

## Ju Li

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- Experience**
- Massachusetts Institute of Technology* Cambridge, MA 02139  
Battelle Energy Alliance Professor of Nuclear Science and Engineering,  
Full Professor (7/2011-present), Department of Nuclear Science and Engineering  
and Department of Materials Science and Engineering
- University of Pennsylvania* Philadelphia, PA 19104  
Associate Professor (9/2007-6/2011),  
Department of Materials Science and Engineering
- Ohio State University* Columbus, OH 43210  
Assistant Professor (9/2002-9/2007),  
Department of Materials Science and Engineering
- Massachusetts Institute of Technology* Cambridge, MA 02139  
Research scientist (4/2002-9/2002), postdoctoral associate (9/2000-4/2002),  
Departments of Nuclear Engineering and Materials Science and Engineering
- Honda R&D Co., Ltd. Wako Research Center* Wako-shi, Saitama, Japan  
Visiting Scientist (1/13-2/14/2002)
- Ames Laboratory, USDOE* Ames, Iowa 50011  
Visiting Scientist  
(7/17-29/96, 6/11-7/3/97, 7/12-8/22/98, 12/19/00-1/19/01, 8/6-20/01, 12/17-24/02,  
10/11-19/03, 7/14-23/05)

- Education**
- Massachusetts Institute of Technology* Cambridge, MA 02139  
Department of Nuclear Engineering (1994-2000) Ph.D., Sept. 2000
- Cumulative GPA: 5.0/5.0 (618 graduate degree credits)  
40 graduate-level courses offered by 8 MIT departments.
- University of Science and Technology of China* Hefei, Anhui 230026, P.R.C.  
Special Class for Gifted Young (1990-1994) B.S. in Physics, 1994

- Honors & Awards**
- MIT *Committed to Caring* Award (2018)
- Fellow of the Materials Research Society (2017)
- 2016 R&D 100 Award, CATEGORY Mechanical/Materials, “Stress-Induced Fabrication of Functionally Designed Nanomaterials”, Hongyou Fan, Willie Luk,

Paul Clem, Tommy Ao, Jack Wise, Randy Hickman, Gordon Leifeste, Dawn Flicker, Sheng Liu, Igal Brener, Kaifu Bian, Leanne Alarid, Michael Sinclair, Hattie Schunk, Christina Ting, Wenbin Li, Ju Li, Zhongwu Wang, Binsong Li, Huimeng Wu.

Fellow of the American Physical Society (2014)

Thomson Reuters *Highly Cited Researchers* 2014, among 147 scientists worldwide in *Materials Science* category based on papers published between 2002-2012, and among “The World’s Most Influential Scientific Minds 2014”

Lee Hsun Young Scientist Lecture Series on Materials Science, Institute of Metal Research, Chinese Academy of Sciences (2011)

Chinese Ministry of Education and Li Ka Shing Foundation Chang Jiang Scholar Award (2009)

TMS Robert Lansing Hardy Award (2009), for “a young person in the broad fields of metallurgy and materials science for exceptional promise of a successful career”

*Technology Review* TR35 award, for 35 “world’s top innovators” under age 35 (2007)

National Academy of Engineering U.S. Frontiers of Engineering Symposium (Microsoft Research, Sept. 24-26, 2007), “that brings together 100 of the nation’s outstanding young engineers (ages 30-45)”, and German-American Frontiers of Engineering Symposium (Oak Ridge, April 22-25, 2010) co-sponsored by the Alexander von Humboldt Foundation.

Materials Research Society (MRS) 2006 Outstanding Young Investigator Award, “to recognize outstanding, interdisciplinary scientific work in materials research by a young scientist or engineer”

Ohio State University College of Engineering 2006 Lumley Research Award

Presidential Early Career Award for Scientists and Engineers (PECASE) 2005, “the highest honor bestowed by the United States Government on scientists and engineers beginning their independent careers”

Outstanding Paper Award in the Fifth International Conference on Advanced Materials 1999, sponsored by the International Union of Materials Research Societies (IUMRS). (10 out of ~ 2,000 papers)

Materials Research Society (MRS) Graduate Student Silver Medalist in 1998.

Sole recipient of the 1996-1997 MIT Nuclear Engineering Department Manson Benedict Fellowship.

Two Letters of Commendation (1996,1997) from MIT Nuclear Engineering Department for outstanding academic performance.

**Advisee Awards**

Best Overall Research Award and Best in Materials Science and Technology Award, Yang Yang, “The Necessity of Full-3D Monte Carlo Simulations for Ion Irradiation,” 2017 American Nuclear Society Student Conference, Pittsburgh, Pennsylvania, April 6-9, 2017.

2016 Del Favero Lecture for the best PhD thesis work in Department of Nuclear Science and Engineering, Mingda Li, “Radiation Explorer and Designer Radiation physics today for material sciences tomorrow,” January 28, 2016.

Best Poster Award, MRS Spring Meeting, April 6-10, 2015, San Francisco, California: Sangtae Kim, Mechanical Energy Harvesters with Extended Current Pulse Duration Based on Electrochemically Alloyed Electrodes.

Best Poster Award, Gordon Research Conferences on Physical Metallurgy, August 2-7, 2009, Proctor Academy, Andover, NH: Erik Bitzek, William T. Cox, Sanket Sarkar, Thomas J. Lenosky, Yunzhi Wang, Ju Li, “Atomic-Scale Modeling of Diffusion-Driven Microstructure Evolution”

**Continued Education**

MIT Professional Education short course *Machine Learning for Big Data and Text Processing*, MIT Campus, July 18-22, 2016.

MIT Professional Education short course *Additive Manufacturing: From 3D Printing To The Factory Floor*, MIT Campus, July 21-25, 2014, taught by Prof. Anastasios John Hart. Won the first place (based on audience vote) on class project “Deployable Fractals” with Dr. Jan Balewski.

MIT Professional Education short course PI.61s *Leadership Skills for Engineering and Science Faculty*, MIT Campus, June 10-11, 2013, taught by Prof. Charles E. Leiserson and Chuck McVinney.

**Teaching**

Instructor, MIT 3.33J/22.73J *Defects in Materials* (Fall Term, 2016)

Instructor, MIT 22.14 *Materials in Nuclear Engineering* (Spring Term, 2017,2018)

Instructor, MIT 22.02 *Introduction to Applied Nuclear Physics* (Spring Term, 2014)

Instructor, MIT 22.101 *Applied Nuclear Physics* (Fall Term, 2012)

Instructor, MIT 3.14/3.40/22.71J *Physical Metallurgy* (Fall Term, 2012,2013,2014)

Instructor, MIT 22.107 *Computational Nuclear Science and Engineering* (Spring Term, 2012,2013)

Instructor, Penn MSE440/540 *Phase Transformations* (Spring Term, 2008, 2009, 2010, 2011)

Instructor, OSU MSE730 *Thermodynamics of Materials* (Wi Qtr., 2004,2005,2006,2007); Penn MSE 530 *Thermodynamics of Materials* (Fall Term, 2008, 2009, 2010)

Instructor (with Suliman Dregia and Yunzhi Wang), OSU *MSE894 Theoretical Methods in Materials Science* (Au Qtr., 2006)

Instructor, OSU *MSE695.01 Senior Design Project I* (Au Qtr., 2003,2004,2005,2006)

Instructor, OSU *MSE533 Modeling of Materials Processing Methods* (Sp Qtr., 2003,2004,2005,2006)

Instructor, OSU *MSE564 Mechanical Behavior and Material Microstructure* (Wi Qtr., 2003)

Instructor, OSU *MSE795 Graduate Seminar and Colloquium* (Au Qtr., 2004)

Instructor, MIT *22.51 Interactions of Radiation with Matter* (Fall 2001)

Course webpage: <http://web.mit.edu/22.51/www/>

Co-instructor, MIT *22.53 Statistical Processes and Atomistic Simulations*

(Fall 2000) Course webpage: <http://web.mit.edu/22.53/www/>

Instructor, GEM<sup>4</sup> Summer School on Cell and Molecular Mechanics in BioMedicine, with a focus on infectious diseases, August 7-18, 2006, MIT, gave four lectures. with a focus on cancer, June 25 - July 6, 2007, National University of Singapore, gave three lectures.

## Advising

PhD adviser of Dr. Liang Qi (Penn MSE, August 2009), Dr. Amit Samanta (Penn MSE, August 2009), Wenbin Li (MIT DMSE), Mingda Li (MIT NSE), Sina Moeini Ardakani (MIT CEE), Yang Yang (MIT NSE), Sangtae Kim (MIT DMSE).

Master's degree adviser of Liang Qi (OSU MSE, March 2007), Amit Samanta (OSU MSE, June 2007), Liu Cao (OSU MSE, September 2007), Zheng Li (Penn MSE, 2008), Wei Liu (Penn MSE, August 2009), Wenbin Li (Penn MSE, May 2011), Cheng-Wei Avis Huang (Penn MSE, May 2011), Hsu-Chung Luker Ko (Penn MSE, May 2011).

Postdoctoral adviser of Dr. James Jianguo Yu (8/2003-10/2004), Dr. Thomas J. Lenosky (8/2006-8/2007), Dr. Erik Bitzek (8/2008-12/2009), Dr. Ji Feng (2/2009-1/2011), Dr. Liang Qi (9/2009-8/2012), Dr. Yu Chieh Lo (11/2009-), Dr. Akihiro Kushima (4/2010-), Dr. JunJie Niu (1/2011-), Dr. Xiaofeng Qian (7/2011-), Dr. Kejie Zhao (9/2012-), Dr. Xiaohui Ning (1/2013-3/2013).

Host of visiting scholars: Prof. Shigenobu Ogata (Osaka University), Dr. Futoshi Shimizu (Japan Atomic Energy Agency), Joshua Fujiwara (Honda), Mitsumoto Kawai (Honda), Prof. ZhengPing Fu (University of Science and Technology of China), Prof. Shotaro Hara (University of Tokyo), Prof. Erik Bitzek (Universitat Erlangen-Nurnberg), Yvonne Ritter (Technische Universitat Darmstadt), Prof. Yonggang Li (Institute of Solid State Physics, Chinese Academy of Sciences, 9/2012-), Prof. JianMing Jia (Huaiyin Normal University, 9/2012-), Prof. Hongyi Li (Beijing University of Technology, 2/2013-).

Host of visiting students: Hyoung Gyu Kim (Korea Advanced Institute of Science and Technology, 1-7/2005), JingShan Qi (Nanjing University of Aeronautics and Astronautics, 6/2009-9/2010), Yi-Gil Cho (Seoul National University, 7/2010-3/2011), Degang Xie (Xi'an Jiaotong University, 9/11-8/12), Akio Ishii (Osaka University, 1/2012-4/2012), Sangchul Yeo (KAIST, 7/2012-10/2012), Dmitry Vasilev (Skoltech, 9/2012-), Ira Zhelavskaya (Skoltech, 2/2013-).

**Presentations** Invited talk at Huazhong University of Science and Technology, Wuhan, China, June 13, 2018.

Invited talk at the 11th International Workshop on Materials Behavior at the Micro- and Nano-Scale, Xian, China, June 9, 2018.

Invited talk at Texas Materials Institute Seminar Series, The University of Texas at Austin, March 28, 2018.

Invited talk at GE Global Research, Niskayuna NY, Feb. 2, 2018.

Invited talk at 2017 MRS Fall Meeting, Boston, November 27, 2017.

Plenary talk, International Forum on Advanced Materials IFAM2017 (<http://ifamat.com>), Xian, China, November 11, 2017.

Invited talk, Institute of Solid State Physics, Chinese Academy of Science, Hefei, China, November 10, 2017.

Invited talk, International Workshop on Physics of Nanofriction and Tribology, International Center for Quantum Design of Functional Materials (ICQD) at University of Science and Technology of China (USTC), Hefei, China, November 8-10, 2017.

Invited talk, Summer school on new algorithms for exploring structure and dynamics of interfaces, The University of British Columbia, Vancouver, Canada, July 31-Aug 1, 2017.

Invited talk, "Interfaces in Environments," Gordon Research Conference on Physical Metallurgy, University of New England, Biddeford, Maine, July 23-28, 2017.

Plenary speaker, "Elastic Strain Engineering", Chinese Materials Conference (C-MRS) 2017, Yinchuan, Ningxia, July 9-12, 2017.

Invited talks, Ningbo Institute of Materials Technology & Engineering, May 27, 2017.

Invited Colloquium, Northwestern Polytechnical University, May 25, 2017.

Stanford Materials Science and Engineering Colloquium, April 21, 2017.

Two invited talks at 2017 MRS Spring Meeting, Phoenix, April 17-21, 2017.

Invited talk at Yale Energy Sciences Institute Symposium, April 10-11, 2017.

Invited talk at Spring ACS Meeting in San Francisco, April 2-6, 2017.

Invited talk at MIT-KAIST symposium on Future of Nuclear Technology, Dept. Nuclear and Quantum Engineering, KAIST, Daejeon, South Korea, March 30, 2017.

Invited talk at Center for Integrated Nanostructure Physics, Sungkyunkwan University, Suwon, South Korea, Jan. 25, 2017.

Invited talk at School of Energy and Chemical Engineering, UNIST, Ulsan, South Korea, Jan. 24, 2017.

Invited talk at 2016 MRS Fall Meeting, Boston, Dec.1, 2016.

Invited talk at General Atomics, San Diego, CA, Oct. 24, 2016.

Invited talk at International Conference on Advanced Lithium Batteries for Automobile Applications (ABAA9), Huzhou, Zhejiang, China, Oct. 19, 2016.

Invited talk at Department of Physics and Texas Center for Superconductivity, University of Houston, Sept. 13, 2016.

Invited talk at Battery Technology Department, Argonne National Laboratory, Aug. 11, 2016.

Invited talk at IBM T.J. Watson Research Center, Yorktown Heights, New York, June 28, 2016.

Invited talk at ExxonMobil Research & Engineering, Annandale, New Jersey, June 27, 2016.

Invited talk at Research, Innovation and Leadership at the Crossroads of Science, Engineering and Medicine, A Conference Honoring Subra Suresh on his sixtieth birthday, Madrid, Spain, June 15-17, 2016.

Invited talk at 9th International Workshop on Materials Behavior at the Micro-and Nano-Scale, Xi'an, China, June 1-3, 2016.

Invited talk at Symposium MD2: Tuning Properties by Elastic Strain Engineering From Modeling to Making and Measuring, 2016 MRS Spring Meeting & Exhibit, March 28-April 1, 2016 Phoenix, Arizona.

Invited talk at 2015 MRS Fall Meeting, Boston, December 1, 2015.

Invited talk at 26th Annual Harry C. Allen, Jr. Symposium, Gustav H. Carlson School of Chemistry, Clark University, October 31, 2015.

Invited talk, Transforming Energy Lectures, University of Maryland, Sept. 2, 2015.

Invited talk, 250th ACS National Meeting & Exposition, Boston, August 16-20, 2015.

Invited talk, 8th International Workshop on Materials Behavior at the Micro- and Nano-scale, Xi'an, China, June 1-3, 2015.

Invited talk, MIT MechE Micro-Nano Seminar, Mar. 11, 2015.

Invited talk, APS March Meeting, San Antonio, March 6, 2015.

Invited talk, School of Materials Science and Engineering, Shanghai Jiaotong University, Jan. 16, 2015.

Invited talk, School of Materials Science and Engineering, Tongji University, Shanghai, Jan. 14, 2015.

Invited talk, Shanghai Institute Of Applied Physics, Chinese Academy of Sciences, Jan. 6, 2015.

Invited talk at Microscience Microscopy Congress 2014 (MMC2014), Manchester, UK, June 30-July 3, 2014.

Invited talks at Korea Institute of Science and Technology (KIST) and Department of Materials Science and Engineering, Seoul National University, Seoul, Korea, June 27-28, 2014.

Keynote talk at the NanoNuclear Materials, Fuels, Applications symposium at Cleantech2014 and TechConnect World 2014, National Innovation Summit, Gaylord National Resort & Convention Center, June 16-19, 2014.

Colloquium and invited talks at Departamento de Fisica, Universidad de Chile, Santiago, Chile, June 2-6, 2014.

Two invited talks, 2014 MRS Spring Meeting, San Francisco, April 21-25, 2014.

Invited talk, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, Apr. 8, 2014.

Two invited talks, King Abdullah University of Science and Technology, Advanced Nanofabrication, Imaging and Characterization Core Lab, Thuwal, Saudi Arabia, March 23 and 24, 2014.

Invited talk, Center for Functional Nanomaterials at Brookhaven National Laboratory, Upton, January 28, 2014.

Invited talk, Idaho National Laboratory, Idaho Falls, August 22, 2013.

Invited talk, Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio, Jan. 22, 2013.

Invited talk, 2012 MRS Fall Meeting, Boston, November 27, 2012.

Plenary talk, “Diffusive Molecular Dynamics (DMD): Simulating Displacive-Diffusive Transformations without Tracking Billions of Hops,” Multiscale Materials Modeling (MMM) 2012 conference, October 15-19, Biopolis, Singapore.

Invited talk, Nanoscale Science and Engineering Seminar Series, University of California at Berkeley, April 13, 2012.

Invited talk, 2012 MRS Spring Meeting, San Francisco, April 9-13, 2012.

Keynote talk, TMS 2012 Annual Meeting & Exhibition, Orlando, March 11-15, 2012.

Invited talk, APS March Meeting, Boston, February 27-March 2, 2012.

Invited talk, Plasticity 2012, San Juan, Puerto Rico, January 3-8, 2012.

Joint MIT ANS Student Chapter / faculty seminar on “Nanoscale electrochemical tests: in situ TEM experiments and modeling”, November 21, 2011.

First Annual Richard K. Osborn Lecture, Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Stamps Auditorium, September 23, 2011.

