Liang Qi

University of Michigan
2158A H. H. Dow Bldg.
2300 Hayward Street
Ann Arbor, MI 48109
Tel: (734) 615-8086
Email:qiliang@umich.edu
Website:http://cms.engin.umich.edu/

Employment

University of Michigan — Ann Arbor, MI
Department of Materials Science and Engineering
Associate Professor (9/2021-), Assistant Professor (1/2015-8/2021)

University of California, Berkeley — Berkeley, CA
Department of Materials Science and Engineering
Assistant Project Scientist (9/2012-12/2014)

Massachusetts Institute of Technology — Boston, MA
Department of Nuclear Science and Engineering
Postdoctoral Associate (9/2011-8/2012)

University of Pennsylvania — Philadelphia, PA
Department of Materials Science and Engineering
Postdoctoral Associate (9/2009-8/2011)

Education

University of Pennsylvania — Philadelphia, PA
Department of Materials Science and Engineering, Ph.D. (2007-2009)

Ohio State University — Columbus, OH
Department of Materials Science and Engineering, M.S. (2003-2007)

Tsinghua University — Beijing, China
Department of Materials Science and Engineering, B.E. (1999-2003)

Awards

TMS MPMD Young Leaders Professional Development Award, 2021

CAREER Award, National Science Foundation, 2019

A finalist for the Rising Stars in Computational Materials Science Special Issue and Prize, 2018

Excellent Graduate Award of Tsinghua University, 2003

Research

Computational materials sciences in fields of metallurgy, mechanical behavior, materials chemistry, and materials processing: first-principles calculations, atomistic simulations, multiscale modeling, and machine learning.

Teaching

Instructor, UMich MSE 350: Structures of Materials (Fall Semester, 2015-2021)

Co-Instructor with Prof. Amit Misra, UMich MSE 520: Advanced Mechanical Behavior (Winter Semester, 2016, 2017, 2020, 2021)

Instructor, UMich MSE 470: Physical Metallurgy (Winter Semester, 2018)

Co-Instructor with Prof. Ju Li, Penn MSE540: Phase Transformations (Spring Term, 2010, 2011)

Service

Co-organizer of the symposium *Grain Boundaries and Interfaces: Metastability, Disorder, and Non-Equilibrium Behavior* in TMS 2022

Lead organizer of the symposium *High-Entropy Alloys and other Novel High-Temperature Structural Alloys* in 2019 MRS Fall Meeting and Exhibit

Lead organizer of the symposium *Computational Approaches for Big Data, Artificial Intelligence and Uncertainty Quantification in Computational Materials Science* in TMS 2019

Co-Guest Editors, JOM Editorial Calendar - Topic Details "Mechanical Properties of Metastable Materials Containing Strong Disorder", 2019

Lead organizer of the symposium *Non-equilibrium Features of Grain Boundaries* in TMS 2018

Member of the Integrated Computational Materials Engineering Committee, TMS-MPMD (3/2018-)

Member of the Computational Materials Science and Engineering Committee, TMS-MPMD (2/2017-)

Member of the Nanomechanical Materials Behavior Committee, TMS-MPMD (2/2017-)

Member of the Mechanical Behavior of Materials Committee, TMS-SMD (2/2017-)

Publications (Google Scholar (Citations = 4869 and h-index = 28 on 9/8/2021) and ResearcherID)

60. A. Chatterjee, **L. Qi**, A. Misra. "In situ transmission electron microscopy investigation of nucleation of GP zones under natural aging in Al-Zn-Mg alloy", submitted to *Scripta Materialia*, (2021)

59. N. Sanders, M. Zhang, K. Mengle, **L. Qi**, E. Kioupakis, "Effect of stacking orientation on the electronic and optical properties of polar 2D III-nitride bilayers", *The Journal of Physical Chemistry C*, **125** (2021) 16837-16842

58. J. Marcial, Y. Zhang , X. Zhao, H. Xu, A. Mesbah, E.T. Nienhuis, S. Szenknect, J.C. Neuefeind, J. Lin, **L. Qi**, A.A. Migdisov, R.C. Ewing, N. Dacheux, J.S. McCloy, and X. Guo, "Thermodynamic non-ideality and disorder heterogeneity in actinide silicate solid solutions", *npj Materials Degradation*,**5** (2021) 34

