

## 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 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 Sergeyevech Baldychev (Penn CBE, 2011), Tingting Qi (Penn Chemistry, 2011), Miguel Angel Mendez Polanco (Penn Chemistry), Kevin Bakhmutsky (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, Washington, 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.

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

Ab initio tight-binding analysis with quasiautomatic orbitals (with Xiaofeng Qian):  
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### Issued Patents

2. Mar 14, 2017: US Patent 9595624 “Strain-engineered bandgaps,” Ju Li, Xiaofeng Qian, Ji Feng.
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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.
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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



45. "Resolving and eliminating precursors to failure of coatings against corrosion," \$316,032, 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," \$195,000, Office of Naval Research MURI (PI: Ritesh Agarwal, University of Pennsylvania, project total: \$3,000,000), 7/31/2017 - 7/30/2022.
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).