024.
(15) Qi, Y.; Konca, E.; Alpas, A. T. Atmospheric effects on the adhesion and friction between non-hydrogenated diamond-like carbon (DLC) coating and aluminum - A first principles investigation. *Surface Science* **2006**, *600* (15), 2955-2965. DOI: 10.1016/j.susc.2006.05.008.

(14) Ward, D. K.; Curtin, W. A.; Qi, Y. Mechanical behavior of aluminum-silicon nanocomposites: A molecular dynamics study. *Acta Materialia* **2006**, *54* (17), 4441-4451. DOI: 10.1016/j.actamat.2006.05.022.

(13) Qi, Y.; Hector, L. G.; Ooi, N.; Adams, J. B. A first principles study of adhesion and adhesive transfer at Al(111)/graphite(0001). *Surface Science* **2005**, *581* (2-3), 155-168. DOI: 10.1016/j.susc.2005.02.048.

(12) Zhang, Q.; Qi, Y.; Hector, L. G., Jr.; Çagin, T.; Goddard, W. A., III. Atomic simulations of kinetic friction and its velocity dependence at Al/Al and α-Al₂O₃/α-Al₂O₃ interfaces - art. no. 045406. *Physical Review B* **2005**, *72* (4). DOI: 10.1103/PhysRevB.72.045406.

(11) Zhang, Q.; Çagin, T.; van Duin, A.; Goddard, W. A., III; Qi, Y.; Hector, L. G., Jr. Adhesion and nonwetting-wetting transition in the Al/α-Al₂O₃ interface - art. no. 045423. *Physical Review B* **2004**, *69* (4). DOI: 10.1103/PhysRevB.69.045423.

(10) Qi, Y.; Hector, L. G. Adhesion and adhesive transfer at aluminum/diamond interfaces: A first-principles study. *Physical Review B* **2004**, *69* (23). DOI: 10.1103/PhysRevB.69.235401.

(9) Qi, Y.; Hector, L. G. Hydrogen effect on adhesion and adhesive transfer at aluminum/diamond interfaces. *Physical Review B* **2003**, *68* (20). DOI: 10.1103/PhysRevB.68.201403.

(8) Qi, Y.; Çagin, T.; Kimura, Y.; Goddard, W. A., III. Viscosities of liquid metal alloys from nonequilibrium molecular dynamics. *Journal of Computer-Aided Materials Design* **2002**, *8* (2-3), 233-243.

(7) Qi, Y.; Çagin, T.; Goddard, W. A., III. MPiSIM: Massively parallel simulation tool for metallic system. *Journal of Computer-Aided Materials Design* **2002**, *8* (2-3), 185-192.

(6) Qi, Y.; Cheng, Y. T.; Çagin, T.; Goddard, W. A., III. Friction anisotropy at Ni(100)/(100) interfaces: Molecular dynamics studies. *Physical Review B* **2002**, *66* (8). DOI: 10.1103/PhysRevB.66.085420.

(5) Qi, Y.; Çagin, T.; Johnson, W. L.; Goddard, W. A., III. Melting and crystallization in Ni nanoclusters: The mesoscale regime. *Journal of Chemical Physics* **2001**, *115* (1), 385-394. DOI: 10.1063/1.1373664.

(4) Qi, Y.; Strachan, A.; Cagin, T.; Goddard, W. A., III. Large scale atomistic simulations of screw dislocation structure, annihilation and cross-slip in FCCNi. *Materials Science and Engineering a-Structural Materials Properties Microstructure and Processing* **2001**, *309*, 156-159. DOI: 10.1016/s0921-5093(00)01716-0.

(3) Qi, Y.; Çagin, T.; Kimura, Y.; Goddard, W. A., III. 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. DOI: 10.1103/PhysRevB.59.3527.

(2) Çagin, T.; Che, J. W.; Qi, Y.; Zhou, Y. H.; Demiralp, E.; Gao, G. H.; Goddard, W. A. Computational materials chemistry at the nanoscale. *Journal of Nanoparticle Research* **1999**, *1* (1), 51-69. DOI: 10.1023/a:1010009630519.

(1) Ikeda, H.; Qi, Y.; Çagin, T.; Samwer, K.; Johnson, W. L.; Goddard, W. A., III. Strain rate induced amorphization in metallic nanowires. *Physical Review Letters* **1999**, *82* (14), 2900-2903. DOI: 10.1103/PhysRevLett.82.2900.

b) Reviewed Conference Papers

- 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.* **2019** DOI: 10.1007/978-3-030-06034-3_4
- 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**.

- 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. DOI: 10.1557/adv.2016.48
- 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, Pg. 2040-2050
- 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.

c) Book Chapters

- 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
- 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

d) Awarded Patents

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