57. Y. Hu, A. Sundar, S. Ogata, **L. Qi**, "Screening of generalized stacking fault energies, surface energies and intrinsic ductile potency of refractory multicomponent alloys", *Acta Materialia*, **210** (2021) 116800

56. A. Sundar, G. Chen, **L. Qi**, "Substitutional adsorptions of chloride at grain boundary sites on hydroxylated alumina surfaces initialize localized corrosion", *npj Materials Degradation*, **5** (2021) 18

55. A. Sundar, **L. Qi**, "Stability of native point defects in α-Al_2O_3 under aqueous electrochemical conditions", *Journal of Applied Electrochemistry*, **51** (2021) 639-651

54. Z. Huang, C. Yang, J. Allison, **L. Qi**, A. Misra, "Dislocation cross-slip in precipitation hardened Mg–Nd alloys", *Journal of Alloys and Compounds*, **859** (2021) 157858

53. L. Jiang, V. Radmilović, J. Sabisch, **L. Qi**, A. Minor, D. Chrzan, M Asta, "Twin nucleation from a single $\langle$c+ a$\rangle$ dislocation in hexagonal close-packed crystals", *Acta Materialia*, **202** (2021) 35-41

52. L. Jiang, Y. Hu, K. Sun, P. Xiu, M. Song, Y. Zhang, W. Boldman, M. Crespillo, P. Rack, **L. Qi**, W. Weber, L. Wang, "Irradiation-Induced Extremes Create Hierarchical Face-/Body-Centered-Cubic Phases in Nanostructured High Entropy Alloys", *Advanced Materials*, **32** (2020) 2002652

51. C. Yang, M. Zhang, **L. Qi**, "Grain boundary structure search by using an evolutionary algorithm with effective mutation methods", *Computational Materials Science*, **184** (2020)109812

50. Y. Hu, G. Zhao, M. Zhang, B. Bin, T. Del Rose, Q. Zhao, Q. Zu, Y. Chen, X. Sun, M. de Jong, **L. Qi**, "Predicting densities and elastic moduli of SiO2-based glasses by machine learning", *npj Computational Materials*, **6** (2020) 25

49. H. Lu, C. Reese, S. Jeon, A. Sundar, Y. Fan, E. Rizzi, Y. Zhuo, **L. Qi**, R. Goldman, "Mechanisms of GaN quantum dot formation during nitridation of Ga droplets", *Applied Physics Letters*, **116** (2020) 062107

48. Y. Hu, G. Zhao, B. Zhang, C. Yang, M. Zhang, Z. Liu, X.F. Qian, **L. Qi**, "Local electronic descriptors for solute-defect interactions in bcc refractory metals", *Nature Communications*, **10** (2019) 4484

47. M. Zhang, L. Hector, Y. Guo, M. Liu, **L. Qi**, "First-principles Search for Alloying Elements that Increase Corrosion Resistance of Mg with Second-Phase Particles of Transition Metal Impurities", *Computational Materials Science*, **165** (2019) 154-166

46. **L. Qi**, "Effects of electronic structures on mechanical properties of transition metals and alloys", *Computational Materials Science*, **163** (2019) 11-16 (*Rising Stars in Computational Materials Science*)

45. C. Wang, T. Yang, C. Tracy, C. Lu, H. Zhang, Y. Hu, L. Wang, **L. Qi**, L. Gu, Q. Huang, J. Zhang, J. Wang, J. Xue, R. Ewing, Y. Wang, "Disorder in $M_{n+1}AX_n$ phases at the atomic scale, *Nature Communications*, **10** (2019) 722

44. C. Yang, **L. Qi**, "Modified embedded-atom method potential of niobium for studies on mechanical properties", *Computational Materials Science*, **161** (2019) 351-363 (*Editor's Choice*)

43. Z. Huang, C. Yang, **L. Qi**, J. Allison, A. Misra, "Dislocation pile-ups at $\beta 1$ precipitate interfaces in Mg-rare earth (RE) alloys", *Materials Science and Engineering: A*, **742** (2019) 278-286