Lee Hsun Young Scientist Lecture Series on Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China, July 18, 2011.

Keynote presentation, ASME McMat2011, symposium on Low Dimensional Carbon NanoMaterials: Properties and Applications, Chicago, May 31-June 2, 2011.

Invited talk, Electron Microscopy and Multiscale Modeling 2011, Granlibakken Conference Center and Lodge, May 22-27, 2011.

Invited talk, Pennergy Symposium “Materials Under Extremes,” April 9, 2011, Philadelphia.

Two invited talks, TMS 2011 Annual Meeting & Exhibition, San Diego, February 27 - March 3, 2011.

Invited talk, Harvard Applied Mechanics Colloquium, February 2, 2011.

Invited talk, MRS Fall Meeting, Boston, November 29 - December 3, 2010.

Microstructure Modelling symposium, MMM2010, the Fifth Conference on Multiscale Material Modelling, Freiburg, Germany, October 7, 2010.

Penn Department of Mechanical Engineering and Applied Mechanics Seminar Series, September 16, 2010.

Invited talk, Physics and Astronomy Colloquium Series at University of Southern California, August 30, 2010.



Invited talk, Department of Engineering Science and Mechanics, Pennsylvania State University, July 16, 2010.

Invited talk, 17th International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM 2010), Zurich, Switzerland, July 4 - 9, 2010.

Invited talk, Sixth International Conference on Materials Structure & Micromechanics of Fracture (MSMF6), Brno, Czech Republic, June 28 - 30, 2010.

Invited talk, Department Werkstoffwissenschaften, Lehrstuhl WWI: Allgemeine Werkstoffeigenschaften, Universitat Erlangen-Nurnberg, Germany, June 24, 2010.

Invited talk, International Workshop on Materials Behavior at Micro- and Nano-Scale, Xi'an, China, June 11, 2010.

Invited talk, International Conference on Mechanical Properties of Materials (ICMPM), Hangzhou, China, May 27, 2010.

Two invited talks, 2010 SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 23, 2010.

Invited talk, Materials Science and Engineering Seminar, University of Tennessee, Knoxville, April 26, 2010.

Invited talk, Materials Science and Engineering Seminar, Rensselaer Polytechnic Institute, Troy, April 7, 2010.

Invited talk, TMS 2010 Annual Meeting & Exhibition, Seattle, February 14-18, 2010.

Keynote talk (40 min), mini-symposium Finite Plasticity & Viscoplasticity of Conventional & Emerging Materials (In celebration of 65 Years of Akhtar Khan), Plasticity 2010, St. Kitts, West Indies, January 3-8, 2010.

Invited talk, MIT Center for Computational Engineering (CCE), December 2, 2009.

Invited talk, MRS Fall Meeting, symposium *Mechanical Behavior of Nanomaterials Experiments and Modeling*, Boston, November 30 - December 4, 2009.

Invited talk, Civil Infrastructure Seminar, School of Civil and Environmental Engineering, Cornell University, November 10, 2009.

Invited talk, Mechanical & Aerospace Engineering Seminar, The University of Texas at Arlington, September 4, 2009.

Invited talk, Department of Mechanical Engineering Seminar, University Of Houston, September 3, 2009.

Invited talk, *Workshop on Probing the Limits of Strength*, Lawrence Berkeley National Laboratory, Berkeley, California, August 11-12, 2009.

Invited talk, “In-situ Observation of Graphene Sublimation and Edge Reconstructions,” mini-symposium *Graphene growth and properties through experiments and simulations*, tenth U.S. National Congress on Computational Mechanics (US-NCCM X), Columbus, July 16-19, 2009.

Invited talk, School of Materials Science and Engineering, Shanghai Jiao Tong University, June 10, 2009.

Invited talk, International Workshop on Size Effect on Materials Mechanical Behavior, Beijing, May 24 - 26, 2009.

Invited talk, “The Coming of Age of Ultra-Strength Materials,” Center for Integrated Nanotechnologies (CINT), Sandia National Laboratories, Albuquerque, New Mexico, May 7, 2009.

Invited talk, Othmer-Jacobs Department of Chemical and Biological Engineering, Polytechnic Institute of NYU, Brooklyn, New York, May 4, 2009.

Invited talk, MRS Spring Meeting, symposium *Probing Mechanics at Nanoscale Dimensions*, San Francisco, April 13-17, 2009.

Invited talk, Shanghai Institute of Ceramics, March 10, 2009.

Invited talk, TMS 2009 Annual Meeting & Exhibition, San Francisco, February 15-19, 2009.

Keynote talk (40 min), “Tensile Ductility of Nanostructured Metals,” Plasticity 2009, St. Thomas, U.S. Virgin Islands, January 3-8, 2009.

Invited talk, Workshop on Mechanical Behaviors of Micro/Nano Materials, XiAn Jiao Tong University, December 30-31, 2008.

Two invited talks, National Sun Yat-sen University, Kaohsiung, Taiwan, December 13-21, 2008.

Invited talk, Georgia Institute of Technology Woodruff School of Mechanical Engineering Seminar, Oct. 23, 2008.

Invited talk, Dislocations 2008, Hong Kong, Oct. 13-17, 2008.

Invited talk, Brown University Joint Materials/Solid Mechanics Seminar, September 12, 2008.

Invited talk, “Plasticity in amorphous and nanocrystalline metals,” Gordon Research Conference on Thin Film & Small Scale Mechanical Behavior, Colby College, Maine, July 27 - August 1, 2008.

Two invited lectures, Workshop on Multi-Scale Modeling of Moving Interfaces in Materials, Katholieke Universiteit Leuven, Belgium, July 2-4, 2008.

Invited talk, 2nd International Conference on Heterogeneous Materials Mechanics (ICHMM-2008), HuangShan, China, June 3-8, 2008.

Invited talk, International Workshop on *in situ* Electron Microscopy in Advanced Materials Research, Beijing, May 31 - June 2, 2008.

Invited talk, NIST 2008 Diffusion Workshop, Gaithersburg, Maryland, May 12-13, 2008.

Invited talk, TMS 2008 Annual Meeting & Exhibition, New Orleans, March 9-13, 2008.

Invited talk, International Workshop on Small Scale Plasticity, Braunwald, Switzerland, September 5-8, 2007.

Keynote talk (45 min), "Cytoskeletal Dynamics Simulations of Red Blood Cell," ninth U.S. National Congress on Computational Mechanics (USNCCM IX), San Francisco, July 22-26, 2007.

Invited seminar at Department of Aerospace and Mechanical Engineering, University of Notre Dame, March 20, 2007.

Los Alamos National Lab Physics & Theoretical Colloquium, March 15, 2007, 2007.

Invited talk, "Shear localization lengthscale in metallic glasses," Center for Advanced Metallic and Ceramic Systems (CAMCS) Seminar, Johns Hopkins University, Baltimore, Maryland, January 3, 2007.

Invited talk, "[Yield Point of Metallic Glass](#)," Pacific Northwest National Laboratory, Richland, WA, September 15, 2006.

Invited talk, "Atomistic Modeling of Rate Dependence of Deformation and Fracture," 232nd ACS National Meeting, San Francisco, September 10-14, 2006.

MRS OYI presentation, "The Mechanics and Physics of Defect Nucleation," San Francisco, April 19, 2006.

Invited talk, "[A minimal mesoscopic model of the self-assembly and micro-rheology of red blood cell cytoskeleton](#)," *First International Conference on Mechanics of Biomaterials & Tissues*, Waikoloa, Hawaii, December 11-15, 2005.

Invited talk, "Modified Frenkel model and ductility of solids," *International Workshop on Nanomechanics*, Asilomar conference grounds, Pacific Grove, California, July 14-17, 2004.

Invited talk, "How bonds break in shear and why it matters," Case Western Reserve University Materials Science and Engineering Departmental Colloquium, September 16, 2003.

Invited talk, AFOSR *Materials Engineering in Affordable New Systems (MEANS)* workshop, Boulder, Colorado, August 6-8, 2003.

Invited talk, “Coupling coarse variables to microscopic simulations,” *Workshop on Algorithm Refinement*, Los Alamos National Laboratory, April 22-24, 2002.

Invited talk, “Consequences of energy locality on atomistic calculations of defect mobility,” *Computational Materials Science Network Workshop on Microstructural Effects on the Mechanics of Materials*, Lawrence Berkeley National Laboratory, June 18-20, 2001.

Conference Fellowship, “Optimal particle controller for coupled continuum/MD fluid simulation,” *First MIT Conference on Computational Fluid and Solid Mechanics*, MIT, June 12-15, 2001.

Invited talk, “Nearly exact solution for coupled continuum/MD fluid simulation,” *NIST Workshop on Hybrid Computational Methods for Multiscale Modeling of Materials*, in Gaithersburg, Maryland, May 12-14, 1999.

## **Service**

Co-director (with Bilge Yildiz), MIT Energy Initiative (MITEI) Low-Carbon Energy Center for Materials in Energy and Extreme Environments (CME), 2016-present.

Member of Editorial Board of *Nano Research* (Mar. 2008-), *Modelling and Simulation in Materials Science and Engineering* (Feb. 2008-), *Science China: Technological Sciences* (Jan. 2013-), *Extreme Mechanics Letters* (Aug. 2014-).

Lead Organizer of 2013 MRS Fall Meeting Symposium YY “Elastic Strain Engineering for Unprecedented Materials Properties” (with Zhiwei Shan, Evan Ma and Oden L. Warren), Dec. 1-5, 2013, Boston.

Lead Guest Editor of *MRS Bulletin* February 2014 special issue on Elastic Strain Engineering (ESE)

Organizer of MRS Webinar on Elastic Strain Engineering on May 6, 2014.

3-Member Executive Board (Oct. 2010-present) and International Advisory Board (Aug. 2009-present) of Multiscale Materials Modeling (MMM) conference series.

MIT NSE Graduate Committee (1/2012-)

Faculty Advisor to Chinese Students and Scholars Association at Penn (CSSAP, 1/2009-6/2011)

Penn MSE Graduate Group Chair (7/1/2009-6/30/2011)

Penn MSE Colloquium Organizer (9/2008-6/2009)

Penn MSE Faculty Search Committee (9/2008-6/2009)

OSU MSE Faculty Meeting Secretary (9/2002-8/2005)

OSU MSE Library and Computing Committee (9/2004-8/2006, 4/2007-9/2007)

OSU MSE Graduate Studies Committee (1/2005-8/2006)

OSU MSE Faculty Search Committee (2/2006-1/2007)

OSU MSE Undergraduate Studies Committee (9/2006-9/2007)

OSE MSE Student Relations Committee (9/2006-4/2007)

OSE MSE Ad Hoc Committee on Undergraduate Curriculum Adjustments (9/2006-2/2007)

Ph.D. candidacy exam committee of: Eunha Lee (OSU MSE 2002), Sudhakar Mahajanam (OSU MSE 2003), James M. Nash (OSU MSE 2004), Mala Seth (OSU MSE 2004), Matthew C. Brandes (OSU MSE 2005), Jonathan P. Blank (OSU MSE 2005), Barbara N. Padgett (OSU MSE 2005), Liang Qi (OSU MSE 2005), Amy M. Hayes (Chemistry 2005), Michael Rauscher (OSU MSE 2005), Lanlin Zhang (OSU MSE 2006), Amit Samanta (OSU MSE 2006), Sungwoo Ahn (OSU Mathematics 2007), Weiqi Luo (OSU MSE 2007); Jae Hong Choi (Penn MSE, 2008)

Ph.D. thesis committee of: Yao Shen (OSU MSE 2004), Tao Liang (OSU MSE 2005), Shanhu Li (OSU MechE 2005), Libor Kovarik (OSU MSE 2006), Carmen M. Carney (OSU MSE 2006); XueLian Zhu (Penn MSE, 2010), Ivan Sergeyevich Baldychev (Penn CBE, 2011), Tingting Qi (Penn Chemistry, 2011), Miguel Angel Mendez Polanco (Penn Chemistry), Kevin Bakhtmutsky (Penn CBE), John Mark Martirez (Penn Chemistry), Tevis Jacobs (Penn MEAM), Vicky Doan-Nguyen (Penn MSE), Matthew A. Caporizzo (Penn MSE), Rubal Dua (Penn CBE), Xiangan Dang (MIT MSE, 2013)

Senior project advisor of: Jaumale L. Daniels (OSU MSE 2005), Danelle Violet (OSU MSE 2006), Joseph Lydon and Arthur Spector, "Building efficiency modeling and materials selection" (Penn MSE 2010).

Undergraduate Research Opportunities (REU) Program advisor of: Miten Mistry (Penn MSE, Jan 2009 - ), Jonathan Rosen (Penn Nano-Bio Interface Center, June 2009 - )

American Chemical Society Project SEED High School Summer Research Experience: Manohjah Blackmanhe

Lead organizer of AFOSR [Workshop on Modeling Materials in Extreme Environment](#), Sept. 24-25, 2005, Washington D.C.

Panel member, [Basic Research Needs for Advanced Nuclear Energy Systems](#) (panel 6: Predictive Modeling and Simulation), July 31 - August 2, 2006, Wash-

ington, D.C., sponsored by the Office of Basic Energy Sciences, Department of Energy.

Panel member, [Advanced High-Strength Steels: Fundamental Research Issues](#) (panel A: Models versus Experiments), October 22-23, 2006, Washington, D.C., sponsored by the National Science Foundation, Department of Energy, and the Auto/Steel Partnership.

Member of DOE-BES Site Review Committee of the BES/Division of Materials Science & Engineering core program at Sandia National Laboratories, Albuquerque, March 22-25, 2010.

Member of Scientific Committee, Third International Conference of Heterogeneous Materials Mechanics (ICHMM 2011), ChongMing Island, China, May 22-26, 2011.

Co-organizer (with Zhiwei Shan, Xiaodong Li and Jun Sun), 4th International Workshop on Materials Behavior at Micro- and Nano-Scale, Xi'an, China, May 19-21, 2011.

Co-organizer (with Erik van der Giessen and Marc G.D. Geers) of symposium "Micromechanics" in MMM2010, the Fifth Conference on Multiscale Material Modelling, Freiburg, Germany, October 4-8, 2010.

Co-organizer (with Sulin Zhang, Gang Bao, Huajian Gao, K. Jimmy Hsia) of symposium "Molecular and Cellular Biomechanics: Adhesion, Cell-ECM Interaction, and Mechanotransduction," 16th US National Congress of Theoretical and Applied Mechanics (USNCTAM), Pennsylvania State University, State College, PA 16801, June 27 - July 2, 2010.

Co-organizer (with Zhiwei Shan, Jun Sun and Evan Ma), International Workshop on Materials Behavior at Micro- and Nano-Scale, Xi'an, China, June 8-11, 2010.

Co-organizer (with Zhiwei Shan, Xiaofeng Zhang, Oden L. Warren, Ming Pan, Shuo Chen, Kai Chen and Jun Sun), Workshop on In Situ Electron Microscopy in Advanced Materials Research, Xi'an, China, June 12-15, 2012.

Co-organizer (with Peter M. Derlet, Mike D. Uchic, Daniel Weygand, Eric Le Bourhis) of Symposium "GG: Plasticity in Confined Volumes - Modeling and Experiments", MRS Fall Meeting, Boston, November 30 - December 4, 2009.

Organizer (with Wei Cai, Ting Zhu, Diana Farkas, Jacob Eapen, Krystyn J. Van Vliet) of symposium "1.1 Multiphysics Materials Modeling from Atoms to Continuum: A Symposium in Honor of Professor Sidney Yip", tenth U.S. National Congress on Computational Mechanics (USNCCM X), July 16-19, 2009.

Local Organizing Committee, tenth U.S. National Congress on Computational Mechanics (USNCCM X), Columbus, Ohio, July 16-19, 2009.

Co-organizer (with George Lykotrafitis, Sulin Zhang, Greg Huber and Ming Dao) of symposium “Mechanics of Biomembranes”, 2009 Joint ASCE-ASME-SES Conference on Mechanics and Materials, Blacksburg, VA, June 24-27, 2009.

Co-organizer (with Shaofan Li and Sukky Jun) of symposium “Recent Developments in Nanoscale Simulations: From Quantum to Coarse-Grained Modeling”, ninth U.S. National Congress on Computational Mechanics (USNCCM IX), San Francisco, July 22-26, 2007.

Co-editor of *Mechanical Behavior at Small Scales - Experiments and Modeling*, Materials Research Society Symposium Proceedings volume 1224, eds. Jun Lou, Erica Lilleodden, Brad Boyce, Lei Lu, Peter M. Derlet, Daniel Weygand, Ju Li, Michael Uchic, and Eric Le Bourhis (Materials Research Society, Warrendale, Pennsylvania, 2010). Symposia FF/GG held on November 30 - December 3, 2009, Boston, USA. ISBN 978-1-60511-197-1.

**Miscellaneous** Listed in *Nanobiomechanics*, one of 10 Emerging Technologies in 2006 according to *Technology Review*.

Author of free molecular visualization software *AtomEye*:  
<http://www.google.com/search?q=AtomEye>

Ab initio tight-binding analysis with quasiatomatic orbitals (with Xiaofeng Qian):  
<http://li.mit.edu/Archive/QO/>

## Issued Patents

4. May 29, 2018: US Patent 9985327, “Air secondary battery,” Tetsuya Koido, Akihiro Kushima, Yoshiya Fujiwara, Ju Li.
3. April 24, 2018: US Patent 9954262, “Air secondary battery including cathode having trap portion,” Tetsuya Koido, Akihiro Kushima, Yoshiya Fujiwara, Ju Li.
2. Mar 14, 2017: US Patent 9595624 “Strain-engineered bandgaps,” Ju Li, Xiaofeng Qian, Ji Feng.
1. Nov.1, 2016: US Patent 9484489 “Engineered band gaps”, Ju Li, Xiaofeng Qian, Menghao Wu.

