Curriculum Vitae

Qiang Cui
Department of Chemistry
Boston University
590 Commonwealth Avenue, Boston, MA 02215
E-mail: qiangcui@bu.edu

Personal

Date and place of birth: 1975, Beijing, P. R. China

Employment

Boston University

Professor of Chemistry, Jan. 2018-

University of Wisconsin, Madison

Professor of Chemistry, Jul. 2010-Dec. 2017; Associate Professor of Chemistry, Jul. 2007-Jun. 2010; Assistant Professor of Chemistry, Aug. 2001-Jun. 2007

Education

Postdoctoral fellow, Oct. 1997- Jul. 2001

Harvard University, Boston, MA Advisor: Martin Karplus

Ph.D. Physical Chemistry, Sept. 1997

Emory University, Atlanta, GA Advisor: Keiji Morokuma

Thesis: Theoretical studies of molecular processes

B. S. Chemical Physics, Jul. 1993

University of Science and Technology of China (USTC), Hefei, Anhui, P. R. China

Awards, Honors and Service

- Kellet Mid-Career Award, UW-Madison (2016-2021)
- Secretary and Treasurer, Physical Chemistry Division (2018-present) Chair, Biophysics subdivision, Physical Chemistry Division, American Chemical Society (2015-2017)
- Vilas Associate, UW-Madison (2014-2016)
- CAPA (Chinese-American Chemistry & Chemical Biology Professors Association) Distinguished Faculty Award, 2010
- H. Romnes Fellow, UW-Madison, 2010-2015
- Member, *Faculty of 1000*, 2008-present
- Editorial Board Member, *Journal of Theoretical and Computational Chemistry*, 2007-2014; Chemical Physics Lett.; 2016-present; *Interdisciplinary Sciences – Computational Life Sciences*, 2008-present; *Journal of Physical Chemistry, B*, 2012-2015; 2018-present; Specialist Editor, Comp. Phys. Comm. 2013-present
- Alfred P. Sloan Research Fellowship, 2004.
- CAREER Award, National Science Foundation, 2004-2009.
- Research Innovation Award, Research Corporation, 2003-2005.
- Graduate student fellowship, Phillips Petroleum Co. 1994 — 1997.
- Lester Award, Department of Chemistry, Emory University, 1996.

- Osborn R. Quayle Award, Department of Chemistry, Emory University, 1995.
- Outstanding student scholarship, USTC, 1989, 1992.

Professional Affiliations

American Physical Society, American Chemical Society, Biophysics Society, American Association for the Advancement of Science, Alpha Phi Simga

Invited University/Institute seminars and Conference presentations (2002-present)

2018 (17)

Dec.	*Computational and Mathematical Approaches for Bioinformatics and Biophysics*	*Sanya, China*
Nov.	*QM/MM workshop*	*Wako, Japan*
Oct.	*CECAM Workshop on Allostery*	*Lugao, Switzerland*
Oct.	*PKU/BU/UW-Madison theoretical chemistry symposium*	*Beijing, China*
Sept.	*CECAM Workshop on structural transitions of proteins*	*Paris, France*
Jul.	*Telluride workshop on Coarse-graining*	*Telluride, CO*
Jul.	*ISRIUM conference*	*Ascona, Switzerland*
Jul.	*CECAM Workshop on Metalloenzymes*	*Lugano, Switzerland*
Jul.	*Telluride workshop on proton transfers*	*Telluride, CO*
Jun.	*Protein Electrostatics*	*Belgrade, Serbia*
Jun.	*Worldwide Chinese Computational Biology & Molecular Simulation Conference*	
Apr.	*Southern Methodist University*	*Dallas, TX*
Apr.	*Brandies University*	*Waltham, MA*
Apr.	*Harvard/MIT/BU seminar*	*Boston, MA*
Mar.	*Japanese Chemical Society Annual Meeting*	*Funabashi, Japan*
Mar.	*ACS National Meeting*	*New Orleans, LA*
Feb.	*Sanibel Symposium*	*St. Simons, GA*

2017 (10)

Nov.	*Castle Reisensburg Electrochemistry workshop*	*Ulm, Germany*
Sept.	*MGM meeting*	*Manchester, UK*
Aug.	*WATOC2017*	*Munich, Germany*
Aug.	*ACS National Meeting*	*Washington DC*
Jul.	*ACTC2017*	*Boston, MA*
Jun.	*Telluride workshop on Protein Electrostatics (cancelled)*	*Telluride, CO*
Jun.	*CECAM workshop on Nano/Bio interface*	*Bremen, Germany*
Apr.	*ACS National Meeting (cancelled)*	*San Francesco, CA*
Mar.	*Department of Chemistry, Boston University*	*Boston, MA*
Feb.	*CECAM workshop on multi-scale simulations (cancelled)*	*Vienna, Austria*

2016 (14)

Dec.	*Theoretical Chemistry Conference (cancelled)*	*India*
Nov.	*DFTB Developer Meeting (cancelled)*	*Beijing*
Oct.	*Bilaterial Conference on Theoretical Chemistry (cancelled)*	*Changsha, China*
Aug.	*ACS National Meeting*	*Philadelphia, PA*
Jul.	*GRC in Comp. Chem.*	*Girona, Spain*