42. M. Zhang, **L. Qi**, "Tuning hydrogen adsorption on pure and doped ZnO $(000\bar{1})$ surfaces by a simple electron counting model", *Journal of Applied Physics*, **124** (2018) 155302

41. LK Aagesen, JF Adams, JE Allison, WB Andrews, V Araullo-Peters, T Berman, Z Chen, S Daly, S Das, S DeWitt, S Ganesan, K Garikipati, V Gavini, A Githens, M Hedstrom, Z Huang, HV Jagadish, JW Jones, J Luce, EA Marquis, A Misra, D Montiel, P Motamarri, AD Murphy, AR Natarajan, S Panwar, B Puchala, **L Qi**, S Rudraraju, K Sagiyama, ELS Solomon, V Sundararaghavan, G Tarcea, GH Teichert, JC Thomas, K Thornton, A Van der Ven, Z Wang, T Weymouth, C Yang, "PRISMS: An Integrated, Open-Source Framework for Accelerating Predictive Structural Materials Science", *JOM*, **70** (2018) 2298-2314

40. C. Yang, **L. Qi**, "Ab initio calculations of ideal strength and lattice instability in W-Ta and W-Re alloys", *Physical Review B*, **97** (2018) 014107

39. E. Chen, L. Williams, A. Olvera, C. Zhang, M. Zhang, G. Shi, J. Heron, **L. Qi**, L. Guo, E. Kioupakis, P. Poudeu, "Sustainable p-type copper selenide solar material with ultra-large absorption coefficient", *Chemical Science*, **9** (2018) 5405-5414

38. L. Zou, C. Yang, Y. Lei, D. Zakharov, J. Wiezorek, D. Su, Q. Yin, J. Li, Z. Liu, E. Stach, J. Yang, **L. Qi**, G. Wang, G. Zhou, "Dislocation nucleation facilitated by atomic segregation", *Nature Materials*, **17** (2018) 56-63

37. W.P. Gao, J.B. Wu, A. Yoon, P. Lu, **L. Qi**, J.G. Wen, D. J. Miller, J. C. Mabon, W. L. Wilson, H. Yang, J. M. Zuo, "Dynamics of Transformation from Platinum Icosahedral Nanoparticles to Larger FCC Crystal at Millisecond Time Resolution", *Scientific Reports*, **7** (2017) 17243

36. Y.H. Dong, **L. Qi**, J. Li, I-W. Chen, "A computational study of yttria-stabilized zirconia: II. Cation diffusion", *Acta Materialia* **126** (2017) 438-450

35. Y.H. Dong, **L. Qi**, J. Li, I-W. Chen, "A computational Study of Yttria-Stabilized Zirconia: I. Using Crystal Chemistry to Search for the Ground State on a Glassy Energy Landscape", *Acta Materialia* **126** (2017) 73-84

34. C. Kinney, K. Pytlewski, **L. Qi**, A.G. Khachaturyan, J.W. Morris, "An Investigation Into 6-Fold Symmetry in Martensitic Steels", *Metallurgical and Materials Transactions A*, **47** (2016) 5266-5270

33. M. de Jong, **L. Qi**, D. Olmsted, A. van de Walle and M. Asta, "Calculations of Planar Defect Energies in Substitutional Alloys Using the Special-Quasirandom-Structure Approach", *Phys. Rev. B*, **93** (2016) 094101.

32. X.F. Guo, E. Tiferet, **L. Qi**, J. M. Solomon, A. Lanzirotti, M. Newville, M. H. Engelhard, R. K. Kukkadapu, D. Wu, E. S Ilton, M. Asta, S. R. Sutton, H. Xu, A. Navrotsky, "U(V) in metal uranates: a combined experimental and theoretical study of MgUO4, CrUO4, and FeUO4", *Dalton Transactions*, **45** (2016) 4622-4632.

31. M. de Jong, J. Kacher, M. Sluiter, **L. Qi**, D. Olmsted, A. van de Walle, J. Morris, Jr., A. Minor and M. Asta, "Electronic Origins of Anomalous Twin Boundary Energies in Hexagonal Close Packed Transition Metals", *Phys. Rev. Lett.*, **115** (2015) 065501.