## Peer-Reviewed Papers<sup>1</sup>

<sup>1</sup> ResearcherID: A-2993-2008    ISI Web of Knowledge search keywords: “Li J” in Author and “nucl same engn same 02139 or mat same 43210 or mat same Univ Penn or 2041 same Columbus” in Address.  
Google Scholar: <http://scholar.google.com/citations?user=SHVhdhoAAAAJ>

321. J. Patra, H-T. Huang, W-J. Xue, C. Wang, A.S. Helal, J. Li and J-K. Chang, “Moderately concentrated electrolyte improves solid-electrolyte interphase and sodium storage performance of hard carbon,” *Energy Storage Materials* **16** (2019) 146-154.
320. L. Li, Y-L. Xu, X-F. Sun, R. Chang, Y. Zhang, X-N. Zhang and J. Li, “Fluorophosphates from Solid-State Synthesis and Electrochemical Ion Exchange: NaVPO<sub>4</sub>F or Na<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>F<sub>3</sub>?” *Advanced Energy Materials* (2018) 1801064.
319. D-T. Wang, K. Wang, L. Sun, H-C. Wu, J. Wang, Y-X. Zhao, L-J. Yan, Y-F. Luo, K-L. Jiang, Q-Q. Li, S-S. Fan, J. Li and J-P. Wang, “MnO<sub>2</sub> nanoparticles anchored on carbon nanotubes with hybrid supercapacitor-battery behavior for ultrafast lithium storage,” *Carbon* **139** (2018) 145-155.
318. X-F. Luo, A.S. Helal, C-T. Hsieh, J. Li and J-K. Chang, “Three-dimensional carbon framework anode improves sodiation/desodiation properties in ionic liquid electrolyte,” *Nano Energy* **49** (2018) 515-522.
317. B-Y. Liu, N. Yang, J. Wang, M. Barnett, Y-C. Xin, D. Wu, R-L. Xin, B. Li, R.L. Narayan, J-F. Nie, J. Li, E. Ma and Z-W. Shan, “Insight from in situ microscopy into which precipitate morphology can enable high strength in magnesium alloys,” *Journal of Materials Science & Technology* **34** (2018) 1061-1066.
316. Z-Q. Liu, N. Li, C. Su, H-Y. Zhao, L-L. Xu, Z-Y. Yin, J. Li and Y-P. Du, “Colloidal synthesis of 1T' phase dominated WS<sub>2</sub> towards enduring electrocatalysis,” *Nano Energy* **50** (2018) 176-181.
315. S. Li, M-W. Jiang, Y. Xie, H. Xu, J-Y. Jia and J. Li, “Developing High-Performance Lithium Metal Anode in Liquid Electrolytes: Challenges and Progress,” *Advanced Materials* **30** (2018) 1706375.
314. Y. Yang, A. Kushima, W-Z. Han, H-L. Xin and J. Li, “Liquid-Like, Self-Healing Aluminum Oxide during Deformation at Room Temperature,” *Nano Letters* **18** (2018) 2492-2497.
313. D. Feng, Y-X. Chen, L-W. Fu, J. Li and J-Q. He, “SnSe + Ag<sub>2</sub>Se composite engineering with ball milling for enhanced thermoelectric performance,” *Rare Metals* **37** (2018) 333342.
312. Y-G. Yao, Z-N. Huang, P-F. Xie, S.D. Lacey, R.J. Jacob, H. Xie, F-J. Chen, A-M. Nie, T-C. Pu, M. Rehwoldt, D-W. Yu, M.R. Zachariah, C. Wang, R. Shahbazian-Yassar, J. Li and L-B. Hu, “Carbothermal shock synthesis of high-entropy-alloy nanoparticles,” *Science* **359** (2018) 1489-1494.
311. \* K.P. So, A. Kushima, J.G. Park, X-H. Liu, D.H. Keum, H.Y. Jeong, F. Yao, S.H. Joo, H.S. Kim, H. Kim, J. Li and Y.H. Lee, “Intragranular Dispersion of Carbon Nanotubes Comprehensively Improves Aluminum Alloys,” *Advanced Science* (2018) 1800115.
310. H-Z. Wang, W.S. Leong, F-T. Hu, L-L. Ju, C. Su, Y-K. Guo, J. Li, M. Li, A-M. Hu and J. Kong, “Low-Temperature Copper Bonding Strategy with Graphene Interlayer,” *ACS Nano* **12** (2018) 2395-2402.



309. T. Dai, Y. Zhao, X-H. Ning, R.L. Narayan, J. Li and Z-W. Shan, "Capacity extended bismuth-antimony cathode for high-performance liquid metal battery," *J. Power Sources* **381** (2018) 38-45.
308. \* W. Gong, B. Fugetsu, Z-P. Wang, I. Sakata, L. Su, X-J. Zhang, H. Ogata, M-D. Li, C. Wang, J. Li, J. Ortiz-Medina, M. Terrones and M. Endo, "Carbon nanotubes and manganese oxide hybrid nanostructures as high performance fiber supercapacitors," *Communications Chemistry* **1** (2018) 16.
307. Q-J. Li, B. Xu, S. Hara, J. Li and E. Ma, "Sample-size-dependent surface dislocation nucleation in nanoscale crystals," *Acta Materialia* **145** (2018) 19-29.
306. L-M. Suo, W-J. Xue, M. Gobet, S.G. Greenbaum, C. Wang, Y-M. Chen, W-L. Yang, Y-X. Li and J. Li, "Fluorine-donating electrolytes enable highly reversible 5V-class Li metal batteries," *PNAS* **115** (2018) 1156-1161.
305. Y. Yang, Y.G. Li, M.P. Short, C-S. Kim, K.K. Berggren and J. Li, "Nano-beam and nano-target effects in ion radiation," *Nanoscale* **10** (2018) 1598-1606.
304. C-H. Yang, Q.D. Nguyen, T-H. Chen, A.S. Helal, J. Li and J-K. Chang, "Functional Group-Dependent Supercapacitive and Aging Properties of Activated Carbon Electrodes in Organic Electrolyte," *ACS Sustainable Chemistry & Engineering* **6** (2018) 1208-1214.
303. \* W-J. Xue, L-X. Miao, L. Qie, C. Wang, S. Li, J-L. Wang and J. Li, "Gravimetric and volumetric energy densities of lithium-sulfur batteries," *Current Opinion in Electrochemistry* **6** (2017) 92-99.
302. L-M. Suo, D. Oh, Y-X. Lin, Z-Q. Zhuo, O. Borodin, T. Gao, F. Wang, A. Kushima, Z-Q. Wang, H-C. Kim, Y. Qi, W-L. Yang, F. Pan, J. Li, K. Xu and C-S. Wang, "How Solid-Electrolyte Interphase Forms in Aqueous Electrolytes," *J. Am. Chem. Soc.* **10** (2017) 18670-18680.
301. G-Y. Xu, A. Kushima, J-R. Yuan, H. Dou, W-J. Xue, X-G. Zhang, X-H. Yan and J. Li, "Ad hoc Solid Electrolyte on Acidized Carbon Nanotube Paper Improves Cycle Life of Lithium-Sulfur Batteries," *Energy & Environmental Science* **10** (2017) 2544-2551.
300. H-Y. Zhao, J-W. Wang, Y-H. Zheng, J. Li, X-G. Han, G. He and Y-P. Du, "Organic Thiocarboxylate Electrodes for a Room-Temperature Sodium-Ion Battery Delivering an Ultrahigh Capacity," *Angew. Chem. Int. Ed.* **56** (2017) 15334-15338.
299. E.D. Cubuk, R.J.S. Ivancic, S.S. Schoenholz, D.J. Strickland, A. Basu, Z.S. Davidson, J. Fontaine, J.L. Hor, Y.-R. Huang, Y. Jiang, N.C. Keim, K.D. Koshigan, J.A. Lefever, T. Liu, X.-G. Ma, D.J. Magagnosc, E. Morrow, C.P. Ortiz, J.M. Rieser, A. Shavit, T. Still, Y. Xu, Y. Zhang, K.N. Nordstrom, P.E. Arratia, R.W. Carpick, D.J. Durian, Z. Fakhraai, D.J. Jerolmack, D. Lee, J. Li, R. Riggelman, K.T. Turner, A.G. Yodh, D.S. Gianola and A.J. Liu, "Structure-property relationships from universal signatures of plasticity in disordered solids," *Science* **358** (2017) 1033-1037.

298. D. Feng, Z-H. Ge, Y-X. Chen, J. Li and J-Q. He, "Hydrothermal synthesis of SnQ (Q=Te, Se, S) and their thermoelectric properties," *Nanotechnology* **28** (2017) 455707.
297. Z-J. Wang, Q-J. Li, Y. Li, L-C. Huang, L. Lu, M. Dao, J. Li, E. Ma, S. Suresh and Z-W. Shan, "Sliding of coherent twin boundaries," *Nature Communications* **8** (2017) 1108.
296. S-T. Wang, W. Quan, Z. Zhu, Y. Yang, Q. Liu, Y. Ren, X-Y. Zhang, R. Xu, Y. Hong, Z-T. Zhang, K. Amine, Z-L. Tang, J. Lu and J. Li, "Lithium titanate hydrates with superfast and stable cycling in lithium ion batteries," *Nature Communications* **8** (2017) 627.
295. J-H. Dou, L. Sun, Y-c. Ge, W-b. Li, C.H. Hendon, J. Li, S. Gul, J. Yano, E.A. Stach and M. Dinca, "Signature of Metallic Behavior in the Metal-Organic Frameworks M<sub>3</sub>(hexaiminobenzene)<sub>2</sub> (M=Ni,Cu)," *J. Am. Chem. Soc.* **139** (2017) 13608-13611.
294. Y-M. Chen, X-Y. Li, K-S. Park, W. Lu, C. Wang, W-J. Xue, F. Yang, J. Zhou, L-M. Suo, T-Q. Lin, H-T. Huang, J. Li and J.B. Goodenough, "Nitrogen-Doped Carbon for Sodium-Ion Battery Anode by Self-Etching and Graphitization of Bimetallic MOF-Based Composite," *Chem* **3** (2017) 152-163.
293. S-L. Zhang, K-J. Zhao, T. Zhu and J. Li, "Electrochemomechanical degradation of high-capacity battery electrode materials," *Progress in Materials Science* **89** (2017) 479-521.
292. Y-H. Zheng, Y-S. Wang, Y-X. Lu, Y-S. Hu and J. Li, "A high-performance sodium-ion battery enhanced by macadamia shell derived hard carbon anode," *Nano Energy* **39** (2017) 489-498.
291. G-Y. Xu, Q-B. Yan, S-T. Wang, A. Kushima, P. Bai, K. Liu, X-G. Zhang, Z-L. Tang and J. Li, "A thin multifunctional coating on a separator improves the cyclability and safety of lithium sulfur batteries," *Chemical Science* **8** (2017) 6619-6625.
290. W-J. Xue, Q-B. Yan, G-Y. Xu, L-M. Suo, Y-M. Chen, C. Wang, C-A. Wang and J. Li, "Double-oxide sulfur host for advanced lithium-sulfur batteries," *Nano Energy* **38** (2017) 12-18.
289. M-J. Lee, E-S. Lho, P. Bai, S-J. Chae, J. Li and J-P. Cho, "Low-Temperature Carbon Coating of Nanosized Li<sub>1.015</sub>Al<sub>0.06</sub>Mn<sub>1.925</sub>O<sub>4</sub> and High-Density Electrode for High-Power Li-Ion Batteries," *Nano Letters* **17** (2017) 3744-3751.
288. W-Z. Han, J. Zhang, M-S. Ding, L. Lv, W-H. Wang, G-H. Wu, Z-W. Shan and J. Li, "Helium Nanobubbles Enhance Superelasticity and Retard Shear Localization in Small-Volume Shape Memory Alloy," *Nano Letters* **17** (2017) 3725-3730.
287. B.Y. Guan, A. Kushima, L. Yu, S. Li, J. Li and X.W. Lou, "Coordination Polymers Derived General Synthesis of Multishelled Mixed Metal-Oxide Particles for Hybrid Supercapacitors," *Advanced Materials* **29** (2017) 1605902.
286. P-Y. Zhao, J. Li, J-W. Hwang and Y-Z. Wang, "Influence of nanoscale structural heterogeneity on shear banding in metallic glasses," *Acta Materialia* **134** (2017) 104-115.

285. P.Y. Zhao, C. Shen, J. Li and Y.Z. Wang, "Effect of nonlinear and noncollinear transformation strain pathways in phase-field modeling of nucleation and growth during martensite transformation," *npj Computational Materials* **3** (2017) 19.
284. T. Yang, Y. Gao, D. Wang, R.P. Shi, Z. Chen, J.F. Nie, J. Li and Y. Wang, "Non-conservative dynamics of lattice sites near a migrating interface in a diffusional phase transformation," *Acta Materialia* **127** (2017) 481-490.
283. Y-H. Dong, L. Qi, J. Li and I-W. Chen, "A computational study of yttria-stabilized zirconia: II. Cation diffusion," *Acta Materialia* **126** (2017) 438-450.
282. Y-H. Dong, L. Qi, J. Li and 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* **127** (2017) 73-84.
281. S-H. Li, W-Z. Han, J. Li, E. Ma and Z-W. Shan, "Small-volume aluminum alloys with native oxide shell deliver unprecedented strength and toughness," *Acta Materialia* **126** (2017) 202-209.
280. W-B. Li, L. Sun, J-S. Qi, P. Jarillo-Herrero, M. Dinca and J. Li, "High temperature ferromagnetism in pi-conjugated two-dimensional metalorganic frameworks," *Chemical Science* **8** (2017) 2859-2867.
279. K. Liu, P. Bai, M.Z. Bazant, C-A. Wang and J. Li, "A soft non-porous separator and its effectiveness in stabilizing Li metal anodes cycling at 10 mA cm<sup>-2</sup> observed in situ in a capillary cell," *Journal of Materials Chemistry A* **5** (2017) 4300-4307.
278. M. Li, D-G. Xie, E. Ma, J. Li, X-X. Zhang and Z-W. Shan, "Effect of hydrogen on the integrity of aluminium-oxide interface at elevated temperatures," *Nature Communications* **8** (2017) 14564.
277. Y. Jin, S. Li, A. Kushima, X-Q. Zheng, Y-M. Sun, J. Xie, J. Sun, W-J. Xue, G-M. Zhou, J. Wu, F-F. Shi, R-F. Zhang, Z. Zhu, K-P. So, Y. Cui and J. Li, "Self-healing SEI enables full-cell cycling of a silicon-majority anode with a coulombic efficiency exceeding 99.9%," *Energy & Environmental Science* **10** (2017) 580-592.
276. A. Kushima, K.P. So, C. Su, P. Bai, N. Kuriyama, T. Maebashi, Y. Fujiwara, M.Z. Bazant and J. Li, "Liquid cell transmission electron microscopy observation of lithium metal growth and dissolution: Root growth, dead lithium and lithium flotsams," *Nano Energy* **32** (2017) 271-279.
275. S-T. Wang, Y. Yang, W. Quan, Y. Hong, Z-T. Zhang, Z-L. Tang and J. Li, "Ti<sup>3+</sup>-free three-phase Li<sub>4</sub>Ti<sub>5</sub>O<sub>12</sub>/TiO<sub>2</sub> for high-rate lithium ion batteries: Capacity and conductivity enhancement by phase boundaries," *Nano Energy* **32** (2017) 294-301.
274. G-Y. Xu, Q-B. Yan, A. Kushima, X-G. Zhang, J. Pan and J. Li, "Conductive graphene oxide-polyacrylic acid (GOPAA) binder for lithium-sulfur battery," *Nano Energy* **31** (2017) 568-574.

273. N. Xu, W-Z. Han, Y-C. Wang, J. Li and Z-W. Shan, "Nanoscratching of copper surface by CeO<sub>2</sub>," *Acta Materialia* **124** (2017) 343-350.
272. Y.G. Li, Y. Yang, M.P. Short, Z.J. Ding, Z. Zeng and J. Li, "Ion radiation albedo effect: influence of surface roughness on ion implantation and sputtering of materials," *Nuclear Fusion* **57** (2017) 016038.
271. M-H. Wu, Z-J. Wang, J-W. Liu, W-B. Li, H-H. Fu, L. Sun, X. Liu, M-H. Pan, H-M. Weng, M. Dinca, L. Fu and J. Li, "Conetronics in 2D metal-organic frameworks: double/half Dirac cones and quantum anomalous Hall effect," *2D Materials* **4** (2017) 015015.
270. S-Z. Li, Q-Y. Li, R.W. Carpick, P. Gumbsch, X.Z. Liu, X-D. Ding, J. Sun and J. Li, "The evolving quality of frictional contact with graphene," *Nature* **539** (2016) 541-545.
269. D. Feng, Z-H. Ge, D. Wu, Y-X. Chen, T-T. Wu, J. Li and J-Q. He, "Enhanced thermoelectric properties of SnSe polycrystals via texture control," *Phys. Chem. Chem. Phys.* **18** (2016) 31821-31827.
268. L. Yang, T. Dai, Y-C. Wang, D-G. Xie, R.L. Narayan, J. Li and X-H. Ning, "Chestnut-like SnO<sub>2</sub>/C nanocomposites with enhanced lithium ion storage properties," *Nano Energy* **30** (2016) 885-891.
267. M-S. Ding, L. Tian, W-Z. Han, J. Li, E. Ma and Z-W. Shan, "Nanobubble fragmentation and bubble-free-channel shear localization in helium-irradiated submicron-sized copper," *Phys. Rev. Lett.* **117** (2016) 215501.
266. D-G. Xie, S-Z. Li, M. Li, Z-J. Wang, P. Gumbsch, J. Sun, E. Ma, J. Li and Z-W. Shan, "Hydrogenated vacancies lock dislocations in aluminium," *Nature Communications* **7** (2016) 13341.
265. P. Bai, J. Li, F.R. Brushett and M.Z. Bazant, "Transition of lithium growth mechanisms in liquid electrolytes," *Energy & Environmental Science* **9** (2016) 3221-3229.
264. X-L. Ding, X-X. Liu, Y-Y. Huang, X-F. Zhang, Q-J. Zhao, X-H. Xiang, G-L. Li, P-F. He, Z-Y. Wen, J. Li and Y-H. Huang, "Enhanced electrochemical performance promoted by monolayer graphene and void space in silicon composite anode materials," *Nano Energy* **27** (2016) 647-657.
263. K.P. So, X-H. Liu, H. Mori, A. Kushima, J.G. Park, H.S. Kim, S. Ogata, Y.H. Lee and J. Li, "Ton-scale metal-carbon nanotube composite: The mechanism of strengthening while retaining tensile ductility," *Extreme Mechanics Letters* **8** (2016) 245-250.
262. X-H. Liu, J-F. Gu, Y. Shen and J. Li, "Crystal metamorphosis at stress extremes: how soft phonons turn into lattice defects," *NPG Asia Materials* **8** (2016) e320.
261. J-Y. Zhang, Y-W. Mao, D. Wang, J. Li and Y-Z. Wang, "Accelerating ferroic ageing dynamics upon cooling," *NPG Asia Materials* **8** (2016) e319.