Jul.	*Protein Electrostatics*	*Berlin, Germany*
Jul.	*Telluride workshop on proton transfers*	*Telluride, CO*
May	*Functional motions in biomolecular machines*	*Hong Kong*
May	*Mathematical & Computational Methods in Quantum Chemistry, New Heaven, CT*	
Apr.	*Lund University*	*Lund, Sweden*
Apr.	*Uppsala University*	*Uppsala, Sweden*
Apr.	*Laufer Center of Quantitative Biology, SUNY-Stony Brooks*	*Stony Brooks, NY*
Apr.	*Department of Biophysics, Johns Hopkins*	*Baltimore, MD*
Mar.	*ACS National Meeting*	*San Diego, CA*
Jan.	*Asia-Pacific Conference of Theoretical and Computational Chemistry, Taiwan*	

2015 (17)

Dec.	*Pacifichem, Metal ions in proteins*	*Hawaii*
Nov.	*MRS Meeting, Simulations and Theory-Driven Design of Soft Materials, Boston, MA*	
Nov.	*ACS Meeting*	*Memphis, TN*
Oct.	*Univ. of Minnesota*	*Duluth, MN*
Oct.	*CECAM workshop on next generation of DFTB*	*Bremen, Germany*
Oct.	*MBI Workshop on Electrostatics*	*Columbus, Ohio*
Sept.	*Protonation Dynamics in Redox Proteins*	*Berlin, Germany*
Aug.	*NYU-ECNU Workshop on Computational Chemistry*	*Shanghai, China*
Aug.	*Zing Conference on Computational Chemical Biology*	*Cairns, Australia*
Jul.	*CECAM workshop on QM based dynamics*	*Bremen, Germany*
Jun.	*Telluride workshop on protein electrostatics*	*Telluride, CO*
Jun.	*Canadian Society for Chemistry Conference*	*Ottawa, Canada*
Jun.	*Satellite meeting of ICQC on biomolecular simulations*	*Changchun, China*
Apr.	*Chemistry, Michigan State*	*Lansing, MI*
Mar.	*ACS National Meeting (3)*	*Denver, CO*
Mar.	*Telluride workshop on membrane biophysics*	*Telluride, CO*
Jan.	*Chemistry, UCSD*	*San Diego, CA*

2014 (16)

Dec.	*International workshop on Computational Science & Engineering (IWCSE 2014)*	*Hong Kong*
Dec.	*Dept. of Chem., HKUST*	*Hong Kong*
Sept.	*Biophysics Society Meeting of Japan*	*Hokkaido, Japan*
Aug.	*ACS National Meeting*	*San Francisco, CA*
Aug.	*Coarse-grained modeling of biological systems*	*Telluride, CO*
July	*Large-scale DFT workshop*	*Aberdeen, MD*
July	*Protein electrostatics workshop*	*Lisbon, Portugal*
Jun.	*Proton Transfer in Biology*	*Telluride, CO*
Jun.	*Molecular simulation summer school*	*Calgary, Canada*
Jun.	*Dept. of Chem. Univ. of Basal*	*Basal, Switzerland*
Jun.	*DFTB developers' workshop*	*Karlsruhe, Germany*
Jun.	*Uppsala Univ.*	*Uppsala, Sweden*
May	*Workshop on potential function developments for materials*	*Madison, WI*
May	*ACS FAME*	*Tampa, FL*

Feb.	*Biophysical Society Meeting*	*San Francisco, CA*
Jan.	*CRC-EC International symposium*	*Atlanta, GA*

2013 (17)

Dec.	*Dept. of Chem., Hong Kong Univ. of Sci. & Tech.*	*Hong Kong*
Dec.	*Workshop on Complex systems*	*Hong Kong*
Nov.	*Univ. of Iowa*	*Iowa City*
Oct.	*Computational Materials Science Initiative*	*Nagoya, Japan*
Sept.	*ACS National Meeting*	*Indianapolis*
Aug.	*ISTCP-VIII*	*Budapest, Hungary*
Aug.	*Beijing University*	*Beijing, PRCHINA*
Jul.	*Dept. of Chem. Kwangwoon University*	*Seoul, Korea*
Jul.	*Snowmass workshop on free energy simulations*	*Snowmass, CO*
May	*University of Washington*	*Seattle, WA*
Apr.	*1st International Symposium on Transformative Biomolecules*	*Nagoya, Japan*
Apr.	*Fukui Institute*	*Kyoto, Japan*
Apr.	*Science on the Edge seminar, MSU*	*East Lansing, MI*
Apr.	*Univ. North. Illinois*	*DeKalb, IL*
Mar.	*APS National Meeting*	*Baltimore, MD*
Mar.	*Telluride workshop on Membrane biophysics*	*Telluride, CO*
Feb.	*University of Minnesota, Chemistry*	*Minneapolis, MN*

2012 (14)

Dec.	*University of Calgary*	*Calgary, Canada*
Nov.	*CECAM workshop on protein dynamics*	*Lugano, Switzerland*
Sept.	*TACC*	*Italy*
Aug.	*MPI Frankfurt*	*Frankfurt, Germany*
Aug.	*ACS National meeting (2)*	*Philadelphia, PA*
Aug.	*Comp Biol 2012*	*Dalian, PRCHINA*
Jul.	*Telluride workshop on proton transports*	*Telluride, CO*
Jun.	*High-performance computing in Chemistry*	*Nanjing, PRCHINA*
Apr.	*Dept. of Chem. Univ. of Maryland*	*College Park, MD*
Mar.	*Dept. of Chem. Univ. of Montana*	*Missoula, MT*
Feb.	*GRC on Protons and Membrane Reactions*	*Ventura, CA*
Feb.	*Multiscale Methods and Validations in Medicine/Biology*	*San Francisco, CA*
Feb.	*Dept. of Chem. Wayne State*	*Detroit, MI*