30. H. Liu, Y.P. Gao, **L. Qi**, Y.Z. Wang and J.F. Nie, "Phase-Field Simulation of Orowan Strengthening by Coherent Precipitate Plates in an Aluminum Alloy",*Metallurgical and Materials Transactions A*, **46** (2015) 3287-3301.

29. Q. Yu, **L. Qi**, R. Mishra, X. Zeng, A. Minor, "Size-dependent mechanical properties of Mg nanoparticles used for hydrogen storage", *Applied Physics Letters*, **106** (2015) 261903.

28. S.Z. Li, Y.G. Li, Y. C. Luo, S. T. Neeraj, R. Srinivasan, X.D. Ding, , J. Sun, **L. Qi**, P. Gumbsch and J. Li, "The interaction of dislocations and hydrogen-vacancy complexes and its importance for deformation-induced proto nano-voids formation in α-Fe", *International Journal of Plasticity*, **74** (2015) 175-191.

27. Q. Yu*, **L. Qi***(*: equal contribution), T. Tsuru, R. Traylor, D. Rugg, J. Morris, M. Asta, D. Chrzan, A. Minor, "Origin of dramatic oxygen solute strengthening effect in Titanium", *Science*, **347** (2015) 635-639.

26. **L. Qi**, A.G. Khachaturyan, J.W. Morris, Jr.,"The microstructure of dislocated martensitic steel: theory", *Acta Materialia*, **76** (2014) 23-39.

25. **L. Qi**, D. Chrzan, "Tuning Ideal Tensile Strengths and Intrinsic Ductility of BCC Refractory Alloys", *Phys. Rev. Lett.* **112** (2014) 115503 (*Featured in Physics* and *Editors' Suggestion*).

24. X. F. Guo, A. H. Tavakolia, S. Sutton, R. K. Kukkadapu, **L. Qi**, A. Lanzirotti, M. Newvilleb, M. Asta and A. Navrotsky, "Cerium substitution in yttrium iron garnet: valence state structure, and energetics", *Chemistry of Materials*, **26** (2014) 1133–1143.

23. J. F. Niu, A. Kushima, X. F. Qian, **L. Qi**, K. Xiang, Y. M. Chiang and J. Li,"In situ electron microscopy of random solid solution region in $LiFePO_4$ battery electrode", *Nano Letters*, **14** (2014) 4005-4010.

22. Q. Yu, **L. Qi**, R. Mishra, J. Li and A. Minor, "Reducing deformation anisotropy to achieve ultrahigh strength and ductility in Mg at the nanoscale", *Proc. Natl. Acad. Sci.*, **110** (2013) 13289-13293.

21. X-C. Ye, J. Chen, M. Engel, A. Millan, W-B Li, **L. Qi**, G-Z. Xing, A-G. Dong, J. Collins, C. Kagan, J. Li, S. Glotzer, C. Murray, "Competition of shape and interaction patchiness for self-assembling nanoplates", *Nature Chemistry*, **5** (2013) 466-473.

20. Y-J. Kang, X-C. Ye, J. Chen, **L. Qi**, R. Diaz, V. Doan-Nguyen, G-Z. Xing, C. Kagan, J. Li, R. Gorte, E. Stach, C. Murray, "Engineering catalytic contacts and thermal stability: gold-iron-oxide binary nanocrystal superlattices for CO Oxidation", *J. Am. Chem. Soc.* **135** (2013) 1499-1505.

19. **L. Qi** and J. Li, "Adsorbate Interactions on Surface Lead to a Flattened Sabatier Volcano Plot in Reduction of Oxygen", *Journal of Catalysis* **295** (2012) 59-69.

18. **L. Qi**, Y-W. Mao and J. Li, "Slip Corona Surrounding Bilayer Graphene Nanopore", *Nanoscale* **4** (2012) 5989-5997.

17. J-B. Wu, **L. Qi**, H-J. You, A. Gross, J. Li, H. Yang, "Icosahedral Platinum Alloy Nanocrystals with Enhanced Electrocatalytic Activities", *J. Am. Chem. Soc.* **134** (2012) 11880-11883.