260. Z-M. Zhu, M-D. Li and J. Li, "Topological semimetal to insulator quantum phase transition in the Zintl compounds Ba<sub>2</sub>X(X = Si,Ge)," *Phys. Rev. B* **94** (2016) 155121.
259. Y-C. Wang, W. Zhang, L-Y. Wang, Z. Zhuang, E. Ma, J. Li and Z-W. Shan, "In situ TEM study of deformation-induced crystalline-to-amorphous transition in silicon," *NPG Asia Materials* **8** (2016) e291.
258. S-X. Huang, Y. Tatsumi, X. Ling, H-H. Guo, Z-Q. Wang, G. Watson, A.A. Puretzky, D.B. Geohegan, J. Kong, J. Li, T. Yang, R. Saito and M.S. Dresselhaus, "In-Plane Optical Anisotropy of Layered Gallium Telluride," *ACS Nano* **10** (2016) 8964-8972.
257. Q-J. Li, J. Li, Z-W. Shan and E. Ma, "Surface Rebound of Relativistic Dislocations Directly and Efficiently Initiates Deformation Twinning," *Phys. Rev. Lett.* **117** (2016) 165501.
256. Q-J. Li, J. Li, Z-W. Shan and E. Ma, "Strongly correlated breeding of high-speed dislocations," *Acta Materialia* **119** (2016) 229-241.
255. B.Y. Guan, L. Yu, J. Li and X.W. Lou, "A universal cooperative assembly-directed method for coating of mesoporous TiO<sub>2</sub> nanoshells with enhanced lithium storage properties," *Science Advances* **2** (2016) e1501554.
254. I.V. Fedotov, C.E. Richman, O.N. Sevryukov, A.N. Suchkov, J. Li, B.A. Kalin, V.T. Fedotov and A.A. Ivannikov, "Brazing Molybdenum and Graphite with a Titanium-Based Powder Filler Metal," *Welding Journal* **95** (2016) 357S-361S.
253. Z-Q. Liu, Z-Y. Yin, C. Cox, M. Bosman, X-F. Qian, N. Li, H-Y. Zhao, Y-P. Du, J. Li and D.G. Nocera, "Room temperature stable CO<sub>x</sub>-free H<sub>2</sub> production from methanol with magnesium oxide nanophotocatalysts," *Science Advances* **2** (2016) e1501425.
252. R.I. Gonzalez, F. Valencia, J. Mella, A.C.T. van Duin, K.P. So, J. Li, M. Kiwi and E.M. Bringa, "Metal-nanotube composites as radiation resistant materials," *Applied Physics Letters* **109** (2016) 033108.
251. H-T. Zhang, J. Tersoff, S. Xu, H-X. Chen, Q-B. Zhang, K-L. Zhang, Y. Yang, C-S. Lee, K-N. Tu, J. Li and Y. Lu, "Approaching the ideal elastic strain limit in silicon nanowires," *Science Advances* **2** (2016) e1501382.
250. Z-M. Zhu, G.W. Winkler, Q-S. Wu, J. Li and A.A. Soluyanov, "Triple Point Topological Metals," *Physical Review X* **6** (2016) 031003.
249. Z. Zhu, A. Kushima, Z-Y. Yin, L. Qi, K. Amine, J. Lu and J. Li, "Anion-redox nanolithia cathodes for Li-ion batteries," *Nature Energy* **1** (2016) 16111.
248. M-S. Ding, J-P. Du, L. Wan, S. Ogata, L. Tian, E. Ma, W-Z. Han, J. Li and Z-W. Shan, "Radiation-Induced Helium Nanobubbles Enhance Ductility in Submicron-Sized Single-Crystalline Copper," *Nano Letters* **16** (2016) 4118-4124.
247. A. Ishii, J. Li and S. Ogata, "Shuffling-controlled versus strain-controlled deformation twinning: The case for HCP Mg twin nucleation," *Int. J. Plasticity* **82** (2016) 32-43.

246. X.L. Wang, F. Jiang, H. Hahn, J. Li, H. Gleiter, J. Sun and J.X. Fang, "Sample size effects on strength and deformation mechanism of Sc<sub>75</sub>Fe<sub>25</sub> nanoglass and metallic glass," *Scripta Materialia* **116** (2016) 95-99.
245. X. Ling, Y-X. Lin, Q. Ma, Z-Q. Wang, Y. Song, L-L. Yu, S-X. Huang, W-J. Fang, X. Zhang, A.L. Hsu, Y-Q. Bie, Y-H. Lee, Y-M. Zhu, L-J. Wu, J. Li, P. Jarillo-Herrero, M. Dresselhaus, T. Palacios and J. Kong, "Parallel Stitching of 2D Materials," *Advanced Materials* **28** (2016) 2322-2329.
244. S-J. Hao, L-S. Cui, H. Wang, D-Q. Jiang, Y-N. Liu, J-Q. Yan, Y. Ren, X-D. Han, D.E. Brown and J. Li, "Retaining Large and Adjustable Elastic Strains of Kilogram-Scale Nb Nanowires," *ACS Appl. Mater. Interfaces* **8** (2016) 2917-2922.
243. H. Wang, G-Y. Gou and J. Li, "Ruddlesden-Popper perovskite sulfides A<sub>3</sub>B<sub>2</sub>S<sub>7</sub>: A new family of ferroelectric photovoltaic materials for the visible spectrum," *Nano Energy* **22** (2016) 507-513.
242. R. He, J-A. Yan, Z-Y. Yin, Z-P. Ye, G-H. Ye, J. Cheng, J. Li and C.H. Lui, "Coupling and Stacking Order of ReS<sub>2</sub> Atomic Layers Revealed by Ultralow-Frequency Raman Spectroscopy," *Nano Letters* **16** (2016) 1404-1409.
241. K.P. So, D. Chen, A. Kushima, M-D. Li, S-T. Kim, Y. Yang, Z-Q. Wang, J.G. Park, Y.H. Lee, R.I. Gonzalez, M. Kiwi, E.M. Bringa, L. Shao and J. Li, "Dispersion of carbon nanotubes in aluminum improves radiation resistance," *Nano Energy* **22** (2016) 319-327.
240. W-B. Li and J. Li, "Ferroelasticity and domain physics in two-dimensional transition metal dichalcogenide monolayers," *Nature Communications* **7** (2016) 10843.
239. Y-M. Chen, S-M. He, C-H. Huang, C-C. Huang, W-P. Shih, C-L. Chu, J. Kong, J. Li and C-Y. Su, "Ultra-large suspended graphene as a highly elastic membrane for capacitive pressure sensors," *Nanoscale* **8** (2016) 3555-3564.
238. J-H. Luo, J-W. Wang, E. Bitzek, J.Y. Huang, H. Zheng, L-M. Tong, Q. Yang, J. Li and S.X. Mao, "Size-Dependent Brittle-to-Ductile Transition in Silica Glass Nanofibers," *Nano Letters* **16** (2016) 105-113.
237. X. Ge, C-D. Gu, Z-Y. Yin, X-L. Wang, J-P. Tu and J. Li, "Periodic stacking of 2D charged sheets: Self-assembled superlattice of NiAl layered double hydroxide (LDH) and reduced graphene oxide," *Nano Energy* **20** (2016) 185-193.
236. C. Wu, H. Wang, J-J. Zhang, G-Y. Gou, B-C. Pan and J. Li, "Lithium-Boron (Li-B) Monolayers: First-Principles Cluster Expansion and Possible Two-Dimensional Superconductivity," *ACS Appl. Mater. Interfaces* **8** (2016) 2526.
235. S-T. Kim, S.J. Choi, K-J. Zhao, H. Yang, G. Gobbi, S-L. Zhang and J. Li, "Electrochemically driven mechanical energy harvesting," *Nature Communications* **7** (2016) 10146.

234. Y-Y. Wang, R.X. Yang, R-G. Quhe, H-X. Zhong, L-X. Cong, M. Ye, Z-Y. Ni, Z-G. Song, J-B. Yang, J-J. Shi, J. Li and J. Lu, “Does p-type ohmic contact exist in WSe<sub>2</sub>-metal interfaces?,” *Nanoscale* **8** (2016) 1179-1191.
233. N-Q. Zhang, Z-L. Zhu, H. Xu, X-P. Mao and J. Li, “Oxidation of ferritic and ferritic-martensitic steels in flowing and static supercritical water,” *Corrosion Science* **103** (2016) 124-131.
232. Y.G. Li, Y. Yang, M.P. Short, Z.J. Ding, Z. Zeng and J. Li, “IM3D: A parallel Monte Carlo code for efficient simulations of primary radiation displacements and damage in 3D geometry,” *Scientific Reports* **5** (2015) 18130.
231. X-G. Wang, K. Chen, Y-Q. Zhang, J-C. Wan, O.L. Warren, J. Oh, J. Li, E. Ma and Z-W. Shan, “Growth Conditions Control the Elastic and Electrical Properties of ZnO Nanowires,” *Nano Letters* **15** (2015) 7886-7892.
230. W. Guo, Z. Wang and J. Li, “Diffusive versus Displacive Contact Plasticity of Nanoscale Asperities: Temperature- and Velocity-Dependent Strongest Size,” *Nano Letters* **15** (2015) 6582-6585.
229. Z. Li, J.T. Zhang, Y.M. Chen, J. Li and X.W. Lou, “Pie-like electrode design for high-energy density lithium-sulfur batteries,” *Nature Communications* **6** (2015) 8850.
228. A. Kushima, T. Koido, Y. Fujiwara, N. Kuriyama, N. Kusumi and J. Li, “Charging/Discharging Nanomorphology Asymmetry and Rate-Dependent Capacity Degradation in Li-Oxygen Battery,” *Nano Letters* **15** (2015) 8260-8265.
227. M-S. Ding, W-Z. Han, J. Li, E. Ma and Z-W. Shan, “In situ study of the mechanical properties of airborne haze particles,” *Science China: Technological Sciences* **58** (2015) 2046-2051.
226. X-F. Qian, Y-Y. Wang, W-B. Li, J. Lu and J. Li, “Modelling of stacked 2D materials and devices,” *2D Materials* **2** (2015) 032003.
225. W-B. Li and J. Li, “Piezoelectricity in two-dimensional group-III monochalcogenides,” *Nano Research* **8** (2015) 3796-3802.
224. R.X. Fei, W-B. Li, J. Li and L. Yang, “Giant piezoelectricity of monolayer group IV monochalcogenides: SnSe, SnS, GeSe, and GeS,” *Applied Physics Letters* **107** (2015) 173104.
223. Z-J. Wang, Q-J. Li, Y-N. Cui, Z-L. Liu, E. Ma, J. Li, J. Sun, Z. Zhuang, M. Dao, Z-W. Shan and S. Suresh, “Cyclic deformation leads to defect healing and strengthening of small-volume metal crystals,” *PNAS* **112** (2015) 13502-13507.
222. Z.T. Tian, M.D. Li, Z.S. Ren, H. Ma, A. Alatas, S.D. Wilson and J. Li, “Inelastic x-ray scattering measurements of phonon dispersion and lifetimes in PbTe<sub>1-x</sub>Sex alloys,” *J. Phys.: Condens. Matter* **27** (2015) 375403.

221. S. Li, J-J. Niu, Y.C. Zhao, K.P. So, C. Wang, C.A. Wang and J. Li, "High-rate aluminium yolk-shell nanoparticle anode for Li-ion battery with long cycle life and ultrahigh capacity," *Nature Communications* **6** (2015) 7872.
220. S-Z. Li, Y-G. Li, Y-C. Lo, 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 alpha-Fe," *Int. J. Plasticity* **74** (2015) 175-191.
219. X-F. Qian, M. Kawai, H. Goto and J. Li, "Effect of twin boundaries and structural polytypes on electron transport in GaAs," *Computational Materials Science* **108** (2015) 258-263.
218. R. Huang, Q-J. Li, Z-J. Wang, L. Huang, J. Li, E. Ma and Z-W. Shan, "Flow Stress in Submicron BCC Iron Single Crystals: Sample-size-dependent Strain-rate Sensitivity and Rate-dependent Size Strengthening," *Materials Research Letters* **3** (2015) 121-127.
217. D-G. Xie, Z-J. Wang, J. Sun, J. Li, E. Ma and Z-W. Shan, "In situ study of the initiation of hydrogen bubbles at the aluminium metal/oxide interface," *Nature Materials* **14** (2015) 899-903.
216. C-C. Wang, Q-J. Li, L. Chen, Y-H. Cheng, J. Sun, Z-W. Shan, J. Li and E. Ma, "Ultrafast shape change and joining of small-volume materials using nanoscale electrical discharge," *Nano Research* **8** (2015) 2143-2151.
215. J. Li, "DISLOCATION NUCLEATION: Diffusive origins," *Nature Materials* **14** (2015) 656-657. News & Views.
214. H. Li, A.W. Contryman, X-F. Qian, S.M. Ardakani, Y-J. Gong, X-L. Wang, J.M. Weisse, C.H. Lee, J-H. Zhao, P.M. Ajayan, J. Li, H.C. Manoharan and X-L. Zheng, "Optoelectronic crystal of artificial atoms in strain-textured molybdenum disulphide," *Nature Communications* **6** (2015) 7381.
213. W-B. Li, J.M. Rieser, A.J. Liu, D.J. Durian and J. Li, "Deformation-driven diffusion and plastic flow in amorphous granular pillars," *Phys. Rev. E* **91** (2015) 062212.
212. W-Z. Han, L. Huang, S. Ogata, H. Kimizuka, Z-C. Yang, C. Weinberger, Q-J. Li, B-Y. Liu, X-X. Zhang, J. Li, E. Ma and Z-W. Shan, "From Smaller is Stronger to Size-Independent Strength Plateau: Towards Measuring the Ideal Strength of Iron," *Advanced Materials* **27** (2015) 3385-3390.
211. M. Wakeda, J. Saida, J. Li and S. Ogata, "Controlled Rejuvenation of Amorphous Metals with Thermal Processing," *Scientific Reports* **5** (2015) 10545.
210. Y-W. Mao, J. Li, Y-C. Lo, X-F. Qian and E. Ma, "Stress-driven crystallization via shear-diffusion transformations in a metallic glass at very low temperatures," *Phys. Rev. B* **91** (2015) 214103.



209. G-X. Wu, Y-G. Cho, I-S. Choi, D-T. Ge, J. Li, H.N. Han, T. Lubensky and S. Yang, "Directing the Deformation Paths of Soft Metamaterials with Prescribed Asymmetric Units," *Adv. Mater.* **27** (2015) 2747-2752.
208. M-D. Li, C-Z. Chang, B.J. Kirby, M.E. Jamer, W-P. Cui, L-J. Wu, P. Wei, Y-M. Zhu, D. Heiman, J. Li and J.S. Moodera, "Proximity-Driven Enhanced Magnetic Order at Ferromagnetic-Insulator-Magnetic-Topological-Insulator Interface," *Phys. Rev. Lett.* **115** (2015) 146802.
207. M-D. Li, C-Z. Chang, L-J. Wu, J. Tao, W-W. Zhao, M.H.W. Chan, J.S. Moodera, J. Li and Y-M. Zhu, "Experimental Verification of the Van Vleck Nature of Long-Range Ferromagnetic Order in the Vanadium-Doped Three-Dimensional Topological Insulator Sb<sub>2</sub>Te<sub>3</sub>," *Phys. Rev. Lett.* **114** (2015) 146802.
206. X-F. Qian, L. Fu and J. Li, "Topological crystalline insulator nanomembrane with strain-tunable band gap," *Nano Research* **8** (2015) 967-979.
205. Z.Y. He, Y.W. Sheng, Y.M. Rong, G-D. Lee, J. Li and J.H. Warner, "Layer-Dependent Modulation of Tungsten Disulfide Photoluminescence by Lateral Electric Fields," *ACS Nano* **9** (2015) 2740-2748.
204. Y. Zhang, C-J. Huang, S-T. Kim, M. Golkaram, M.W.A. Dixon, L. Tilley, J. Li, S-L. Zhang and S. Suresh, "Multiple stiffening effects of nanoscale knobs on human red blood cells infected with *Plasmodium falciparum* malaria parasite," *PNAS* **112** (2015) 6068-6073.
203. C. Wang, X-S. Wang, Y. Yang, A. Kushima, J-T. Chen, Y-H. Huang and J. Li, "Slurryless Li<sub>2</sub>S/Reduced Graphene Oxide Cathode Paper for High-Performance Lithium Sulfur Battery," *Nano Letters* **15** (2015) 1796-1802.
202. K. He, H.L. Xin, K.J. Zhao, X.Q. Yu, D. Nordlund, T-C. Weng, J. Li, Y. Jiang, C.A. Cadigan, R.M. Richards, M.M. Doeff, X-Q. Yang, E.A. Stach, J. Li, F. Lin and D. Su, "Transitions from Near-Surface to Interior Redox upon Lithiation in Conversion Electrode Materials," *Nano Letters* **15** (2015) 1437-1444.
201. A. Kushima, X-F. Qian, P. Zhao, S.L. Zhang and J. Li, "Ripplocations in van der Waals Layers," *Nano Letters* **15** (2015) 1302-1308.
200. Y.Y. Wang, Z.Y. Ni, Q.H. Liu, R.G. Quhe, J.X. Zheng, M. Ye, D.P. Yu, J.J. Shi, J.B. Yang, J. Li and J. Lu, "All-Metallic Vertical Transistors Based on Stacked Dirac Materials," *Advanced Functional Materials* **25** (2015) 68-77.
199. H.X. Zong, X.D. Ding, T. Lookman, J. Li and J. Sun, "Uniaxial stress-driven coupled grain boundary motion in hexagonal close-packed metals: A molecular dynamics study," *Acta Materialia* **82** (2015) 295-303.
198. X.L. Wang, F. Jiang, H. Hahn, J. Li, H. Gleiter, J. Sun and J.X. Fang, "Plasticity of a scandium-based nanoglass," *Scripta Materialia* **98** (2015) 40-43.