2011 (18)

Nov.	*UW-Eau Claire*	*Eau Claire, WI*
Aug.	*Dalian Institute of Chemical Physics*	*Dalian, PRCHINA*
Aug.	*Telluride workshop on Molecular machines*	*Telluride, CO*
Jul.	*IUPAC 2011*	*Puerto Rico*
Jul.	*WATOC2011*	*Spain*
Jun.	*Dept. of Chem. Fudan Univ.*	*Shanghai, PRCHINA*
Jun.	*CAPA meeting 2011*	*Guiyang, PRCHINA*

Jun.	*QM/MM workshop*	*Beijing, PRCHINA*
Jun.	*Materia Medica, Chinese Academy of Sciences*	*Shanghai, PRCHINA*
Jun.	*ACS Regional Meeting*	*Indianapolis, IN*
May	*DOE workshop*	*Denver, CO*
May	*Dept. of Chem. Marquett*	*Milwaukee, WI*
Apr.	*Dept. of Chem., Univ. Colorado-Denver*	*Denver, CO*
Apr.	*Dept. of Biochem. Iowa State*	*Ames, IA*
Mar.	*A*Research Institute*	*Singapore*
Mar.	*Dept. of Chemistry, NUS*	*Singapore*
Mar.	*Dept. of Chemistry, NTU*	*Singapore*
Mar.	*Dept. of Material Science, NTU*	*Singapore*

2010 (16)

Dec.	*Hamilton College*	*Clinton, NY*
Nov.	*University of Delaware*	*Delaware, DE*
Nov.	*University of Missouri*	*Columbia, MO*
Oct.	*International workshop on DFTB methods*	*Thailand*
Sept.	*CECAM workshop on DFTB*	*Breman, Germany*
Sept.	*Gordon Conference on Computational Chemistry*	*Switzerland*
Aug.	*ACS National Meeting*	*Boston, MA*
Aug.	*4th Shanghai International Conference on Biophycis*	*Shanghai, PRC*
Aug.	*Telluride workshop on proton transfers*	*Telluride, CO*
Jul.	*Telluride workshop on coarse-grained models*	*Telluride, CO*
Jun.	*Telluride workshop on energy landscape*	*Telluride, CO*
Jun.	*Telluride workshop on phosphoryl transfers (organizer)*	*Telluride, CO*
Jun.	*From Computational Biophysics to Systems Biology*	*Traverse City, MI*
Jun.	*German-American Conference on Frontier of Science*	*Berlin, Germany*
Mar.	*Telluride workshop on Membrane Biophysics (organizer)*	*Telluride, CO*
Feb.	*Workshop on proton mobility in Chemistry and Biology*	*Israel*

2009 (22)

Dec.	*6th Xiamen Workshop on Surface Science*	*Xiamen, PRChina*
Dec.	*5th WCTCC*	*Xiamen, PRChina*
Dec.	*CAS-MPG Partner Institute of Computational Biology*	*Shanghai, PRC*
Dec.	*Workshop on "Theoretical Methods Developments"*	*Hongkong*
Nov.	*Dept. of Physics, SUNY-Buffalo*	*Buffalo, NY*
Sept.	*Dept. of Biophysics, Univ. of Bochum*	*Bochum, Germany*
Sept.	*MPI workshop on "Future of Computational Biology"*	*Berlin, Germany*
Sept.	*University of Tokyo*	*Tokyo, Japan*
Sept.	*Riken Institute*	*Toyko, Japan*
Sept.	*Workshop on Biomolecular Motors*	*Kyoto, Japan*
Aug.	*ACS National Meeting*	*Washington, DC*
Jul.	*China KITPC program on protein function & dynamics*	*Beijing, PRC*
Jul.	*Morokuma birthday symposium*	*Kyoto, Japan*
Jul.	*Telluride workshop on pKa prediction*	*Telluride, CO*
Apr.	*Dept. of Chem., MIT*	*Boston, MA*

Apr.	*Dept. of Chem., Arizona State Univ.*	*Tempe, AZ*
Apr.	*Dept. of Physiol., UW-Madison*	*Madison, WI*
Mar.	*Dept. of Chem. West Michigan Univ.*	*Kalamazoo, MI*
Mar.	*Dept. of Chem., Cornell*	*Ithaca, NY*
Mar.	*Sanibel Symposium*	*Georgia*
Feb.	*Proton Transfer Gordon Conference*	*Ventura, CA*
Jan.	*Mesilla Workshop on Multi-scale modeling in Biology*	*Mesilla, NM*

2008 (17)

Dec.	*Dept. of Bioeng., Univ. Texas, Austin*	*Austin, TX*
Sept.	*TCAA 2008*	*Shanghai, China*
Sept.	*Dept. of Chem., Xiamen Univ.*	*Xiamen, China*
Aug.	*ACS National Meeting*	*Philadelphia, PA*
Jul.	*ISTCP-VI*	*Vancouver, Canada*
Jul.	*ACTC 2008*	*Evanston, IL*
Jul.	*Telluride Workshop*	*Telluride, CO*
Jul.	*Telluride Workshop*	*Telluride, CO*
Jun.	*ISQBP 2008*	*Ascona, Switzerland*
May	*National Conference on Quantum Chemistry*	*Nanjing, China*
May	*Enzyme Dynamics & Function*	*New York*
Apr.	*Dept. of Chem. Univ. of Miami*	*Miami, FL*
Apr.	*Dept. of Chem. Univ. of Nebraska*	*Lincoln, NE*
Apr.	*Dept. of Chem. Ohio State University*	*Columbus, OH*
Mar.	*Telluride Workshop*	*Telluride, CO*
Mar.	*Basel Computational Biology Conference*	*Basael, Switzerland*
Feb.	*Ibaraki Univ.*	*Japan*

