Curriculum Vitae

Qiang Cui
Department of Chemistry
University of Wisconsin, Madison
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Personal

Date and place of birth: Jan. 28. 1975, Beijing, P. R. China

Employment

Associate Professor of Chemistry, 2007-present
Assistant Professor of Chemistry, 2001-2007
University of Wisconsin, Madison

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

- I. H. Romnes Fellow, UW-Madison, 2010-2015
- Member, *Faculty of 1000*, 2008-present
- Advisory Editorial Board Member, *Journal of Theoretical and Computational Chemistry*, 2007-present; *Interdisciplinary Sciences – Computational Life Sciences*, 2008-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)

2010 (17)

Nov.	*University of Delaware,*	*Delaware, DE*
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*
May	*International workshop on Solvation*	*Armenia*
Apr.	*Dept. of Chem., Marquett*	*Milwaukee, WI*
Mar.	*Mixed quantum/classical methods, IPAM workshop*	*Maryland, MD*
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

- Chair, Computer Committee of Chemistry Department [2007-present]
- Member, Graduate Student Faculty Liaison Committee [2006-present]
- Member, Graduate Recruiting Committee (responsible for international recruiting for physical chemistry division) [2001-present]
- Organizer, Theoretical Chemistry Institute Seminar Series [2001-present]
- Member, Library Committee of Chemistry Department [2002-2006]

- Member, Steering Committee of Graduate Program in Biophysics [2006-present]
- Member, University Appeal Committee [2007-present]
- Alternate member of UW Faculty Senate [2006-2007]
- Member, Committee for Cluster Hire in "Materials by Design" [2006-2007]

- Thesis committee members for students in Chemistry, Biophysics, Biochemistry, Materials Science, Physiology.
- Member of training grants in: BACTER (Bring Advanced Computations to Environment/Energy Research), CIBM (Computations and Informatics in Biology and Medicine), Molecular Biophysics, Chemical Biology

Professional Activities

2010 Co-organizer (with D. York and D. Herschlag), Telluride Workshop on "Phosphoryl transfers"
2008,2010 Co-Organizer (with A. Yethiraj, N. Baker), 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 Co-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 Graduate Students

Mr. Jejoong Yoo (Biophysics, 2005-present)
Mr. Shuo Yang (Chemistry, 2006-present)
Mr. Guanhua Hou (Chemistry, 2007-present)
Mr. Zhe Wu (Chemistry, 2007-present, joint with Prof. A. Yethiraj)
Ms. Puja Goyal (Chemistry, 2008-present)

Current Postdoctoral Fellows

Dr. Demian Riccardi (CIBM fellow, joint with Prof. G. Phillips, 01/07-present)
Dr. Michael Daily (CIBM fellow, joint with Prof. G. Phillips, 07/08-present)
Dr. Jan Zienau (04/10-present)

Undergraduate Students

Mr. M. Wolfsen (2004-2006)	Graduate student, MIT
Mr. N. Schaefer (2008)	Graduate student, UCSD

Former Graduate Students

Ms. Megan Hyland (Chemistry) (2002-2004), M. S.	PPD, Inc., WI
Ms. Patricia Schaefer (Chemistry) (2002-2005), M. S.	UW-Madison, 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	UW-Madison (CIBM)
Dr. Adam Van Wynsberghe (Biophysics, 2001-2006), Ph.D. 12/06	Hamilton (Asst. Prof.)
Ms. Junjun Yu (Chemistry, 2005-2009), M.S. 08/09	
Dr. Nilanjan Ghosh (Chemistry) (2003-2009), Ph.D., 01/09	U. Colorado
Dr. Yang Yang (Chemistry, 2004-2008), Ph.D. 12/08	UW-Madison (Geology)
Dr. Liang Ma (Biophysics, 2004-2009), Ph.D. 08/09	UW-Madison (Business)
Dr. Xiao Zhu (Chemistry, joint with Prof. A. Yethiraj, 2004-2009) Ph.D. 01/10	Northwestern

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 (Asst. 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)	Univ. of Chicago
Dr. Dmitry Kondrashov (CIBM postdoctoral fellow)	Univ. of Chicago

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

Active Support

1. NIH-R01: *Coupling between conformation and chemistry in enzymes*
   $976,423 total cost, 03/01/05-02/28/10 [No cost extension to 08/31/10]

2. DOE: *Bringing Advanced Computational Techniques to Environmental Research*
   PI: J. Mitchell, Co-PIs: M. Craven, Q. Cui, T. Donohue, P. Milewski, D. Nelson, G. Phillips, S. Wright
   $5,678,802 total cost, 09/01/07-08/31/10 [Support one graduate student]

3. 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, 09/01/04-08/31/09 [No cost extension to 08/31/10]

4. NIH-ARRA-R01: *QM/MM analysis of redox driven proton pumping*
   PI: Q. Cui, Co-PI: M. Gunner (CUNY)
   $550,000 total cost, 09/30/09-8/31/11

5. NSF-Chem: *New methods for treating electrostatics and adaptive partitioning in QM/MM simulations*, $496,812 total cost, 01/01/10-12/31/12