197. Y.G. Cho, J-H. Shin, A. Costa, T.A. Kim, V. Kunin, J. Li, S.Y. Lee, S. Yang, H.N. Han, I-S. Choi and D.J. Srolovitz, "Engineering the shape and structure of materials by fractal cut," *PNAS* **111** (2014) 17390-17395.
196. X-F. Qian, J-W. Liu, L. Fu and J. Li, "Quantum spin Hall effect in two-dimensional transition metal dichalcogenides," *Science* **346** (2014) 1344-1347.
195. J. Sun, L-B. He, Y-C. Lo, T. Xu, H-C. Bi, L-T. Sun, Z. Zhang, S. X. Mao and J. Li, "Liquid-like pseudoelasticity of sub-10-nm crystalline silver particles," *Nature Materials* **13** (2014) 1007-1012.
194. J-J. Niu, A. Kushima, M-D. Li, Z-Q. Wang, W-B. Li, C. Wang and J. Li, "Scalable synthesis of a sulfur nanosponge cathode for a lithium-sulfur battery with improved cyclability," *J. Mater. Chem. A* **2** (2014) 19788-19796.
193. W-B. Li, X-F. Qian and J. Li, "Envelope function method for electrons in slowly-varying inhomogeneously deformed crystals," *J. Phys.: Condensed Matter* **26** (2014) 455801.
192. S.C. Yeo, Y.C. Lo, J. Li and H.M. Lee, "Theoretical study of the ammonia nitridation rate on an Fe (100) surface: A combined density functional theory and kinetic Monte Carlo study," *J. Chem. Phys.* **141** (2014) 134108.
191. S-Z. Li, X-D. Ding, J. Ren, X. Moya, J. Li, J. Sun and E.K.H. Salje, "Strain-controlled thermal conductivity in ferroic twinned films," *Scientific Reports* **4** (2014) 6375.
190. M-H. Wu, X-F. Qian and J. Li, "Tunable Exciton Funnel Using Moire Superlattice in Twisted van der Waals Bilayer," *Nano Letters* **14** (2014) 5350-5357.
189. W-B. Li, H-Y. Fan and J. Li, "Deviatoric Stress-Driven Fusion of Nanoparticle Superlattices," *Nano Letters* **14** (2014) 4951-4958.
188. H-Y. Li, J-S. Wang, M. Liu, H. Wang, P-L. Su, J-S. Wu and J. Li, "A nanoporous oxide interlayer makes a better Pt catalyst on a metallic substrate: Nanoflowers on a nanotube bed," *Nano Research* **7** (2014) 1007-1017.
187. C. Shen, J. Li and Y-Z. Wang, "Predicting structure and energy of dislocations and grain boundaries," *Acta Materialia* **74** (2014) 125-131.
186. J-J. Niu, A. Kushima, X-F. Qian, L. Qi, K. Xiang, Y-M. Chiang and J. Li, "In Situ Observation of Random Solid Solution Zone in LiFePO<sub>4</sub> Electrode," *Nano Letters* **14** (2014) 4005-4010.
185. H-X. Zong, X-D. Ding, T. Lookman, J. Li, J. Sun, E.K. Cerreta, A.P. Escobedo, F.L. Addessio and C.A. Bronkhorst, "Collective nature of plasticity in mediating phase transformation under shock compression," *Physical Review B* **89** (2014) 220101.
184. P. Nukala, R. Agarwal, X-F. Qian, M.H. Jang, S. Dhara, K. Kumar, A.T.C. Johnson, J. Li and R. Agarwal, "Direct Observation of Metal-Insulator Transition in Single-Crystalline Germanium Telluride Nanowire Memory Devices Prior to Amorphization," *Nano Letters* **14** (2014) 2201-2209.

183. P-Y. Zhao, J. Li and Y-Z. Wang, "Extended defects, ideal strength and actual strengths of finite-sized metallic glasses," *Acta Materialia* **73** (2014) 149-166.
182. X-W. Fu, C. Su, Q. Fu, X-L. Zhu, R. Zhu, C-P. Liu, Z-M. Liao, J. Xu, W-L. Guo, J. Feng, J. Li and D-P. Yu, "Tailoring Exciton Dynamics by Elastic Strain-Gradient in Semiconductors," *Advanced Materials* **26** (2014) 2572-2579.
181. B-Y. Liu, J. Wang, B. Li, L. Lu, X-Y. Zhang, Z-W. Shan, J. Li, C-L. Jia, J. Sun and E. Ma, "Twinning-like lattice reorientation without a crystallographic twinning plane," *Nature Communications* **5** (2014) 3297.
180. Z.J. Wang, Z.W. Shan, J. Li, J. Sun and E. Ma, "An index for deformation controllability of small-volume materials," *Science China Technological Sciences* **57** (2014) 663-670.
179. J.P. Lin, X.D. Li, G.J. Qiao, Z. Wang, J. Carrete, Y. Ren, L.Z. Ma, Y.J. Fei, B.F. Yang, L. Lei and J. Li, "Unexpected High-Temperature Stability of beta-Zn4Sb3 Opens the Door to Enhanced Thermoelectric Performance," *J. Am. Chem. Soc.* **136** (2014) 1497-1504.
178. \*\* J. Li, Z-W. Shan and E. Ma, Guest Editors, "Elastic strain engineering for unprecedented materials properties," *MRS Bulletin* **39** (2014) 108-162.
177. L.F. Liu, X.D. Ding, J. Li, T. Lookmand and J. Sun, "Direct observation of hierarchical nucleation of martensite and size-dependent superelasticity in shape memory alloys," *Nanoscale* **6** (2014) 2067-2072.
176. C-C. Wang, Y-W. Mao, Z-W. Shan, M. Dao, J. Li, J. Sun, E. Ma and S. Suresh, "Real-time, high-resolution study of nanocrystallization and fatigue cracking in a cyclically strained metallic glass," *PNAS* **110** (2013) 19725-19730.
175. W.T. Liang, L. Hong, H. Yang, F.F. Fan, Y. Liu, H. Li, J. Li, J.Y. Huang, L-Q. Chen, T. Zhu and S.L. Zhang, "Nanovoid Formation and Annihilation in Gallium Nanodroplets under Lithiation-Delithiation Cycling," *Nano Letters* **13** (2013) 5212-5217.
174. M. Gu, A. Kushima, Y.Y. Shao, J-G. Zhang, J. Liu, N.D. Browning, J. Li and C.M. Wang, "Probing the Failure Mechanism of SnO2 Nanowires for Sodium-Ion Batteries," *Nano Letters* **13** (2013) 5203-5211.
173. J-H. Seo, H. S. Park, Y. Yoo, T-Y. Seong, Ju Li, J-P. Ahn, B. Kim and I-S. Choi, "Origin of Size Dependency in Coherent-Twin-Propagation-Mediated Tensile Deformation of Noble Metal Nanowires," *Nano Letters* **13** (2013) 5112-5116.
172. Y.J. Zhu, J.W. Wang, Y. Liu, X.H. Liu, A. Kushima, Y.H. Liu, Y.H. Xu, S.X. Mao, J. Li, C.S. Wang and J.Y. Huang, "In Situ Atomic-Scale Imaging of Phase Boundary Migration in FePO4 Microparticles During Electrochemical Lithiation," *Advanced Materials* **25** (2013) 5461-5466.
171. Q. Yu, L. Qi, R.K. Mishra, J. Li and A.M. Minor, "Reducing deformation anisotropy to achieve ultrahigh strength and ductility in Mg at the nanoscale," *PNAS* **110** (2013) 13289-13293.

170. Y.G. Cho, T.H. Ahn, H.H. Cho, J.H. Shin, J.H. Moon, S. Yang, I-S. Choi, H.N. Han and J. Li, "Study of architectural responses of 3D periodic cellular materials," *Modelling Simul. Mater. Sci. Eng.* **21** (2013) 065018.
169. L. Tian, J. Li, J. Sun, E. Ma and Z-W. Shan, "Visualizing size-dependent deformation mechanism transition in Sn," *Scientific Reports* **3** (2013) 2113.
168. S. Huang, F. Fan, J. Li, S. Zhang and T. Zhu, "Stress generation during lithiation of high-capacity electrode particles in lithium ion batteries," *Acta Materialia* **61** (2013) 4354-4364.
167. L. Wan and J. Li, "Shear responses of [110]-tilt  $\{115\}/\{111\}$  asymmetric tilt grain boundaries in fcc metals by atomistic simulations," *Modelling and Simulation in Materials Science and Engineering* **21** (2013) 055013.
166. X.C. Ye, J. Chen, M. Engel, J.A. Millan, W.B. Li, L. Qi, G.Z. Xing, J.E. Collins, C.R. Kagan, J. Li, S.C. Glotzer and C.B. Murray, "Competition of shape and interaction patchiness for self-assembling nanoplates," *Nature Chemistry* **5** (2013) 466-473.
165. J.Y. Huang, Y-C. Lo, J.J. Niu, A. Kushima, X.F. Qian, L. Zhong, S.X. Mao and J. Li, "Nanowire Liquid Pumps," *Nature Nanotechnology* **8** (2013) 277-281.
164. S.J. Hao, L.S. Cui, D.Q. Jiang, X.D. Han, Y. Ren, J. Jiang, Y.N. Liu, Z.Y. Liu, S.C. Mao, Y.D. Wang, Y. Li, X.B. Ren, X.D. Ding, S. Wang, C. Yu, X.B. Shi, M.S. Du, F. Yang, Y.J. Zheng, Z. Zhang, X.D. Li, D.E. Brown and J. Li, "A Transforming Metal Nanocomposite with Large Elastic Strain, Low Modulus, and High Strength," *Science* **339** (2013) 1191-1194.
163. A. Ishii, J. Li and S. Ogata, "Conjugate Channeling Effect in Dislocation Core Diffusion: Carbon Transport in Dislocated BCC Iron," *PLoS ONE* **8** (2013) e60586.
162. Y.J. Kang, X.C. Ye, J. Chen, L. Qi, R.E. Diaz, V. Doan-Nguyen, G.Z. Xing, C.R. Kagan, J. Li, R.J. Gorte, E.A. Stach and C.B. Murray, "Engineering Catalytic Contacts and Thermal Stability: Gold/Iron Oxide Binary Nanocrystal Superlattices for CO Oxidation," *J. Am. Chem. Soc.* **135** (2013) 1499-1505.
161. P.Y. Zhao, J. Li and Y.Z. Wang, "Heterogeneously randomized STZ model of metallic glasses: Softening and extreme value statistics during deformation," *Int. J. Plasticity* **40** (2013) 1-22.
160. P. Liu, J. Li and Y-W. Zhang, "Breakup of spherical vesicles caused by spontaneous curvature change," *Acta Mechanica Sinica* **28** (2012) 1545-1550.
159. R. M. Mutiso, M. C. Sherrott, J. Li and K. I. Winey, "Simulations and generalized model of the effect of filler size dispersity on electrical percolation in rod networks," *Phys. Rev. B* **86** (2012) 214306.
158. J. Feng, X-F. Qian, C-W. Huang and J. Li, "Strain-engineered artificial atom as a broad-spectrum solar energy funnel," *Nature Photonics* **6** (2012) 866-872.

157. A. Kushima, J.Y. Huang and J. Li, "Quantitative fracture strength and plasticity measurements of lithiated silicon nanowires by in situ TEM tensile experiments," *ACS Nano* **6** (2012) 9425-9432.
156. I-W. Chen, S-W. Kim, J. Li, S-J. L. Kang and F.Q. Huang, "Ionomigration of Neutral Phases in Ionic Conductors," *Adv. Energy Mater.* **2** (2012) 1383-1389.
155. J. Li and L-Y. Bai, "DNA Nanotechnology: A metamaterial with memory," *Nature Nanotechnology* **7** (2012) 773-774.
154. X.H. Liu, J.W. Wang, S. Huang, F.F. Fan, X. Huang, Y. Liu, S. Krylyuk, J. Yoo, S.A. Dayeh, A.V. Davydov, S.X. Mao, S.T. Picraux, S.L. Zhang, J. Li, T. Zhu and J.Y. Huang, "In situ atomic-scale imaging of electrochemical lithiation in silicon," *Nature Nanotechnology* **7** (2012) 749-756.
153. L. Qi and J. Li, "Adsorbate interactions on surface lead to a flattened Sabatier volcano plot in reduction of oxygen," *J. Catalysis* **295** (2012) 59-69.
152. L. Qi, Y.W. Mao and J. Li, "Slip Corona Surrounding Bilayer Graphene Nanopore," *Nanoscale* **4** (2012) 5989-5997.
151. T. Neeraj, R. Srinivasan and J. Li, "Hydrogen embrittlement of ferritic steels: Observations on deformation microstructure, nanoscale dimples and failure by nanovoiding," *Acta Mater.* **60** (2012) 5160-5171.
150. X.H. Liu, J.W. Wang, Y. Liu, H. Zheng, A. Kushima, S. Huang, T. Zhu, S.X. Mao, J. Li, S.L. Zhang, W. Lu, J. M. Tour and J. Y. Huang, "In situ transmission electron microscopy of electrochemical lithiation, delithiation and deformation of individual graphene nanoribbons," *Carbon* **50** (2012) 3836-3844.
149. S. Sarkar, J. Li, W.T. Cox, E. Bitzek, T.J. Lenosky and Y.Z. Wang, "Finding activation pathway of coupled displacive-diffusional defect processes in atomistics: Dislocation climb in fcc copper," *Phys. Rev. B* **86** (2012) 014115.
148. J. Feng, W-B. Li, X-F. Qian, J-S. Qi, L. Qi and J. Li, "Patterning of graphene," *Nanoscale* **4** (2012) 4883-4899.
147. C-C. Wang, J. Ding, Y-Q. Cheng, J-C. Wan, L. Tian, J. Sun, Z-W. Shan, J. Li, E. Ma, "Sample size matters for Al<sub>88</sub>Fe<sub>7</sub>Gd<sub>5</sub> metallic glass: Smaller is stronger," *Acta Mater.* **60** (2012) 5370-5379.
146. X.H. Liu, Y. Liu, A. Kushima, S.L. Zhang, T. Zhu, J. Li and J.Y. Huang, "In Situ TEM Experiments of Electrochemical Lithiation and Delithiation of Individual Nanostructures," *Adv. Energy Mater.* **2** (2012) 722-741.
145. J-B. Wu, L. Qi, H-J. You, A. Gross, J. Li and H. Yang, "Icosahedral Platinum Alloy Nanocrystals with Enhanced Electrocatalytic Activities," *J. Am. Chem. Soc.* **134** (2012) 11880-11883.