2007 (15)

Nov.	*Dept. of Chem. East Carolina Univ.*	
Nov.	*BioGen, Inc.*	*Boston, MA*
Oct.	*Center of Bioinformatics, Kansas State*	
Sept.	*Multi-scale simulations in Biology*	*Imperial College, London*
Sept.	*Quantum Systems in Chemistry and Physics*	*University of London*
Aug.	*QM/MM Workshop*	*Phildelphia, PA*
Aug.	*ACS National Meeting*	*Boston, MA*
Jul.	*Telluride Workshop in "Proton Transfer"*	*Telluride, CO*
May	*Dept. of Chem. NYU*	*New York, NY*
Apr.	*Center of Bioinformatics and Biostatics, Iowa State*	*Ames, IA*
Apr.	*Dept. of Chem. Purdue Univ.*	*Lafayette, IN*
Mar.	*ACS National Meeting*	*Chicago, IL*
Mar.	*Biophysical Society National Meeting*	*Baltimore, MD*
Feb.	*Dept. of Biochemistry, Univ. of Minnesota*	*Minneapolis, MN*
Feb.	*Quantitative Computations in Biophysics*	*Tallahassee, FL*

2006 (20)

Nov.	*Dept. of Chem. Univ. of Notre Dame*	*Notre Dame, IN*

Nov.	*Beckeman Institute, UIUC*	*Urbana, IL*
Nov.	*Dept. of Mechanical Eng., Johns Hopkins*	*Baltimore, MD*
Oct.	*Dept. of Chem., Univ. of Chicago*	*Chicago, IL*
Oct.	*Center of Theoretical Biophysics, UCSD*	*San Diego, CA*
Oct.	*Dept. of Mol. Biol., Scripps*	*San Diego, CA*
Sept.	*ACS National Meeting*	*San Francisco, CA*
Aug.	*Dept. of Biochem., Univ. of Iowa*	*Iowa City, IW*
Aug.	*4th World Wide Chinese Theoretical and Computational Chemistry Conference*	*Kunming, China*
Jun.	*Cross-strait biophysics conference BITS 5,*	*Sun-Moon-Lake, Taiwan*
Jun.	*International symposium "Biomolecules: Proteins, DNA/RNA, and Their Interactions",*	*Taipei, Taiwan*
Jun.	*Midwest Theoretical Chemistry Conference*	*Columbus, OH*
Jun.	*Trends in Enzymology*	*Como, Italy*
Jun.	*Mitsubishi Chemical*	*Tokyo, Japan*
May	*Dept. of Informatics, Kobe Univ.*	*Kobe, Japan*
May	*Satellite meeting for International Congress of Quantum Chemistry*	*Kyoto, Japan*
Apr.	*Dept. of Chem., Florida State Univ.*	*Tallahassee, FL*
Apr.	*Dept. of Chem., Univ. Pittsburgh*	*Pittsburgh, PA*
Mar.	*APS National Meeting*	*Baltimore, MD*
Mar.	*Gordon Research Conference "Protons & Membrane Reactions", poster selected for talk,*	*Harbortown, CA*
2005	***(13)***	
Dec.	*M2CELL: Modeling from Macromolecules to Cells*	*Paris, France*
Oct.	*International workshop "Multi-scale simulation of biological systems"*	*Snowbird, Utah*
Sept.	*Dept. of Chem., Univ. of Detroit Mercy*	*Detroit, MI*
Aug.	*ACS National Meeting*	*Washington, D.C.*
Aug.	*Telluride Workshop on "Vibrational Dynamics"*	*Telluride, CO*
Jul.	*International symposium "Protein folding, dynamics and function"*	*Beijing, China*
May	*Workshop on "Enzyme dynamics", Mathematical Bioscience Institute, Ohio-State University*	*Columbus, OH*
Apr.	*Dept. of Biochem. & Mol. Biophys., Washington Univ.*	*St. Louise, MO*
Apr.	*Dept. of Chem., Jackson State Univ.*	*Jackson, MS*
Mar.	*Dept. of Chem., Univ. of Penn.*	*Philadelphia, PA*
Mar.	*Dept. of Biochem., Michigan State Univ.*	*East Lansing, MI*
Jan.	*WATOC 2005*	*Cape Town, South Africa*
Jan.	*International symposium "Theoretical and computational chemistry of complex systems"*	*Hongkong*
2004	***(11)***	
Nov.	*Triangle symposium*	*Chapel Hill, NC*
Oct.	*NSF Workshop on "Molecular basis of life processes"*	*Oakridge, TN*
Sept.	*Worshop on "Towards Accurate calculation of biomolecular recognition and reactivity"*	*Manchester, UK*

Sept. *CIBM Program seminar series, Univ. of Wisc. Madison* *Madison, WI*
Aug. *ACS National Meeting* *Philadelphia, PA*
Aug. *4th Conference for Worldwide Chinese Young Chemists* Chengdu, China
Jul. *German-American Symposium on Frontiers of Chemistry* *Seeon, Germany*
Jul. *DKFZ* *Heidelberg, Germany*
May *UCLA-IPAM Proteomics Workshop: Molecular Machine* *Los Angles, CA*
May *Dept. of Chem., SUNY, Stony Brook* *Stony brook, NY*
Mar. *Dept. of Chem., Penn. State Univ.* *University Park, PA*