16. J. Feng, W-B. Li, X-F. Qian, J-S. Qi, **L. Qi**, and J. Li, "Patterning of Graphene", *Nanoscale* **4** (2012) 4883-4899.

15. S-W. Nam, H-S. Chung, Y-C. Lo, **L. Qi**, J. Li, Y. Lu, A.T. C. Johnson, Y. Jung, P. Nukala, and R. Agarwal, "Electrical Wind Force-Driven and Dislocation-Templated Amorphization in Phase-Change Nanowires", *Science* **336** (2012) 1561-1566

14. Y-J. Kang, **L. Qi**, M. Li, R. Rivas, R. Adzic, E. Stach, J. Li, C.B. Murray, "Highly active Pt_3Pb and core-shell Pt_3Pb-Pt electrocatalysts for formic acid oxidation", *ACS Nano* **6** (2012) 2818-2825

13. J-S. Qi, X-F. Qian, **L. Qi**, F. Ji, D-N. Shi and J. Li, "Strain-Engineering of Band Gaps in Piezoelectric Boron Nitride Nanoribbons", *Nano Letters* **12** (2012) 1224-1228

12. Q. Yu*, **L. Qi***(*: equal contribution), K. Chen, R. Mishra, J. Li and A. Minor, "The Nanostructured Origin of Deformation Twinning", *Nano Letters* **12** (2012) 887-892.

11. C. He, **L. Qi**, W.X. Zhang and H. Pan, "Effect of electric and stress field on structures and quantum conduction of Cu nanowires", *Appl. Phys. Lett.* **99** (2011) 073105

10. J-Y. Huang, L. Zhong, C-M. Wang, J. P. Sullivan, W. Xu, L-Q. Zhang, S. X. Mao, N. S. Hudak, X-H. Liu, A. Subramanian, H-Y. Fan, **L. Qi**, A. Kushima, J. Li, "In situ observation of the electrochemical lithiation of a single SnO_2 nanowire electrode", *Science* **330** (2010) 1515-1520.

9. **L. Qi**, J-Y. Huang, J. Feng and J. Li, "In-situ observations of the nucleation and growth of atomically sharp graphene bilayer edges", *Carbon* **48** (2010) 2354-2360.

8. J-Y. Huang, **L. Qi** and J. Li, "In-situ imaging layer-by-layer sublimation of suspended graphene", *Nano Research* **3** (2010) 43.

7. J. Feng, **L. Qi**, J-Y. Huang and J. Li, "Geometric and Electronic Structures of Graphene Bilayer Edges", *Phys. Rev. B* **80** (2009) 165407.

6. J-Y. Huang, D. Feng, B. I. Yakobson, P. Lu, **L. Qi**, and J. Li, "In-situ observation of graphene sublimation and multi-layer edge reconstructions: genesis of interconnected carbon nanostructures", *Proc. Natl. Acad. Sci.* **106** (2009) 10103-10108.

5. X-F. Qian, J. Li, **L. Qi**, C-Z. Wang, T-L. Chan, Y-X. Yao, K-M. Ho and S. Yip, "Quasiatomic orbitals for *ab initio* tight-binding analysis", *Phys. Rev. B* **78** (2008) 245112.

4. **L. Qi**, X-F. Qian and J. Li, "Near-neutrality of oxygen molecule adsorbed on Pt(111) surface", *Phys. Rev. Lett.* **101** (2008) 146101.

3. **L. Qi**, J-G. Yu and J. Li, "Coverage dependence and hydroperoxyl-mediated pathway of catalytic water formation on Pt (111) surface", *J. Chem. Phys.* **125** (2006) 054701.

2. C-A. Wang, A-G. Zhou, **L. Qi**, Y. Huang, "Quantitative phase analysis in the Ti-Al-C ternary system by X-ray diffraction", *Powder Diffraction* **20** (2005) 218.

1. C-A. Wang, **L. Qi**, A-G. Zhou, Y. Huang, "Fabrication of Ti_3AlC_2 powder by pressureless synthesis method", *Rare Metal Materials and Engineering* **32** (2003) 607 Suppl. 1.