144. S-W. Nam, H-S. Chung, Y.C. Lo, L. Qi, J. Li, Y. Lu, A.T.C. Johnson, Y. Jung, P. Nukala, R. Agarwal, "Electrical Wind Force-Driven and Dislocation-Templated Amorphization in Phase-Change Nanowires," *Science* **336** (2012) 1561-1566.
143. H. Yang, S. Huang, X. Huang, F.F. Fan, W.T. Liang, X. H. Liu, L-Q. Chen, J. Y. Huang, J. Li, T. Zhu and S.L. Zhang, "Orientation-Dependent Interfacial Mobility Governs the Anisotropic Swelling in Lithiated Silicon Nanowires," *Nano Letters* **12** (2012) 1953-1958.
142. J.S. Qi, X.F. Qian, L. Qi, J. Feng, D.N. Shi and J. Li, "Strain-Engineering of Band Gaps in Piezoelectric Boron Nitride Nanoribbons," *Nano Letters* **12** (2012) 1224-1228.
141. Y.J. Kang, L. Qi, M. Li, R.E. Diaz, D. Su, R. R. Adzic, E. Stach, J. Li and C. B. Murray, "Highly Active Pt<sub>3</sub>Pb and Core-Shell Pt<sub>3</sub>Pb-Pt Electrocatalysts for Formic Acid Oxidation," *ACS Nano* **6** (2012) 2818-2825.
140. Z-J. Wang, Z-W. Shan, J. Li, J. Sun and E. Ma, "Pristine-to-pristine regime of plastic deformation in submicron-sized single crystal gold particles," *Acta Mater.* **60** (2012) 1368-1377.
139. Q. Yu, L. Qi, K. Chen, R.K. Mishra, J. Li and A.M. Minor, "The Nanostructured Origin of Deformation Twinning," *Nano Letters* **12** (2012) 887-892.
138. A. Ishii, S. Ogata, H. Kimizuka and J. Li, "Adaptive-boost molecular dynamics simulation of carbon diffusion in iron," *Phys. Rev. B* **85** (2012) 064303.
137. Z-J. Wang, Q-J. Li, Z-W. Shan, J. Li, J. Sun and E. Ma, "Sample size effects on the large strain bursts in submicron aluminum pillars," *Applied Physics Letters* **100** (2012) 071906.
136. L. Tian, Y-Q. Cheng, Z-W. Shan, J. Li, C-C. Wang, X-D. Han, J. Sun and E. Ma, "Approaching the ideal elastic limit of metallic glasses," *Nature Communications* **3** (2012) 609.
135. L. Huang, Q-J. Li, Z-W. Shan, J. Li, J. Sun and E. Ma, "A new regime for mechanical annealing and strong sample-size strengthening in body centred cubic molybdenum," *Nature Communications* **2** (2011) 547.
134. A. Kushima, X. H. Liu, G. Zhu, Z. L. Wang, J.Y. Huang and J. Li, "Leapfrog Cracking and Nanoamorphization of ZnO Nanowires during in Situ Electrochemical Lithiation," *Nano Letters* **11** (2011) 4535-4541.
133. X.H. Liu, S. Huang, S.T. Picraux, J. Li, T. Zhu and J.Y. Huang, "Reversible nanopore formation in Ge nanowires during lithiation-delithiation cycling: an in situ transmission electron microscopy study," *Nano Letters* **11** (2011) 3991-3997.
132. Y. Liu, H. Zheng, X. H. Liu, S. Huang, T. Zhu, J. W. Wang, A. Kushima, N. S. Hudak, X. Huang, S.L. Zhang, S. X. Mao, X.F. Qian, J. Li, and J.Y. Huang, "Lithiation-Induced Embrittlement of Multiwalled Carbon Nanotubes," *ACS Nano* **5** (2011) 7245-7253.
131. J. Li, S. Sarkar, W. T. Cox, T. J. Lenosky, E. Bitzek and Y.Z. Wang, "Diffusive molecular dynamics and its application to nanoindentation and sintering," *Phys. Rev. B* **84** (2011) 054103.

130. A. Kushima, J. Eapen, J. Li, S. Yip and T. Zhu, "Time scale bridging in atomistic simulation of slow dynamics: viscous relaxation and defect activation," *Eur. Phys. J. B* **82** (2011) 271-293.
129. X.H. Liu, H. Zheng, L. Zhong, S. Huang, K. Karki, L.Q. Zhang, Y. Liu, A. Kushima, W.T. Liang, J.W. Wang, J.-H. Cho, E. Epstein, S.A. Dayeh, S.T. Picraux, T. Zhu, J. Li, J.P. Sullivan, J. Cumings, C.S. Wang, S.X. Mao, Z.Z. Ye, S.L. Zhang and J.Y. Huang, "Anisotropic Swelling and Fracture of Silicon Nanowires during Lithiation," *Nano Letters* **11** (2011) 3312-3318.
128. A.T. Jennings, J. Li and J.R. Greer, "Emergence of strain-rate sensitivity in Cu nanopillars: Transition from dislocation multiplication to dislocation nucleation," *Acta Mater.* **59** (2011) 5627-5637.
127. X.H. Liu, L. Zhong, L.Q. Zhang, A. Kushima, S.X. Mao, J. Li, Z.Z. Ye, J.P. Sullivan and J.Y. Huang, "Lithium fiber growth on the anode in a nanowire lithium ion battery during charging," *Appl. Phys. Lett.* **98** (2011) 183107.
126. N. Zhou, C. Shen, M.J. Mills, J. Li and Y.Z. Wang, "Modeling displacive-diffusional coupled dislocation shearing of gamma-prime precipitates in Ni-base superalloys," *Acta Mater.* **59** (2011) 3484-3497.
125. J.S. Qi, J.Y. Huang, J. Feng, D.N. Shi and J. Li, "The Possibility of Chemically Inert, Graphene-Based All-Carbon Electronic Devices with 0.8 eV Gap," *ACS Nano* **5** (2011) 3475-3482.
124. J. Li, A. Kushima, J. Eapen, X. Lin, X.F. Qian, J. C. Mauro, P. Diep and S. Yip, "Computing the Viscosity of Supercooled Liquids: Markov Network Model," *PLoS ONE* **6** (2011) e17909.
123. 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 and J. Li, "In situ observation of the electrochemical lithiation of a single SnO<sub>2</sub> nanowire electrode," *Science* **330** (2010) 1515-1520.
122. S.Z. Li, X.D. Ding, J.K. Deng, T. Lookman, J. Li, X.B. Ren, J. Sun and A. Saxena, "Superelasticity in BCC nanowires by a reversible twinning mechanism," *Phys. Rev. B* **82** (2010) 205435.
121. X.F. Qian, J. Li and S. Yip, "Calculating phase-coherent quantum transport in nanoelectronics with ab initio quasiatomic orbital basis set," *Phys. Rev. B* **82** (2010) 195442.
120. S. Hara and J. Li, "Adaptive strain-boost hyperdynamics simulations of stress-driven atomic processes," *Phys. Rev. B* **82** (2010) 184114.
119. P. A. Gordon, T. Neeraj, Y. Li and J. Li, "Screw dislocation mobility in BCC metals: the role of the compact core on double-kink nucleation," *Modelling Simul. Mater. Sci. Eng.* **18** (2010) 085008.

118. H.Y. Yuan, J. Li, G. Bao and S.L. Zhang, "Variable Nanoparticle-Cell Adhesion Strength Regulates Cellular Uptake," *Phys. Rev. Lett.* **105** (2010) 138101.
117. S. I. White, R. M. Mutiso, P. M. Vora, D. Jahnke, S. Hsu, J. M. Kikkawa, J. Li, J. E. Fischer and K. I. Winey, "Electrical percolation behavior in silver nanowire-polystyrene composites: simulation and experiment," *Adv. Funct. Mater.* **20** (2010) 2709-2716.
116. C. Zheng, P. Liu, J. Li and Y-W. Zhang, "Phase Diagrams for Multi-Component Membrane Vesicles: A Coarse-Grained Modeling Study," *Langmuir* **26** (2010) 12659-12666.
115. H.Y. Yuan, C.J. Huang, J. Li, G. Lykotrafitis and S.L. Zhang, "One-particle-thick, solvent-free, coarse-grained model for biological and biomimetic fluid membranes," *Phys. Rev. E* **82** (2010) 011905.
114. S. Z. Li, X. D. Ding, J. Li, X. B. Ren, J. Sun, E. Ma and T. Lookman, "Inverse martensitic transformation in Zr nanowires," *Phys. Rev. B* **81** (2010) 245433.
113. T. Zhu and J. Li, "Ultra-strength materials," *Progress in Materials Science* **55** (2010) 710-757.
112. J-Y. Zhang, G. Liu, R. H. Wang, J. Li, J. Sun and E. Ma, "Double-inverse grain size dependence of deformation twinning in nanocrystalline Cu," *Phys. Rev. B* **81** (2010) 172104
111. S. Z. Li, X. D. Ding, J. Li, X. B. Ren, J. Sun and E. Ma, "High-efficiency mechanical energy storage and retrieval using interfaces in nanowires," *Nano Letters* **10** (2010) 1774-1779.
110. 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.
109. Q. Yu, Z.-W. Shan, J. Li, X.X. Huang, L. Xiao, J. Sun and E. Ma, "Strong crystal size effect on deformation twinning," *Nature* **463** (2010) 335-338.
108. J. Y. Huang, L. Qi and J. Li, "*In situ* imaging of layer-by-layer sublimation of suspended graphene," *Nano Research* **3** (2010) 43-50.
107. Y. Wang and J. Li, "Phase field modeling of defects and deformation," *Acta Mater.* **58** (2010) 1212-1235. Overview No. 150.
106. Y. Mishin, M. Asta and J. Li, "Atomistic modeling of interfaces and their impact on microstructure and properties," *Acta Mater.* **58** (2010) 1117-1151. Overview No. 148.
105. X.H. Liu, J.F. Gu, Y. Shen, J. Li and C.F. Chen, "Lattice dynamical finite-element method," *Acta Mater.* **58** (2010) 510-523.
104. S. Ogata and J. Li, "Toughness scale from first principles", *J. Appl. Phys.* **106** (2009) 113534.
103. A. Kushima, X. Lin, J. Li, X-F. Qian, J. Eapen, J. C. Mauro, P. Diep and S. Yip, "Computing the viscosity of supercooled liquids. II. Silica and strong-fragile crossover behavior," *J. Chem. Phys.* **131** (2009) 164505.



102. J. Feng, L. Qi, J. Y. Huang and J. Li, "Geometric and electronic structure of graphene bilayer edges," *Phys. Rev. B* **80** (2009) 165407.
101. P. Liu, J. Li and Y-W. Zhang, "Pressure-temperature phase diagram for shapes of vesicles: A coarse-grained molecular dynamics study," *Appl. Phys. Lett.* **95** (2009) 143104.
100. J. Y. Huang, F. Ding, B. I. Yakobson, P. Lu, L. Qi and J. Li, "In situ observation of graphene sublimation and multi-layer edge reconstructions," *PNAS* **106** (2009) 10103-10108.
99. L. Kovarik, R.R. Unocic, J. Li, P. Sarosi, C. Shen, Y. Wang and M.J. Mills, "Microtwinning and other shearing mechanisms at intermediate temperatures in Ni-based superalloys," *Progress in Materials Science* **54** (2009) 839-873.
98. A. Kushima, X. Lin, J. Li, J. Eapen, J. C. Mauro, X.F. Qian, P. Diep and S. Yip, "Computing the viscosity of supercooled liquids," *J. Chem. Phys.* **130** (2009) 224504.
97. L. Lu, M. Dao, T. Zhu and J. Li, "Size dependence of rate-controlling deformation mechanisms in nanotwinned copper," *Scripta Mater.* **60** (2009) 1062-1066.
96. T. Zhu, J. Li, S. Ogata and S. Yip, "Mechanics of Ultra-Strength Materials," *MRS Bulletin* **34** (March 2009) 167-172.
95. P.M. Derlet, P. Gumbsch, R. Hoagland, J. Li, D.L. McDowell, H. van Swygenhoven and J. Wang, "Atomistic Simulations of Dislocations in Confined Volumes," *MRS Bulletin* **34** (March 2009) 184-189.
94. L. Kovarik, R. R. Unocic, J. Li and M. J. Mills, "The Intermediate Temperature Deformation of Ni-Based Superalloys: Importance of Reordering," *JOM* **61** (2009) 42-48.
93. S. L. Zhang, J. Li, G. Lykotrafitis, G. Bao and S. Suresh, "Size-Dependent Endocytosis of Nanoparticles," *Adv. Mater.* **21** (2009) 419-424.
92. C-Z. Wang, G-D. Lee, J. Li, S. Yip and K-M. Ho, "Atomistic simulation studies of complex carbon and silicon systems using environment-dependent tight-binding potentials," *Scientific Modeling and Simulation* **15** (2008) 97-121.
91. C-Z. Wang, W-C. Lu, Y-X. Yao, J. Li, S. Yip and K-M. Ho, "Tight-binding Hamiltonian from first-principles calculations," *Scientific Modeling and Simulation* **15** (2008) 81-95.
90. 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.
89. S. Suresh and J. Li, "Deformation of the ultra-strong," *Nature* **456** (2008) 716-717.
88. L. Qi, X-F. Qian and J. Li, "Near-neutrality of oxygen molecule adsorbed on Pt(111) surface," *Phys. Rev. Lett.* **101** (2008) 146101.
87. R.R. Unocic, G.B. Viswanathan, P.M. Sarosi, S. Karthikeyan, J. Li and M.J. Mills, "Mechanisms of creep deformation in polycrystalline Ni-base disk superalloys," *Mater. Sci. Eng. A* **483-484** (2008) 25-32.

86. J. Li, T.J. Lenosky, C.J. Först and S. Yip, "Thermochemical and Mechanical Stabilities of the Oxide Scale of ZrB<sub>2</sub>+SiC and Oxygen Transport Mechanisms," *J. Am. Ceram. Soc.* **91** (2008) 1475-1480.
85. Z. W. Shan, J. Li, Y. Q. Cheng, A. M. Minor, S. A. Syed Asif, O. L. Warren and E. Ma, "Plastic flow and failure resistance of metallic glass: Insight from *in situ* compression of nanopillars," *Phys. Rev. B* **77** (2008) 155419.
84. C. Shen, J. Li and Y-Z. Wang, "Finding Critical Nucleus in Solid-State Transformations," *Metall. Mater. Transactions A* **39** (2008) 976-983. "Editors' Choice" article.
83. H. Kimizuka, S. Ogata and J. Li, "Hydrostatic compression and high-pressure elastic constants of coesite silica," *J. Appl. Phys.* **103** (2008) 053506.
82. T. Zhu, J. Li, A. Samanta, A. Leach and K. Gall, "Temperature and Strain-Rate Dependence of Surface Dislocation Nucleation," *Phys. Rev. Lett.* **100** (2008) 025502. Cover article.
81. J. Eapen, J. Li and S. Yip, "Beyond the Maxwell limit: thermal conduction in nanofluids with percolating fluid structures," *Phys. Rev. E* **76** (2007) 062501.
80. H. Verweij, M. C. Schillo and J. Li, "Fast Mass Transport through Carbon Nanotube Membranes," *Small* **3** (2007) 1996-2004. Concepts article.
79. T.-L. Chan, Y. X. Yao, C. Z. Wang, W. C. Lu, J. Li, X. F. Qian, S. Yip and K. M. Ho, "Highly localized quasiatomic minimal basis orbitals for Mo from ab initio calculations," *Phys. Rev. B* **76** (2007) 205119.
78. F. Shimizu, S. Ogata and J. Li, "Theory of Shear Banding in Metallic Glasses and Molecular Dynamics Calculations," *Materials Transactions - JIM* **48** (2007) 2923-2927.
77. H. Kaburaki, J. Li, S. Yip and H. Kimizuka, "Dynamical thermal conductivity of argon crystal," *J. Appl. Phys.* **102** (2007) 043514.
76. H. Mori, S. Ogata, J. Li, S. Akita and Y. Nakayama, "Plastic bending and shape-memory effect of double-wall carbon nanotubes," *Phys. Rev. B* **76** (2007) 165405.
75. F. Liu, P.B. Ming and J. Li, "Ab initio calculation of ideal strength and phonon instability of graphene in tension," *Phys. Rev. B* **76** (2007) 064120.
74. J. Li, P. G. Kevrekidis, C. W. Gear and I. G. Kevrekidis, "Deciding the Nature of the Coarse Equation through Microscopic Simulations: The Baby-Bathwater Scheme," *SIAM Review* **49** (2007) 469-487.
73. E. Silva, C. Först, J. Li, X. Lin, T. Zhu and S. Yip, "Multiscale Materials Modeling: Case Studies at the Atomistic and Electronic Structure Levels," *Mathematical Modelling and Numerical Analysis* **41** (2007) 427-445.
72. Y.M. Wang, J. Li, A.V. Hamza and T.W. Barbee, Jr., "Ductile crystalline-amorphous nanolaminates," *PNAS* **104** (2007) 11155-11160.

71. A. C. Lawson, D. P. Butt, J. W. Richardson and J. Li, "Thermal expansion and atomic vibrations of zirconium carbide to 1600K," *Philos. Mag.* **87** (2007) 2507-2519.
70. T. Kadoyoshi, H. Kaburaki, F. Shimizu, H. Kimizuka, S. Jitsukawa and J. Li, "Molecular dynamics study on the formation of stacking fault tetrahedra and unfauling of Frank loops in fcc metals," *Acta Mater.* **55** (2007) 3073-3080.
69. J. Li, G. Lykotrafitis, M. Dao and S. Suresh, "Cytoskeletal Dynamics of Human Erythrocyte," *PNAS* **104** (2007) 4937-4942.
68. A. Gouldstone, N. Chollacoop, M. Dao, J. Li, A. Minor and Y.-L. Shen, "Indentation Across Size Scales and Disciplines: Recent Developments in Experimentation and Modeling," *Acta Mater.* **55** (2007) 4015-4039. Overview No. 142.
67. H. Kimizuka, S. Ogata, J. Li and Y. Shibutani, "Complete set of elastic constants of alpha-quartz at high pressure: A first-principles study," *Phys. Rev. B* **75** (2007) 054109.
66. T. Zhu, J. Li, A. Samanta, H.G. Kim and S. Suresh, "Interfacial Plasticity Governs Strain Rate Sensitivity and Ductility in Nanostructured Metals," *PNAS* **104** (2007) 3031-3036. Cover article.
65. J. Li, "The Mechanics and Physics of Defect Nucleation," *MRS Bulletin* **32** (2007) 151-159.
64. J. Eapen, J. Li and S. Yip, "Mechanism of thermal transport in dilute nanocolloids," *Phys. Rev. Lett.* **98** (2007) 028302.
63. H. Mori, S. Ogata, J. Li, S. Akita and Y. Nakayama, "Energetics of plastic bending of carbon nanotubes," *Phys. Rev. B* **74** (2006) 165418.
62. W.M. Zhu, D.E. Taylor, A.R. Al-Derzi, K. Runge, S.B. Trickey, T. Zhu, J. Li and S. Yip, "Encoding electronic structure information in potentials for multi-scale simulations: SiO<sub>2</sub>," *Comp. Mater. Sci.* **38** (2006) 340-349.
61. E.C.C.M. Silva, J. Li, D. Liao, S. Subramanian, T. Zhu and S. Yip, "Atomic scale chemomechanics of silica: nano-rod deformation and water reaction," *J. Computer-Aided Materials Design* **13** (2006) 135-159.
60. J. Li, "Spectral method for thermal conductivity calculations," *J. Computer-Aided Materials Design* **12** (2005) 141-159.
59. A. Samanta, T. Furuta and J. Li, "Theoretical assessment of the elastic constants and hydrogen storage capacity of some metal-organic framework materials," *J. Chem. Phys.* **125** (2006) 084714.
58. 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.
57. F. Shimizu, S. Ogata and J. Li, "Yield Point of Metallic Glass," *Acta Mater.* **54** (2006) 4293-4298.