2003 (10)

Dec. *Dept. of Chem. Univ. of Michigan* *Ann Arbor, MI*
Nov. *Dept. of Chem. Univ. of Nevada-Reno* *Reno, NV*
Nov. *Center for Comput. Biol., Univ. of Pittsburgh* *Pittsburgh, PA*
Sept. *Dept. of Chem. Univ. of Wisc. Madison* *Madison, WI*
Aug. *Workshop on "Grand challenges in modeling the assembly and properties of nanomaterials"* *Argonne, IL*
Aug. *Workshop on "Excited state processes in electronic and bio nano-materials"* *Las Alamos, NM*
Aug. *Satellite meeting for International Congress of Quantum Chemistry* *Mulheim, Germany*
Aug. *CECAM workshop* *Lyon, France*
Mar. *ACS National Meeting* *New Orleans, LA*
Feb. *Sanibel Symposium* *Augusta, FL*

2002 (9)

Oct. *Dept. of Mathematics, Univ. of Wisc. Madison* *Madison, WI*
Oct. *Dept. of Chem., College of Staten Island, CUNY* *Staten Island, NY*
Oct. *Dept. of Chem., Univ. New Mexico* *Albuquerque, NM*
Sept. *2nd Worldwide Chinese Theoretical and Computational Chemistry Conference* *Taipei, Taiwan*
Aug. *2nd German American Symposium on the frontier of Chemistry, Durham, NH*
Jul. *Gordon Research Conference in Comput. Chem.* *Durham, NH*
Jun. *Great-Lake regional ACS meeting* *Minneapolis, MN*
Apr. *Dept. of Chem., Eng. Univ. of Wisc. Madison* *Madison, WI*
Apr. *Dept. of Chem., Univ. of Iowa* *Iowa City, IW*

Departmental/University Service [UW-Madison]

- Member, Finance Committee of Chemistry Department [2016-2017]
- Graduate Program of Biophysics; Chair, graduate program admission committee [2011-present]; Steering committee [2006-2017]
- Member, Computer Committee of Chemistry Department [2007-2017]
- Member, Graduate Student Faculty Liaison Committee [2006-2010]
- Member, Graduate Recruiting Committee (responsible for international recruiting for physical chemistry division) [2001-2017]
- Organizer, Theoretical Chemistry Institute Seminar Series [2001-2017]
- Member, Library Committee of Chemistry Department [2002-2006]
- Member, University Appeal Committee [2007-2009]
- Alternate member of UW Faculty Senate [2006-2007, 2010-2017]
- Member, Committee for Cluster Hire in "Materials by Design" [2006-2007]
- Thesis committee members for students in Chemistry, Biophysics, Biochemistry, Materials Science, Neuroscience.
- Member of training grants in: CIBM (Computations and Informatics in Biology and Medicine), Molecular Biophysics, Chemical Biology

Professional Activities

2018 Co-organizer (with D. M. York, G. H. Li and M. Elstner), Telluride Workshop on Multi-scale computations, Telluride, CO

2017 Co-organizer (with R. J. Hamers, J. A. Pedersen and T. Fraunheim), CECAM workshop on "Tackling complexity of the Nano/Bio interface", Bremen, Germany

2016 Co-organizer (with X. Huang and H. Yang), HKUST-IAS workshop on "Functional Dynamics of Biomolecular Machines"

2015 Organizer (with M. Meuwly, Y. Q. Gao, T. Allen), Pacifichem symposium on "Metal ions and protein function"

2014 Editor (with M. Meuwly, P. Ren), Monograph on "Many-Body Effects and Electrostatics in Biomolecules"

2014 Organizer (with B. Garcia-Moreno), Telluride Workshop on "Proton transfers in biology"

2014 Co-chair (with S. Hammes-Schiffer), symposium in Biophysical Society Meeting on "Application of Quantum Mechanics to Biophysical Problems"

2012 Organizer (with M. Meuwly, M. Elstner), CECAM Workshop on "Protein Dynamics"

2011 Organizer (with H. Yang, S. Sun), Telluride Workshop on "Rise of the Machines"

2010 Organizer (with D. York and D. Herschlag), Telluride Workshop on "Phosphoryl transfers"

2008, 2010, 2013 Organizer (with A. Yethiraj), Telluride Workshop on "Frontiers of Molecular Simulations"

2006 Co-Organizer (with G. Phillips, J. Mitchell, R. Jernigan), 32nd Steenbock symposium on "Dynamics of proteins and macromolecular assemblies"

2005 Organizer (with J. M. Bowman, Emory Univ.), Telluride Workshop on "Vibrational Dynamics of Biomolecules"

2004 Editor (with I. Bahar, Univ. of Pittsburgh), Monograph on "Normal Mode Analysis: Theory and Applications to Biological and Chemical Systems"

2003 Organizer, ACS National Meeting, "Physical Chemistry of Biomolecular Motors"

Current Postdoctoral Fellows

Dr. Mesele Oluwaseun (8/17-), Dr. M. Huynh (9/17-), Dr. Shingo Ito (03/18-)
Dr. Mandal Taraknath (4/18-), Dr. Rui Lai (6/18-)