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

Pending Support

1. NIH-R01: Renewal: *Coupling between conformation and chemistry in enzymes*
   $1,807,750 total cost, 09/01/10-08/31/15

2. NIH-R01: *Conformational duality in the human chemokine hLtn/XCL1*
   PI: B. Volkman, Co-PI: Q. Cui
   $307,992 total cost to UW-Madison, 12/01/10-11/31/15

3. NIH-R01: Accelerating QM/MM molecular dynamics sampling of protein-ligand interactions,
   PI: W. Yang (Florida State), Co-PI: Q. Cui
   $310,000 total cost to UW-Madison, 11/01/10-10/31/15

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

Publication List

Qiang Cui
Department of Chemistry and Theoretical Chemistry Institute
University of Wisconsin, Madison
1101 University Ave, Madison, WI 53706

April 9, 2010

Univ. of Wisconsin-Madison (08/2001 - present, * indicates corresponding author) Hirsch index: 38

132. Iron-Catalyzed Oxidation Intermediates Captured in A DNA Repair Monooxygenase, C. Yi, G. Jia, G. Hou, Q. Dai, G. Zheng, X. Jian, C. G. Yang, Q. Cui, and C. He*, *Science*, Submitted

131. Disruption and formation of surface salt bridges are coupled to DNA binding in integration host factor (IHF): a computational analysis, L. Ma, M. T. Record, Jr., N. Sundlass, R. T. Raines and Q. Cui*, *J. Mol. Biol.*, Submitted

130. An implicit solvent model for SCC-DFTB with Charge-Dependent Radii, G. Hou, X. Zhu and Q. Cui*, *J. Chem. Theo. Comp.*, Submitted

129. Elastic Network Models of Proteins in Crystals, D. Riccardi*, Q. Cui and G. N. Phillips, Jr. *Proc. Natl. Acad. Sci. USA*, Submitted

128. Sequence-dependent interaction of β-peptides with membranes, J. Mondal, X. Zhu, Q. Cui and A. Yethiraj*, *J. Am. Chem. Soc.*, Submitted

127. QM/MM Alchemical free energy simulations: Challenges and Recent Developments, W. Yang*, Q. Cui, D. Min and H. Li, *Annual Reports in Comput. Chem.* Submitted **Invited Review**

126. A new coarse-grained model for water: The importance of electrostatic interactions, Z. Wu, Q. Cui* and A. Yethiraj*, *J. Phys. Chem. B* Submitted

125. Conservation and Variation of Structural Flexibility in Protein Families, A. Van Wynsberghe and Q. Cui, *Structure*, 18, 281-283 (2010) **Invited Commentary**

124. Many low-barrier local motions cooperate to produce the adenylate kinase conformational transition, M. D. Daily, G. N. Phillips, Jr, Q. Cui*, *J. Mol. Biol.*, Submitted

123. How does bone sialoprotein promote the nucleation of hydroxyapatite? A molecular dynamics study using model peptides of different conformations, Y. Yang, Q. Cui and N. Sahai*, *Langmuir*, Submitted

122. Sequence control in random copolymers from chain exchange and adsorption: Insight from a lattice model, X. Zhu, Q. Cui* and A. Yethiraj*, *J. Phys. Chem. C*, Submitted

121. Preferential interactions between small solutes and the protein backbone: A computational analysis, L. Ma, L. M. Pegram, M. T. Record, Jr., Q. Cui*, *Biochem.*, 49, 1954-1962 (2010)

120. Establishing effective simulation protocols for β- and α/β-peptides. III. Molecular Mechanical (MM) model for a non-cyclic β-residue, X. Zhu, P. König, M. Hoffman, A. Yethiraj* and Q. Cui*, *J. Comp. Chem.*, In press

119. Proton Transfer Function of Carbonic Anhydrase: Insights from QM/MM simulations, D. Riccardi, S. Yang and Q. Cui*, *BBA-Prot. & Proteomics, Invited special issue on "Carbonic Anhydrase and Superoxide Dismutase"*, 1804, 342-351 (2010)

118. Curvature Generation and Pressure Profile in Membrane with lysolipids: Insights from coarse-grained simulations, J. Yoo and Q. Cui*, *Biophys. J.* 97, 2267-2276 (2009)

117. The hydrolysis activity of Adenosine triphosphate in myosin: a theoretical analysis of anomeric effects and the nature of transition state, Y. Yang* and Q. Cui*, *J. Phys. Chem. A (R. M. Pitzer Festschrift)*, 113, 12439-12446 (2009)

116. CHARMM: The biomolecular simulation program, B. R. Brooks, et al., Q. Cui, et al., M. Karplus, *J. Comp. Chem.* 30, 1545-1614 (2009)

115. Multi-scale methods for the description of chemical events in biological systems, M. Elstner* and Q. Cui*, in NIC (John von Neumann Institut für Computing) series. (2009) **Invited Book Chapter**

114. Does water relayed proton transfer play a role in phosphoryl transfer reactions? A theoretical analysis of uridine 3'-*m*-nitrobenzyl phosphate isomerization in water and *tert*-butanol, Y. Yang and Q. Cui*, *J. Phys. Chem. B* 113, 4930-4939 (2009)