56. C.-Z. Wang, J. Li, K.-M. Ho and S. Yip, "Undissociated screw dislocation in Si: glide or shuffle-set?" *Appl. Phys. Lett.* **89** (2006) 051910.
55. M. Dao, J. Li and S. Suresh, "Molecularly based analysis of deformation of spectrin network and human erythrocyte," *Mater. Sci. Eng. C* **26** (2006) 1232-1244.
54. A. Romano, J. Li and S. Yip, "Atomistic simulation of rapid compression of fractured silicon carbide," *J. Nucl. Mater.* **352** (2006) 22-28.
53. S. Ogata, F. Shimizu, J. Li, M. Wakeda and Y. Shibutani, "Atomistic Simulation of Shear Localization in Zr-Cu Bulk Metallic Glass," *Intermetallics* **14** (2006) 1033-1037.
52. X. Lin, J. Li, C. J. Först and S. Yip, "Multiple Self-Localized Electronic States in Trans-Polyacetylene," *PNAS* **103** (2006) 8943-8946.
51. A. Bongiorno, C.J. Först, R.K. Kalia, J. Li, J. Marschall, A. Nakano, M.M. Opeka, I.G. Talmy, P. Vashishta and S. Yip, "A Perspective on Modeling Materials in Extreme Environments: Oxidation of Ultra-High Temperature Ceramics," *MRS Bulletin* **31** (2006) 410-418.
50. T. Zhu, J. Li and S. Yip, "Atomistic characterization of three-dimensional lattice trapping barriers to brittle fracture," *Proc. R. Soc. A* **462** (2006) 1741-1761.
49. D.S. Xu, R. Yang, J. Li, J.P. Chang, H. Wang, D. Li and S. Yip, "Atomistic simulation of the influence of pressure on dislocation nucleation in bcc Mo," *Comp. Mater. Sci.* **36** (2006) 60-64.
48. X.-F. Qian, J. Li, X. Lin and S. Yip, "Time-dependent density functional theory with ultrasoft pseudopotentials: Real-time electron propagation across a molecular junction," *Phys. Rev. B* **73** (2006) 035408.
47. J. Eapen, J. Li and S. Yip, "Statistical Field Estimators for Multiscale Simulations," *Phys. Rev. E* **72** (2005) 056712.
46. X. Lin, J. Li and S. Yip, "Controlling Bending and Twisting of Conjugated Polymers via Solitons," *Phys. Rev. Lett.* **95** (2005) 198303.
45. Y. Umeno, A. Kushima, T. Kitamura, P. Gumbsch and J. Li, "Ab initio study of the surface properties and ideal strength of (100) silicon thin films," *Phys. Rev. B* **72** (2005) 165431.
44. T. Zhu, J. Li and S. Yip, "Nanomechanics of Crack Front Mobility," *J. Appl. Mech.* **72** (2005) 932-935.
43. S.V. Dmitriev, J. Li, N. Yoshikawa and Y. Shibutani, "Theoretical strength of 2D hexagonal crystals: application to bubble raft indentation," *Phil. Mag.* **85** (2005) 2177-2195.
42. S. Ogata, J. Li and S. Yip, "Energy landscape of deformation twinning in bcc and fcc metals," *Phys. Rev. B* **71** (2005) 224102.
41. T. Zhu, J. Li, X. Lin and S. Yip, "Stress-dependent molecular pathways of silica-water reaction," *J. Mech. Phys. Solids* **53** (2005) 1597-1623.

40. J. Li, M. Dao, C. T. Lim and S. Suresh, "Spectrin-level analysis of shape evolution and large deformation elasticity of erythrocyte," *Biophys. J.* **88** (2005) 3707-3719.
39. X. Lin, J. Li, E. Smela and S. Yip, "Polaron-induced conformation change in single polypyrrole chain: an intrinsic actuation mechanism," *Int. J. Quantum Chem.* **102** (2005) 980-985.
38. S.V. Dmitriev, J. Li, N. Yoshikawa, Y. Tanaka, Y. Kagawa, T. Kitamura and S. Yip, "Breaking atomic bonds through vibrational mode localization," *Defect and Diffusion Forum* **233-234** (2004) 49-60.
37. S.V. Dmitriev, T. Kitamura, J. Li, Y. Umeno, K. Yashiro and N. Yoshikawa, "Near-surface lattice instability in 2D fiber and half-space," *Acta Mater.* **53** (2005) 1215-1224.
36. D.-S. Xu, J.-P. Chang, J. Li, R. Yang, D. Li and S. Yip, "Dislocation slip or deformation twinning: confining pressure makes a difference," *Mater. Sci. Eng. A* **387** (2004) 840-844.
35. T. Zhu, J. Li and S. Yip, "Atomistic configurations and energetics of crack extension in silicon," *Phys. Rev. Lett.* **93** (2004) 205504.
34. S. Ogata, J. Li and S. Yip, "Twinning pathway in BCC molybdenum," *Europhys. Lett.* **68** (2004) 405-411.
33. J. Li, C.-Z. Wang, J.-P. Chang, W. Cai, V.V. Bulatov, K.-M. Ho and S. Yip, "Core energy and Peierls stress of a screw dislocation in bcc molybdenum: A periodic-cell tight-binding study," *Phys. Rev. B* **70** (2004) 104113.
32. S. Ogata, J. Li, N. Hirosaki, Y. Shibutani and S. Yip, "Ideal shear strain of metals and ceramics," *Phys. Rev. B* **70** (2004) 104104.
31. H. Kimizuka, H. Kaburaki, F. Shimizu and J. Li, "Crack-tip dislocation nanostructures in dynamical fracture of fcc metals: A molecular dynamics study," *J. Computer-Aided Materials Design* **10** (2003) 143-154. (printed in 2004).
30. R.D. Boyer, J. Li, S. Ogata and S. Yip, "Analysis of shear deformations in Al and Cu: empirical potentials versus density functional theory," *Modelling Simul. Mater. Sci. Eng.* **12** (2004) 1017-1029.
29. T. Zhu, J. Li and S. Yip, "Atomistic study of dislocation loop emission from a crack tip," *Phys. Rev. Lett.* **93** (2004) 025503.
28. J. Li, "Transformation strain by chemical disordering in silicon carbide," *J. Appl. Phys.* **95** (2004) 6466-6469.
27. T. Zhu, J. Li, K.J. Van Vliet, S. Ogata, S. Yip and S. Suresh, "Predictive modeling of nanoindentation-induced homogeneous dislocation nucleation in copper," *J. Mech. Phys. Solids* **52** (2004) 691-724.
26. J. Li, T. Zhu, S. Yip, K.J. Van Vliet and S. Suresh, "Elastic criterion for dislocation nucleation," *Mater. Sci. Eng. A* **365** (2004) 25-30.

25. Y. Choi, K.J. Van Vliet, J. Li and S. Suresh, "Size effects on the onset of plastic deformation during nanoindentation of thin films and patterned lines," *J. Appl. Phys.* **94** (2003) 6050-8.
24. J. Li, A.H.W. Ngan and P. Gumbsch, "Atomistic modeling of mechanical behavior," *Acta Mater.* (Golden Jubilee Issue) **51** (2003) 5711-42.
23. N.H. de Leeuw, Z.M. Du, J. Li, S. Yip and T. Zhu, "Computer modeling study of the effect of hydration on the stability of a silica nanotube," *Nano Letters* **3** (2003) 1347-52.
22. C.W. Gear, J. Li and I.G. Kevrekidis, "The gap-tooth method in particle simulations," *Physics Letters A* **316** (2003) 190-5.
21. T. Zhu, J. Li, S. Yip, R.J. Bartlett, S.B. Trickey and N.H. de Leeuw, "Deformation and fracture of a SiO<sub>2</sub> nanorod," *Molecular Simulation* **29** (2003) 671-6.
20. J. Li, P.G. Kevrekidis, C.W. Gear and I.G. Kevrekidis, "Deciding the nature of the coarse equation through microscopic simulations: the baby-bathwater scheme," *Multiscale Modeling and Simulation* **1** (2003) 391-407.
19. J. Li and S. Yip, "Response to Comment on Theoretical evaluation of hydrogen storage capacity in pure carbon nanostructures," *J. Chem. Phys.* **120** (2004) 9430-9432.
18. J. Li, T. Furuta, H. Goto, T. Ohashi, Y. Fujiwara and S. Yip, "Theoretical evaluation of hydrogen storage capacity in pure carbon nanostructures," *J. Chem. Phys.* **119** (2003) 2376-85.
17. J. Li, D.Y. Liao, S. Yip, R. Najafabadi and L. Ecker, "Force-based many-body interatomic potential for ZrC," *J. Appl. Phys.* **93** (2003) 9072-85.
16. K.J. Van Vliet, J. Li, T. Zhu, S. Yip and S. Suresh, "Quantifying the early stages of plasticity through nanoscale experiments and simulations," *Phys. Rev. B* **67** (2003) 104105.
15. W. Cai, V.V. Bulatov, J.-P. Chang, J. Li and S. Yip, "Periodic image effects in dislocation modelling," *Phil. Mag.* **83** (2003) 539-67.
14. J. Li, "AtomEye: an efficient atomistic configuration viewer," *Modelling Simul. Mater. Sci. Eng.* **11** (2003) 173-7.
13. S. Ogata, J. Li and S. Yip, "Ideal pure shear strength of aluminum and copper," *Science* **298** (2002) 807-11.
12. J. Li, K.J. Van Vliet, T. Zhu, S. Yip and S. Suresh, "Atomistic mechanism governing elastic limit and incipient plasticity in crystals," *Nature* **418** (2002) 307-10.
11. J. Li and S. Yip, "Atomistic measures of materials strength," *Computer Modeling in Engineering & Sciences* **3** (2002) 219-227.
10. A. Romano, J. Li and S. Yip, "Atomistic simulation of matter under stress: cross-over from hard to soft materials," *Physica A* **304** (2002) 11-22.

9. S. Yip, J. Li, M. Tang and J. Wang, "Mechanistic aspects and atomic-level consequences of elastic instabilities in homogeneous crystals," *Mater. Sci. Eng. A* **317** (2001) 236-40.
8. W. Cai, V.V. Bulatov, J.-P. Chang, J. Li and S. Yip, "Anisotropic elastic interactions of a periodic dislocation array," *Phys. Rev. Lett.* **86** (2001) 5727-30.
7. J. Li, D.Y. Liao and S. Yip, "Nearly exact solution for coupled continuum/MD fluid simulation," *J. Computer-Aided Materials Design* **6** (1999) 95-102.
6. J. Li, L.J. Porter and S. Yip, "Atomistic modeling of finite-temperature properties of crystalline  $\beta$ -SiC: II. thermal conductivity and effects of point defects," *J. Nucl. Mater.* **255** (1998) 139-52.
5. J. Li, D.Y. Liao and S. Yip, "Coupling continuum to molecular-dynamics simulation: reflecting particle method and the field estimator," *Phys. Rev. E* **57** (1998) 7259-67.
4. J. Li and S. Yip, "Order-N method to calculate the local density of states," *Phys. Rev. B* **56** (1997) 3524-7.
3. L.J. Porter, J. Li and S. Yip, "Atomistic modeling of finite-temperature properties of  $\beta$ -SiC: I. lattice vibrations, heat capacity, and thermal expansion," *J. Nucl. Mater.* **246** (1997) 53-9.
2. J.H. Wang, J. Li, S. Yip, S. Phillpot and D. Wolf, "Unifying two criteria of Born: elastic instability and melting of homogeneous crystals," *Physica A* **240** (1997) 396-403.
1. J.H. Wang, J. Li, S. Yip, S. Phillpot and D. Wolf, "Mechanical instabilities of homogeneous crystals," *Phys. Rev. B* **52** (1995) 12627-35.

### Conference Proceeding Papers

16. H. Kaburaki, J. Li, S. Yip and H. Kimizuka, "Dynamical Behavior of Heat Conduction in Solid Argon," 11th Granada Seminar on Computational and Statistical Physics in La Heradura, Spain, September 13-17, 2010.
15. R.R. Unocic, L. Kovarik, C. Shen, P.M. Sarosi, Y.Z. Wang, J. Li, S. Ghosh and M.J. Mills, "Deformation Mechanisms in Ni-Base Disk Superalloys at Higher Temperatures," in *Superalloys 2008*, 11th International Symposium on Superalloys, September 14-18, 2008, Champion, Pennsylvania, USA, edited by Roger C. Reed, Kenneth A. Green, Pierre Caron, Timothy P. Gabb, Michael G. Fahrman, Eric S. Huron, and Shiela A. Woodard, p. 377-386.
14. C. Shen, J. Li, M.J. Mills and Y. Wang, "Modeling shearing of gamma prime in Ni-based superalloys," in *Integral Materials Modeling: Towards Physics-Based Through-Process Models*, ed. G. Gottstein (Wiley-VCH, Heidelberg, 2007), pp. 243-252. ISBN: 3527317112.
13. F. Shimizu, S. Ogata, H. Kimizuka, T. Kano, J. Li and H. Kaburaki, "First-principles Calculation on Screw Dislocation Core Properties in BCC Molybdenum," *Journal of the Earth Simulator* **7** (2007) 17-21.

12. A. J. H. McGaughey and J. Li, “Molecular dynamics prediction of the thermal resistance of solid-solid interfaces in superlattices,” ASME publications HTD (Heat Transfer Division) vol. **377** (2006) part 1, pages 315-324. IMECE2006-13590.
11. J. Eapen, J. Li and S. Yip, “Probing transport mechanism in nanofluids by molecular dynamics simulations,” 7th ISHMT-ASME Heat and Mass Transfer Conference at Indian Institute of Technology Guwahati, January 4-6, 2006.
10. I.G. Kevrekidis, J. Li and S. Yip, “Nonlinear dynamics analysis through molecular dynamics simulations,” *Multiscale Modelling and Simulation*, eds. S. Attinger and P. Koumoutsakos, Lecture Notes in Computational Science and Engineering, vol. **39** (Springer, Berlin, 2004). ISBN: 3540211802.
9. S. Ogata, J. Li, Y. Shibutani and S. Yip, “Ab initio study of ideal shear strength,” *IUTAM Symposium on Mesoscopic Dynamics of Fracture Process and Materials Strength*, eds. H. Kitagawa and Y. Shibutani, Solid Mechanics and Its Applications **115** (Kluwer, Dordrecht, 2004). ISBN: 1402020376.
8. J.-P. Chang, T. Zhu, J. Li, X. Lin, X.-F. Qian and S. Yip, “Multiscale modeling of defect nucleation and reaction: bulk to nanostructures,” *IUTAM Symposium on Mesoscopic Dynamics of Fracture Process and Materials Strength*, eds. H. Kitagawa and Y. Shibutani, Solid Mechanics and Its Applications **115** (Kluwer, Dordrecht, 2004), pp. 223-233. ISBN: 1402020376.
7. Shuhong Xu, Ju Li, Chonghe Li and Frank Chan, “Immersive visualisation of nano-indentation simulation of Cu,” *Recent Advances in Computational Science and Engineering*, eds. H.P. Lee and K. Kumar, Proceedings of the International Conference on Scientific and Engineering Computation (IC-SEC) 2002 (World Scientific, Singapore, 2003). ISBN: 1860943454.
6. J. Li, W. Cai, J. Chang and S. Yip, “Commentary on atomistic simulations of materials strength and deformation: prospects for mechanistic insights,” in Proceedings of International Symposia on Materials Science for the 21th Century (ISMS-21), vol. A (The Society of Materials Science, Japan, Suita, Japan, 2001), p. 220-233.
5. S. Yip, J. Li, W. Cai, J.-P. Chang and D.Y. Liao, “Atomistic measures of mechanical deformation and thermal transport processes,” in *Computational Fluid and Solid Mechanics : Proceedings, First MIT Conference on Computational Fluid and Solid Mechanics, June 12-15, 2001*, ed. K. J. Bathe (Elsevier, New York, 2001). ISBN: 0080439446.
4. J. Li, D.Y. Liao and S. Yip, “Optimal particle controller for coupled continuum/MD fluid simulation,” in *Computational Fluid and Solid Mechanics : Proceedings, First MIT Conference on Computational Fluid and Solid Mechanics, June 12-15, 2001*, ed. K. J. Bathe (Elsevier, New York, 2001). ISBN: 0080439446.
3. F. Shimizu, H. Kimizuka, H. Kaburaki, J. Li and S. Yip, “Parallel molecular dynamics simulation on elastic properties of solid argon,” *SNA 2000*. Proceedings of the Fourth International Conference on Supercomputing in Nuclear Applications, September 4-7, 2000, Tokyo, Japan.



2. H. Kaburaki, J. Li and S. Yip, "Thermal conductivity of solid argon by classical molecular dynamics," *Mater. Res. Soc. Symp. Proc.* **538** (1999) 503-8.
1. J. Li, D.Y. Liao and S. Yip, "Imposing field boundary conditions in MD simulation of fluids: optimal particle controller and buffer zone feedback," *Mater. Res. Soc. Symp. Proc.* **538** (1999) 473-8.