Current Graduate Students

Mr. Darren Demapan (Chemistry, 2014-present)
Ms. Gladys Vazquez (Biophysics, 2014-present, joint with Prof. A. Senes)
Mr. Dongyue Liang (Chemistry, 2015-present)
Mr. Tanmoy Pal (Chemistry, 2016-present)

Undergraduate Students

Mr. M. Wolfsen (2004-2006)	Graduate student, MIT
Mr. N. Schaefer (2008)	PhD, UCSD
Ms. Jane (Yi-Chen) Lin (2014)	
Mr. S. Slattery (2012-2016)	
Ms. Lixue Cheng (2014-2017, joint with Prof. M. T. Record, Jr.)	Graduate student, Cal Tech
Mr. Rishi Ragsdale (2014-2016); Mr. Stephen Pan (2015-2017)	

Former Graduate Students

Ms. Megan Hyland (Chemistry) (2002-2004), M. S.	PPD, Inc., WI
Ms. Patricia Schaefer (Chemistry) (2002-2005), M. S.	High-school teacher, WI
Dr. Mark S. Formaneck (Chemistry) (2001-2005), Ph.D. 02/06	Epic Systems, WI
Dr. Demian Riccardi (Chemistry) (2001-2006), Ph.D. 12/06	NIST
Dr. Adam Van Wynsberghe (Biophysics, 2001-2006), Ph.D. 12/06	Hamilton (Asso. Prof.)
Ms. Junjun Yu (Chemistry, 2005-2009), M.S. 08/09	
Dr. Nilanjan Ghosh (Chemistry) (2003-2009), Ph.D., 01/09	Intel
Dr. Yang Yang (Chemistry, 2004-2008), Ph.D. 12/08	Haverford Coll. (Visit. Prof.)
Dr. Liang Ma (Biophysics, 2004-2009), Ph.D. 08/09	S. Carolina (Asst. Prof.)
Dr. Xiao Zhu (Chemistry, joint with Prof. A. Yethiraj, 2004-2009) Ph.D. 01/10	Computer Center, Purdue
Dr. Jejoong Yoo (Biophysics, 2005-2010), Ph. D. 06/10	IBS Fellow, Korea
Dr. Guanhua Hou (Chemistry, 2007-2012), Ph. D. 06/12	Micron
Dr. Zhe Wu (Chemistry, 2007-2012, joint with Prof. A. Yethiraj) Ph.D. 08/12	Merck Co.
Mr. Shuo Yang (Chemistry, 2006-2013)	Huawei Inc.
Dr. Puja Goyal (Chemistry, 2008-2013), Ph. D. 08/13	SUNY-Binghamton (Asst. Prof.)
Dr. Xueqin Pang (Visiting student, DICP, 2011-2013)	UW-Madison, Pharmacy
Ms. Fang He (Visiting student from National University of Singapore, 2012-2013)	
Dr. Leili Zhang (Chemistry, 2010-2015, joint with Prof. A. Yethiraj) Ph. D. 09/15	IBM
Dr. Elif Nihal Korkmaz (Biophysics, 2010-2016), Ph. D. 05/16	U. Washington
Dr. Xiya Lu (Chemistry, 2010-2016), Ph.D. 06/17	LinkedIn Co.
Mr. Runze Liu (DICP visiting graduate student, 2014-2016)	DICP
Mr. Haiyun Jin (Chemistry, 2013-2017), M.S. 06/17	Amazon, Seattle
Mr. Jiewei Hong (Chemistry, 2014-2017), M. S. 08/17	UW-Madison, CS

Mr. Ruochen Lin (Chemistry, 2016-2017)	UW-Madison, CS
Mr. Mingren Shen (Biophysics, 2016-2017)	UW-Madison, Biophysics
Dr. Changyun Son (Chemistry, 2012-2017, joint with Prof. A. Yethiraj)	Cal Tech
Dr. Yuqing Zheng (Biophysics, 2012-2017)	Schneider, Inc.

Former Postdoctoral Fellows

Dr. Xiaodong Zhang (2001-2002)	UC-Santa Barbara, CA
Dr. Guohui Li (2001-2003)	Dalian Inst. Of Chem. Phys. (Principal Investigator)
Dr. Demitry Khoroshun (2002-05/2004)	MPI-Mulheim, Germany
Dr. Xavier Prat-Resina (2005-2006)	Univ. Minnesota-Rochester (Asso. Prof.)
Dr. Justin Hoerter (joint with Prof. S. Stahl, 11/2004-05/2007)	Dupont
Dr. Peter König (BACTER postdoctoral fellow, 01/2006-06/2007)	P & G
Dr. Haibo Yu (01/2005-09/2007)	Wollongong (Asst. Prof.)
Dr. Dmitry Kondrashov (CIBM postdoctoral fellow)	Univ. of Chicago (Lecturer)
Dr. Demian Riccardi (06/10-12/10)	NIST
Dr. Michael Daily (CIBM fellow, 07/08-06/11)	Monsanto
Dr. Jan Zienau (05/10-08/12)	Frankfurt
Dr. M. Gauss (11/11-03/13)	SAP, Germany
Dr. T. Mori (10/12-11/13)	IMS, Japan (Asst. Prof.)
Dr. C. Mahajan (11/13-07/14)	Deceased
Dr. A. S. Christensen (9/14-9/16)	Basel, Switzerland
Dr. D. Fang (10/14-9/16)	Jingtai Inc., China
Dr. D. Roston (9/13-12/17)	UW-Madison