113. Microscopic pK_a analysis of Glu 286 in Cytochrome c Oxidase (*Rhodobacter sphaeroids*): towards a consistent molecular model, N. Ghosh, X. Prat-Resina, M. Gunner and Q. Cui*, *Biochem.*, 48, 2468-2485 (2009)

112. A combined continuum mechanics and continuum electrostatics (CM/CE) computational framework for macromolecules: application to the salt concentration dependence of DNA bendability, L. Ma, Y. Tang, A. Yethiraj, X. Chen* and Q. Cui*, *Biophys. J.* 96, 3543-3554 (2009)

111. Application of elastic network models to proteins in the crystalline state, D. Riccardi, Q. Cui and G. Phillips, Jr.* *Biophys. J.* 96, 464-475 (2009)

110. Mechanochemical coupling in molecular motors: insights from molecular simulations of the myosin motor domain, H. Yu, Y. Yang, L. Ma and Q. Cui*, Book Chapter in "*Energy Flows in Proteins*", Eds. D. Leitner and J. E. Straub, CRC Press (2008) **Invited Book Chapter**

109. Description of phosphate hydrolysis reactions with the Self-Consistent-Charge Density-Functional-Tight-Binding (SCC-DFTB) theory. 1. Parameterization, Y. Yang, H. Yu, D. York, M. Elstner* and Q. Cui*, *J. Chem. Theo. Comp.,* 4, 2067-2084 (2008)

108. Computational Molecular Biomechanics: A Hierarchical Multiscale Framework with Applications to Gating of Mechanosensitive Channels of Large Conductance, X. Chen* & Q. Cui*, in *Trends in Computational NanoMechanics*, Ed. T. Dumitrica, *Springer Series: Challenges and Advances in Computational Chemistry and Physics,* (2008) **Invited Book Chapter**

107. Mechanosensitive Channels: Insights from Continuum-Based Simulations, Y. Tang, J. Yoo, A. Yethiraj, Q. Cui* and X. Chen*, *Cell Biochem. & Biophys.*, 52, 1-18 (2008) **Invited Review**

106. Amino acids with an intermolecular proton bond as the proton storage site in bacteriorhodopsin, P. Phatak‡, N. Ghosh‡, H. Yu, Q. Cui* and M. Elstner*, *Proc. Natl. Acad. Sci. USA*, 105, 19672-19677 (2008) [‡These authors contributed equally]

105. Extensive conformational changes are required to turn on ATP hydrolysis in myosin, Y. Yang, H. Yu and Q. Cui*, *J. Mol. Biol.*, 381, 1407-1420 (2008)

104. pK_a of residue 66 in *Staphylococal nuclease*: insights from QM/MM simulations with conventional sampling, N. Ghosh, Q. Cui*, *J. Phys. Chem. B*, 112, 8387-8397 (2008) **Cover**

103. Gating Mechanisms of Mechanosensitive Channels of Large Conductance Part II: Systematic Study of Conformational Transitions, Y. Tang, J. Yoo, A. Yethiraj, Q. Cui and X. Chen*, *Biophys. J.*, 95, 581-596 (2008) **Cover**

102. Gating Mechanisms of Mechanosensitive Channels of Large Conductance Part I: A Continuum Mechanics-Based Hierarchical Framework, X. Chen*, Q. Cui, Y. Tang, J. Yoo and A. Yethiraj, *Biophys. J.*, 95, 563-580 (2008)

101. QM/MM and multi-scale methods for the simulation of biochemical processes in complex environments, Q. Cui* and M. Elstner*, in *Solvation effects on molecules and biomolecules: Computational methods and applications*, Ed. S. Canuto, *Springer Series: Challenges and Advances in Computational Chemistry and Physics,* (2008) **Invited Book Chapter**

100. "Multi-scale" QM/MM methods with the Self-Consistent-Charge Density-Functional-Tight-Binding (SCC-DFTB) Method, Q. Cui* and M. Elstner*, in *Multi-scale Quantum Models for Biocatalysis*, Eds. D. York, T. Lee (2008) **Invited Book Chapter**

99. Does Arg remain protonated in the lipid membrane? Insights from microscopic pK_a calculations, J. Yoo and Q. Cui*, *Biophys. J. Lett*, L61-L63 (2008)

98. Establishing effective simulation protocols for β- and α/β-peptides. II. Molecular Mechanical

(MM) model for a Cyclic β-residue, X. Zhu, P. König, S. Gellman, A. Yethiraj* and Q. Cui*, *J. Phys. Chem. B*, 112, 5439-5448 (2008)

97. Allostery and Cooperativity Revisited, Q. Cui*, M. Karplus*, *Protein Sci.*, 17, 1295-1307 (2008)

96. Functional Motions in Biomolecules: Insights from Computational Studies at Multiple Scales, A. W. van Wynsberghe, L. Ma, X. Chen and Q. Cui*, in *Computational Structural Biology*, Eds. T. Schwede, M. Peitsch, pp253-298 World Scientifc (2008) **Invited Book Chapter**

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