### Book Chapters, Reviews and Monographs

7. W. Cai, J. Li and S. Yip, "Molecular Dynamics," in *Comprehensive Nuclear Materials*, edited by R.J.M. Konings (Elsevier, Amsterdam, 2012), vol. 1, p. 249-265. ISBN: 9780080560335.
6. T. Zhu, J. Li and S. Yip, "Atomistic Reaction Pathway Sampling: The Nudged Elastic Band Method and Nanomechanics Applications," in *Nano and Cell Mechanics: Fundamentals and Frontiers*, edited by Horacio D. Espinosa and Gang Bao (Wiley, 2013), Chap. 12, p. 313-338. ISBN: 9781118460399.
5. J. Li, "Atomistic visualization," Chap. 2.31 in *Handbook of Materials Modeling*, ed. S. Yip (Springer, Dordrecht, 2005), pp. 1051-1068. ISBN: 1402032870. Mistake free version at <http://alum.mit.edu/www/liju99/Papers/05/Li05-2.31.pdf>
4. J. Li, "Atomistic calculation of mechanical behavior," Chap. 2.19 in *Handbook of Materials Modeling*, ed. S. Yip (Springer, Dordrecht, 2005), pp. 773-792. ISBN: 1402032870. Mistake free version at <http://alum.mit.edu/www/liju99/Papers/05/Li05-2.19.pdf>
3. J. Li, "Basic molecular dynamics," Chap. 2.8 in *Handbook of Materials Modeling*, ed. S. Yip (Springer, Dordrecht, 2005), pp. 565-588. ISBN: 1402032870. Mistake free version at <http://alum.mit.edu/www/liju99/Papers/05/Li05-2.8.pdf>
2. W. Cai, V.V. Bulatov, J.-P. Chang, J. Li and S. Yip, "Dislocation Core Effects on Mobility," in *Dislocations in Solids* vol. **12**, eds. F.R.N. Nabarro and J.P. Hirth (Elsevier, Amsterdam, 2004), chap 64, pp. 1-80. ISBN: 044451483X.
1. J. Li, W. Cai, J.-P. Chang and S. Yip, "Atomistic Measures of Materials Strength and Deformation," in *Computational Materials Science*, ed. C.R.A. Catlow and E.A. Kotomin (IOS Press, Amsterdam, 2003), pp. 359-387. NATO Science Series, Series III: Computer and Systems Sciences **187**. ISBN: 1586033352.

### Research Grants

49. "Determination of Molecular Structure and Dynamics of Molten Salts by Advanced Neutron and X-ray Scattering Measurements and Computer Modeling," \$, USDOE Nuclear Energy University Program (NEUP) Reactor Concepts Research Development and Demonstration (PI: Boris Khaykovich, MIT, project total: \$800,000), 10/01/2018 - 09/30/2021.

48. "Blueprint for design and assembly of multifunctional, adaptive materials using the nanocrystal periodic table," \$435,000, Office of Naval Research MURI (PI: Christopher B. Murray, University of Pennsylvania, project total: \$), 06/01/2018 - 05/31/2021.
47. "Low-temperature Electrochemical Activation of Ethane for Co-production of Chemicals/Fuels and Hydrogen," \$150,000, USDOE EERE (PI: Dong Ding, Idaho National Laboratory, project total: \$), 05/01/2018 - 09/30/2019.
46. "Grid-scale Energy Storage with New Battery Formulations," \$375,000, General Electric Company, 04/01/2018 - 08/14/2021.
45. "Resolving and eliminating precursors to failure of coatings against corrosion," \$421,376, The Dow Chemical Company through the MIT Energy Initiative (PI: Bilge Yildiz, MIT, project total: \$1,264,128), 11/15/2017 - 11/14/2020.
44. "New Developments in Electrochemical Energy Systems," \$41,640+\$249,840, Wuxi Weifu High-Technology Group, 8/1/2017 - 12/31/2019.
43. "Modeling porous media impedance spectra," \$50,000, Idaho National Lab and Battelle Energy Alliance, LLC, 08/09/2017 - 09/30/2018.
42. "New phase change materials for photonics: from in-silico design to novel device concepts," \$435,000, Office of Naval Research MURI (PI: Ritesh Agarwal, University of Pennsylvania, project total: \$3,000,000), 8/1/2017 - 7/31/2020.
41. "Lithium-Sulfur Batteries," Samsung Advanced Institute of Technology, \$400,000, 08/01/2016 - 07/31/2018.
40. "Machine Learning Elastic Strain Engineering," Skolkovo Institute of Science and Technology, \$332,905, 12/01/2016 - 11/30/2019.
39. "LCEC Materials - Two-prong Approach to Making Steel Surfaces Hydrogen-repellent: Electrochemical Pumping and Hydrogen Resistant Coatings," \$655,071, Exelon Corporation through the MIT Energy Initiative (PI: Bilge Yildiz, MIT, project total: \$1,965,213), 10/01/2016 - 09/30/2019.
38. "Collaborative Research: Electrochemically driven Mechanical Energy Harvesting," NSF ECCS-1610806 (\$270,000, Ju Li) and DMR-1610331 (\$180,000, Sulin Zhang, Penn State), July 15, 2016 - June 30, 2019.
37. "MIT-Harvard Center for Excitonics: 2D metal-organic frameworks," Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Basic Energy Sciences under award no. DE-SC0001088, April 1, 2015 - present.
36. "Collaborative Research: Design of Low-Hysteresis High-Susceptibility Materials by Nanodomain Engineering," NSF DMR-1410636 (\$300,000, Ju Li) and DMR-1410322 (\$307,851, Yunzhi Wang, Ohio State), Division of Materials Research, Condensed Matter & Materials Theory, National Science Foundation, September 1, 2014 - August 31, 2017.

35. "Atomistic Modeling of White Etch Area/Cracking of Steels," Timken (project total: \$250,000), 1/1/2014 - 12/31/2015.
34. "Thermo-mechanical Optimization of Thorium-based Fuel Systems," Lockheed Martin Corporation (PI: Mujid S. Kazimi, MIT, project total: \$300,000), 4/1/2013 - 9/30/2014.
33. "A novel design for Lithium-ion Nanobattery," Kuwait-MIT Center for Natural Resources and the Environment, April 1, 2013 - March 31, 2015, \$200,000.
32. "Skoltech Strategic Development Project in Nuclear Systems and Materials," Skolkovo Foundation, 01/01/2013 - 12/31/2014, \$1,200,000. (with Michael W. Golay, Ronald G. Ballinger, Emilio Baglietto)
31. "In-situ TEM observation of the positive electrode reactions of Li-air battery," Honda R&D Co., Ltd., Japan, \$263,000, Oct.1, 2012 - Sept.30, 2014.
30. "Computational Study of the Feasibility of Nanotwinning in Titanium," Honda R&D Co., Ltd., Japan, \$270,000, Oct. 1, 2012 to March 31, 2015.
29. "Collaborative Research: Developing A Complete Membrane-Cytoskeleton Model for Human Erythrocyte," NSF CBET-1066469/CBET-1240696 (\$220,000, Ju Li) and CBET-1067523 (\$240,000, Sulin Zhang, Penn State), Division of Chemical, Bioengineering, Environmental, and Transport Systems (CBET), National Science Foundation, August 1, 2011 - July 31, 2014.
28. "Finding optimal combinations of electrode, electrolyte and operating condition for high-performance Li-ion batteries," Honda R&D Co., Ltd., Japan, 09/01/2011-08/31/2014, \$562,500.
27. "Modeling Nanowire Growth and Electrical Conduction," Honda R&D Co., Ltd., Japan, 08/01/2011-07/31/2013, \$300,000.
26. "IRG-3: Mechanical Failure in Disordered Packings," Penn CEMRI (Center of Excellence for Materials Research and Innovation), \$360,000 (PI: Arjun Yodh, University of Pennsylvania, \$21,180,000, NSF DMR-1120901, 09/15/2011 - 08/31/2017).
25. "Modeling Creep-Fatigue-Environment Interactions in Steam Turbine Rotor Materials for Advanced Ultrasupercritical Coal Power Plants," Department of Energy, 12/1/2010-11/30/2013, \$220,000 (PI: Liang Jiang, General Electric Global Research, project total: \$1,199,940 + \$299,988 GE cost share).
24. "Materials World Network: Collaborative Research: Modeling Ferroelastic Strain Glasses," DMR-1008349 (\$309,000, Yunzhi Wang) and DMR-1008104/DMR-1240933 (\$288,000, Ju Li), Condensed Matter and Materials Theory (CMMT), National Science Foundation, 9/15/2010-08/31/2014.
23. "Modeling Microscopic Damage in Hydrogen Embrittlement," ExxonMobil Research & Engineering Company, 5/15/2010-5/14/2011, \$155,000.

22. "Modeling Nanowire Growth and Electrical Conduction," Honda R&D Co., Ltd., Japan, 04/15/2010-04/14/2013, \$450,000.
21. Penn MRSEC (Materials Research Science and Engineering Center) seed grant, 1/1/2010, \$7,500 (PI: Arjun Yodh, University of Pennsylvania, \$20,052,603, NSF DMR-0520020, 10/1/2005 - 9/30/2011).
20. "Metamaterials: a computational alchemy approach," Honda Research Institute of America, 1/1/2008-12/31/2010, \$341,609.
19. "Modeling-assisted new catalyst discovery - phase III," Honda Research Institute of America, 1/1/2008-12/31/2010, \$436,774.
18. "AHSS: Multi-scale Modeling of Deformation Mechanism for Design of New Generation of Steels," NSF CMMI - Mechanics & Structure of Materials (award number CMMI-0728069), 6/1/2008-5/31/2012, \$430,000. (PI: Ju Li, \$215,000; Co-PI: Yunzhi Wang, Ohio State University, \$215,000). A supplemental funding of \$181,421 was approved on Sept. 30, 2011, making the total award \$611,421.
17. "Atomistic and First-Principles Modeling of Materials under Extreme Environments," Idaho National Laboratory LDRD (award number TM105), 12/26/06-12/27/09, \$254,850 (PI: Paul Meakin, Idaho National Laboratory, project total: \$405,000).
16. "First-principles modeling of mechanics and chemistry of materials," Presidential Early Career Award for Scientists and Engineers (PECASE), Department of Defense / Air Force Office of Scientific Research (award number FA9550-07-1-0007, FA9550-08-1-0325), 12/01/06 - 11/30/11, \$500,000.
15. "First-principles modeling of phonon heat conduction in nanoscale crystalline structures," Department of Energy Basic Energy Sciences (award number DE-FG02-06ER46330), 9/1/06-08/31/09, approximately \$150,000 (PI: Sandip Mazumder, Department of Mechanical Engineering, OSU, project total: \$330,000).
14. "University computational materials consortium - ab-initio and atomistic modeling of solute and impurity effects on the fracture toughness of Ni-Fe alloys," Department of Energy National Energy Technology Laboratory DE-AM26-04NT41817, 1/9/06-12/31/06, \$68,500 (PI: David S. Sholl, Carnegie Mellon University, project total: \$342,500).
13. "Metallurgical Research Fund (MRF)," ExxonMobil Research & Engineering Company, \$15,000 (12/15/05) + \$15,000 (01/25/06) + \$25,000 (03/19/08) + \$20,000 (04/29/09).
12. "Multi-scale Analysis of Cellular Force Transmission and Biochemical Activation," National Institutes of Health (award number 1-R01-GM-076689-01), 09/01/05-08/31/08, consultant charging 1-month summer salary (PI: Roger D. Kamm, MIT, project total: \$1,098,263).
11. "Ab-initio modeling of metal-organic frameworks," Honda R&D Co., Ltd., Japan, 04/15/05-04/14/06, \$22,219.

10. "Nanomeso: A NSF-EC Cooperative Activity in Computational Research to Study Nano/Meso Length Scale Effects on Crystal Plasticity," National Science Foundation (award number DMR-0502711), 06/15/05-06/14/08, approximately \$140,000 (PI: Peter M. Anderson, OSU, project total: \$546,000).
9. "Modeling-assisted new catalyst discovery - phase II," Honda Research Institute of America, 01/01/05-12/31/07, \$547,801.
8. "Defense University Research Initiative on NanoTechnology (DURINT): Damage-resistant and failure-resistant nanostructures and interfacial materials," Office of Naval Research, \$15,000 administrated by Nitin P. Padture, 05/01/05- (PI: Subra Suresh, MIT).
7. "Experimental and Computational Tools for the Digital Representation and Prediction of Microstructure and its Incorporation in the Designer's Knowledge Base," Office of Naval Research (award number N00014-05-1-0504), 05/01/05-04/30/10, approximately \$400,000 (PI: Hamish L. Fraser, OSU, project total: \$5,553,111).
6. "Materials Engineering for Affordable New Systems II (MEANS2): Development of Microstructure- and Micromechanism-Sensitive Property Models and Their Integration Into the Design of Advanced Disk and Blade Systems", Air Force Office of Scientific Research (award number FA9550-05-1-0135), 02/15/05-10/31/07, approximately \$100,000 (PI: Michael J. Mills, OSU, project total: \$1,100,000).
5. "Molecular Modeling of High-Temperature Oxidation of Refractory Borides", Air Force Office of Scientific Research (award number FA9550-05-1-0026), 11/15/04-11/14/07, \$256,268.
4. "NER: Hydrogen in Carbon Nanotubes - NMR and Multiscale Simulations," National Science Foundation (award number 0403809), 07/01/04-06/30/05, \$15,000 (PI: David Cory, MIT, project total: \$100,000).
3. "MOF Modeling Fund (MMF)," Honda Research Institute USA, Inc., 06/01/04-12/31/04, \$20,000.
2. "Computational Research Fund (CRF)," Honda Research Institute USA, Inc., \$50,000 (05/01/04) + \$52,199 (03/18/05) + \$20,000 (03/22/06) + \$20,000 (06/07/06) + \$40,000 (09/26/2008).
1. "Modeling-assisted new catalyst discovery - phase I," Honda R&D Co., Ltd., Japan, 01/01/03-12/31/04, \$298,418.

## Other Grants

9. 2,000,000 CPU hours on TACC Dell PowerEdge C8220 Cluster with Intel Xeon Phi coprocessors (Stampede), National Science Foundation Extreme Science and Engineering Discovery Environment (XSEDE), "First-principles investigation of materials for solar cells and lithium-ion batteries," Apr 01, 2013 - Apr 01, 2014 (with Kejie Zhao).

8. Department of Energy user proposal “Patterning Multiple Layers of Graphene”, with Dr. Jianyu Huang, Center for Integrated Nanotechnologies (CINT) operated by Los Alamos National Laboratory and Sandia National Laboratories, Albuquerque, New Mexico (CINT User project number RA2009A029 and C2010B1042), Aug. 27, 2009 - June 30, 2012.
7. \$17,036 from National Science Foundation (award number 0714540) to organize an International Workshop on Strength and Plasticity at Nanometer and Sub-Micron Scales, Braunschweig, Switzerland; September 4-7, 2007. (PI: Peter M. Anderson).
6. \$1,000 NSF travel grant to attend 210th Meeting of The Electrochemical Society in Cancun, Mexico, October 29-November 3, 2006.
5. Major Grant of 30,000 RUs (Nov. 14, 2005) + 30,000 RUs (July 13, 2007) + 30,000 RUs (June 1, 2009) (1 Resource Unit = 20 dedicated CPU hours on 2.4 GHz Xeon, cash equivalent: \$5) from Ohio Supercomputer Center (award number PAS0167), “Materials Design for Aero-Propulsion, Fuel Cells and Advanced Energy Storage”.
4. \$27,044 from Air Force Office of Scientific Research (award number FA9550-05-1-0446) to organize a Workshop on Modeling Materials in Extreme Environment, Sept. 24-25, 2005, Washington D.C.
3. Travel grant from American Chemical Society Petroleum Research Fund to attend the Time-Dependent Density-Functional Theory and the Dynamics of Complex Systems (TDDFT 2004) Summer School in Santa Fe, NM, June 5-10, 2004.
2. Initiated and mediated a \$25,000 donation (03/01/04) from Honda Research Institute USA, Inc. to establish the HRI-USA Scholarship at Dept. Materials Science and Engineering.
1. With W. Windl and Y. Wang: “Highly parallel multiscale modeling suite for the simulation of real materials,” 52-CPU Myrinet Beowulf cluster (Cluster Ohio Rev. 3) equipment grant from Ohio Supercomputer Center, hardware worth ~\$100,000, Feb. 4, 2004.

### **Projects Participated as Graduate Student and Post-doc at MIT**

9. Modeling molecular actuation in conducting polymers (2002-2004, sponsored by Honda R&D, Inc.)
8. Theoretical analysis of conductance of molecular junctions (2002-2004, sponsored by the Office of Naval Research / Defense Advanced Research Projects Agency).
7. Defense University Research Initiative on NanoTechnology (DURINT): Damage-resistant and failure-resistant nanostructures and interfacial materials (2001-2005, sponsored by the Office of Naval Research).
6. First-principles theoretical evaluation of hydrogen storage capacity of carbon nanotubes (2000-2002, sponsored by the Honda Motor Company).

5. Construction of a many-body interatomic potential for  $ZrC_X$  starting from first principles, then compute its thermal conductivity (1999-2000, sponsored by the Knolls Atomic Power Laboratory).
4. Strengths of crystalline/amorphous/nanocrystalline materials with applications to SiC fiber matrix composites (1996-2002, sponsored by the Air Force Office of Scientific Research).
3. Multiscale techniques to couple continuum PDE with molecular dynamics in MEMS micro-channel flow modeling (1996-1998, sponsored by the Sandia National Laboratory).
2. Calculation of the lattice thermal conductivity of SiC before and after irradiation (1995-1997, sponsored by the Knolls Atomic Power Laboratory).
1. Molecular dynamics study of water and ice (1994-1995, sponsored by the American Chemical Society Petroleum Research Fund).