Research Funding and Support **(***PI: Q. Cui unless otherwise stated*)

Current:

Project: Phase II Center for Chemical Innovation, A Molecular Basis for Sustainable Nanotechnology
Source: National Science Foundation (PI: Hamers)
Total Award: $20,000,000 Period: 9/1/15-8/31/20
Location: UW-Madison
Commitment to Project: 0.5 SM

Project: Multi-scale simulation methods for energy transduction and macromolecular assembly
Source: National Science Foundation Period: 8/1/17-7/31/20
Total Award: $450,000
Location: UW-Madison
Commitment to Project: 0.5 SM

Project: Collaborative Research: Multi-scale models of membrane fission catalyzed by the ESCRT complexes
Source: NSF (PIs: Cui, Audhya, Spagnolie)
Total Award: $1,200,000 Period: 07/1/17-6/30/21
Location: UW-Madison
Commitment to Project: 0.8 SM

Project: Development and application of QM/MM methods for metalloenzymes
Source: NIH
Total Award: $290,736 per year Period: 09/1/13-7/31/21
Location: UW-Madison
Commitment to Project: 1.0 SM

Pending Grants

Project: Toward a biomolecular force field based on many-body expansion models
PI: F. Paesani (UCSD), Co-PI: Q. Cui
Source: NIH
Total Award: $275,000 direct cost Period: 07/1/18-6/31/20
Location: UW-Madison
Commitment to Project: 0.5 SM

Completed Grants

1. ACS-PRF-G: *Probing conformational dynamics and luminescent reactions in photoproteins with novel QM/MM methods*
   $35,000 direct cost, 09/01/02-08/31/04

2. Research Corporation: *Understanding allosteric transition in biomolecules with novel molecular simulation methods*
   $35,000 direct cost, 06/01/03-11/18/06

3. NSF-MCB: *Collaborative research of proton transfers in enzymes: A synergestic theory-experiment approach*
PI: Q. Cui, Co-PIs: H. Guo (Univ. of New Mexico), R. Viola (University of Toledo)
$174, 235 total cost to Cui, 09/01/03-08/31/06

4. Alfred P. Sloan Foundation: *Sloan research fellowship*
$40,000 direct cost, 09/01/2004-08/31/2008

5. NSF-CHEM-CAREER: *Theoretical analysis of oxygen chemistry in biological systems*
$510,000 total cost, 03/01/04-08/31/09

6. Graduate school funding: *continuum mechanics models of proteins*
Supporting one graduate student, 07/01/08-06/30/09

7. NIH-R01: *Coupling between conformation and chemistry in enzymes*
$976,423 total cost, 03/01/05-08/31/10

8. NSF-CRC: *Catalytic manipulation of amide-based molecules and materials*
PI: S. Gellman, Co-PIs: S. Stahl, Q. Cui, A. Yethiraj, A. E. Barron (Northwestern)
$2,325,000 total cost, 09/01/04-08/31/10

9. DOE-BACTER: Bringing Advanced Computational Techniques to Environmental Research
PI: J. Mitchell; Co-PI: Cui and 7 others
$4,200,000 total cost, 08/01/08-03/31/12

10. NIH-ARRA: QM/MM analysis of redox driven proton pumping
PI: Q. Cui, Co-PI: M. Gunner (CUNY)
$549,556 total cost, 09/30/09-08/31/12

11. NIH: Conformational duality of the human chemokine lymphotactin
PI: B. Volkman, Co-PI: Q. Cui
$57,592 total cost, 08/01/11-06/30/12

12. I. H. Romnes Fellowship, UW-Madison, $50,000, 07/01/10-06/30/15

13. Graduate school funding: *QM/MM models for DNA repair enzymes*
Supporting one graduate student, 07/01/11-06/30/12

14. NSF: New methods for treating electrostatics and adaptive partitioning in QM/MM simulations
PI: Q. Cui
$410,001 total cost, 01/15/10-08/31/13

15. NSF: UW NSEC
$60,000 to Cui research, 09/01/13-08/31/14

16. NSF-CHE: Development of multi-scale models for enzyme catalysis in complex environments
$405,000 total cost, 08/1/13-7/31/17

17. NSF: UW CEMRI on Structured Interfaces
PI: Abbott & 28 co-PIs), $18,000,000 ($53,153 to Cui research annually), 01/01/13-08/31/17

18. NSF-DMS: FRG: Collaborative Research: Variational multiscale approaches to biomolecular structure, dynamics and transport
PI: J Mitchell, co-PI: Q Cui, $321,054 total 09/15/12-08/31/17

Publication List

Qiang Cui
Department of Chemistry
Boston University
590 Commonwealth Avenue, Boston, MA 02215

February 16, 2018

Boston University (01/2018-present); Univ. of Wisconsin-Madison (08/2001 - 12/2017), * indicates corresponding author)
Google Scholar Profile: http://scholar.google.com/citations?hl=en&user=4x1QeogAAAAJ
h-index: 66 (Google Scholar); 57 (Web of Science)

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231. Essence of Small Molecule-Mediated Control of Hydroxyapatite Growth: Free Energy Calculations of amino acid side chain analogs, Z. J. Xu*, Q. C. Wei, W. L. Zhao, Q. Cui and N. Sahai*, *J. Phys. Chem. C*, In press (2018) [DOI: 10.1021/acs.jpcc.7b12142]

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Approach for the Determination of Surface Charge of Nanomaterials, J. W. Hong, R. J. Hamers, J. A. Pedersen and Q. Cui*, *J. Phys. Chem. C*, 121, 3584-3596 (2017)

218. Microscopic Mechanisms that Govern the Titration Response and pK_a Values of Buried Residues in Staphylococcal Nuclease Mutants, Y. Q. Zheng and Q. Cui*, *Proteins: Struct., Funct. & Bioinform.*, 85, 268-281 (2017) ***Cover***

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208. Towards a Barrier Height Benchmark Set for Biologically Relevant Systems, J. C. Kromann, A. S. Christensen, Q. Cui and J. H. Jensen*, *Peer J.*, e1994 (2016)

207. Gating Mechanism of Mechanosensitive Channel of Large Conductance: A Coupled Continuum Mechanical-Continuum Solvation Approach, L. Zhu, J. Wu, Y. Liu, Y. Yan, Q. Cui and X. Chen*, *Biomechan.& Modeling in Mechanobio.*, 15, 1557-1576 (2016)

206. First Principles United Atom Force Field for the Ionic Liquid $[BMIM^+][BF_4^-]$: An Alternative to Charge Scaling, C. Y. Son, J. McDaniel, J. R. Schmidt, Q. Cui and A. Yethiraj*, *J. Phys. Chem. B*, 120, 3560-3568 (2016)

205. Semi-empirical Quantum Mechanical Methods for Non-covalent Interactions for Chemical and Biochemical Applications, A. S. Christensen, T. Kubar, Q. Cui* and M. Elstner*, *Chem. Rev.*, 116, 5301-5337 (2016)

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201. Copper Oxidation/Reduction in Water and Protein: Studies with DFTB3/MM and VALBOND Molecular Dynamics Simulations, H. Jin, P. Goyal, A. Kumar Das, M. Gaus, M. Meuwly* and Q. Cui*, *J. Phys. Chem. B* ***Bruce Garrett Festschrift***, 120, 1894-1910 (2016)

200. Comparison of Native and Non-native Ubiquitin Oligomers Reveals Analogous Structures and Reactivities, G. H. Pham, A. S. J.B. Rana, E. N. Korkmaz, V. H. Trang, Q. Cui, and E. R. Strieter*, *Prot. Sci.*, 25, 456-471 (2016)

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197. Electronic Polarization Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins, V. Ngo, M. C. da Silva, M. Kubillus, M. Elstner, H. Li, B. Roux, Q. Cui*, D. R. Salahub* and S. Noskov*, *J. Chem. Theory Comp.* 11, 4992-5001 (2015)

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194. DFTB3 Parametrization for Copper: the Importance of Orbital Angular Momentum Dependence of Hubbard Parameters, M. Gaus, H. Jin, D. Demapan, A. S. Christensen, P. Goyal, M. Elstner and Q. Cui*, *J. Chem. Theory Comp.* 11, 4205-4219 (2015)

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192. Skip Residues Modulate the Structural Properties of the Myosin Rod and Guide Thick Filament Assembly, K. C. Taylor, M. Buvoli, N. Korkmaz, A. Buvoli, Y. Q. Zheng, N. T. Heinz, Q. Cui*, L. A. Leinwand*, and I. Rayment*, *Proc. Natl. Acad. Sci. USA* E3806-E3815 (2015)

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189. Histone H3 N-terminal Tail: a Computational Analysis of Free Energy Landscape and Kinetics, Y. Zheng and Q. Cui*, *Phys. Chem. Chem. Phys.*, 17, 13689 - 13698 (2015)

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187. Parameterization of DFTB3/3OB for Magnesium and Zinc for Chemical and Biological Applications, X. Lu, M. Gaus, M. Elstner and Q. Cui*, *J. Phys. Chem. B*, ***Bill Jorgensen Festschrift***, 119, 1062-82 (2015)

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185. Microscopic Basis for Kinetic Gating in Cytochrome c Oxidase: Insights from QM/MM Analysis, P. Goyal, S. Yang and Q. Cui*, *Chem. Sci.*, 6, 826-841 (2015)

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182. Molecular simulation of water and hydration effects in different environments: challenges and developments for DFTB based models, P. Goyal, H-J. Qian, S. Irle, X. Lu, D. Roston, T. Mori, M. Elstner and Q. Cui*, *J. Phys. Chem. B* **Featured Articles**, 118, 11007-11027 (2014)

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and R. Nussinov*, *PLoS Comp. Biol.* 10, e1003786 (2014)

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Comp., 9, 5059-5069 (2013)

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166. Contribution of Electrostatics to the Binding of Pancreatic-Type Ribonucleases to Membranes, N. K. Sundlass, C. H. Eller, Q. Cui and R. T. Raines*, *Biochem.* 52, 6304-6312 (2013)

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163. Molecular Simulation of Biomineral Nucleation and Crystal Growth: Modern Computational Challenges and Approaches, Y. Yang, Z. J. Xu, Q. Cui and N. Sahai, *Characterization of Biominerals and Biomimetic Materials*, Eds. L. Gower, E. DiMasi, Taylor & Francis, In press (2013) **Invited Review**

162. Toward quantitative analysis of metalloenzyme function using MM and hybrid QM/MM methods: challenges, methods and recent applications, M. Gaus, P. Goyal, G. Hou, X. Lu, X. Pang, J. Zienau, X. Xu, M. Elstner and Q. Cui*, "*Molecular Modeling at the Atomic Scale: Methods and Applications in Quantitative Biology*", Ed. Ruhong Zhou, In press (2013) **Invited Review**

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