Curriculum Vitae

Benzhuo Lu

ADDRESS

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EDUCATION

2006 - Present	Research associate. **Howard Hughes Medical Institute,** University of California at San Diego, San Diego.
2003 - 2006	Postdoctoral researcher. **University of California at San Diego, San Diego.**
1997 - 2002	PhD in Biochemistry and Molecular Biology. **University of Science and Technology of China, Hefei, China** Dept. of Astronomy and Applied Physics.
1989 - 1993	B.S. in Physics. **East China Normal University, Shanghai, China** Department of Physics.

DISSERTATION

"Studies on computational methods of electrostatics in molecular modeling and on protein folding prediction".

PROFESSIONAL ACTIVITIES

Reviews:
Reviewer for *Journal of Computational Physics, Physical Chemistry Chemical Physics, Journal of Chem. Phys., Communications in Computational Physics, Journal of Phys. Chem.*

Member of the **American Chemical Society, Biophysical Society and Protein Society**.

RESEARCH INTERESTS

- Theory and numerical approaches for continuum modeling of biomolecular/cellular systems and processes such as electrodiffusion described by Poisson-Nernst-Planck equation and beyond. Some fundamental biophysical problems and (e.g., hydrophobicity, solvation free energy) and abnormal phenomena (e.g., like-charge attraction) are also aimed to be treated in this frame through prediction of the solution structure including ions, water, and biomolecules.
- Molecular biophysics and molecular dynamics simulation study on specific system such as protein kinase. An example problem is how the dynamics and fluctuating energy landscape correlate with the reaction rate.

TEACHING EXPERIENCE

07/2004 - 08/2006	**Co-supervisor**, University of California at San Diego, San Diego. Co-supervised a student research project on ligand binding to protein kinase.
09/1999 - 07/2002	**Co-supervisor,** University of Science and Technology of China and Beijing Polytechnic University, China. Co-supervised a number of postgraduate masters student and undergraduate research projects.
09/1998 - 01/1999	**Teaching assistant**, University of Science and Technology of China. *Quantum mechanics.*
07/1993 - 09/1997	**Lecturer**, Yunnan Agriculture University, Kunming, China. Taught courses: *general physics* and *calculus*; Mentored a number of *experimental courses of basic physics.* Instructed students' *social investigation.*

HONORS AND AWARDS

2006 Travel award, ICAM workshop on Multiscale Interactions and Dynamics in Biological Systems at Washington University in St. Louis on May 27-29, 2006.

2001 Research paper award of young researcher, Conference on Biomedical Engineering 2001 (CBME), Wuhan, China.

2000 Guanghua Education Scholarship in University of Science and Technology of China.

1999 Visiting Student program (3 months), the International Center for Theoretical Physics (ICTP), Trieste, Italy.

SELECTED PUBLICATIONS

Invited review:

1. B. Z. Lu, Y. C. Zhou, Michael J. Holst, and J. A. McCammon. Recent progress in numerical solution of the Poisson-Boltzmann equation for biophysical applications. *Commun. in Comput. Phys.*, 3(5):9731009, 2008.

Journal paper:

[1] B. Z. Lu and J. A. McCammon. Molecular surface-free continuum model for electrodiffusion processes. *Chem. Phys. Lett.*, 451(4-6):282–286, 2008.

[2] Y. C. Zhou, B. Z. Lu, Gary A. Huber, Michael J. Holst, and J. A. McCammon. Continuum simulations of acetylcholine consumption by acetylcholinesterase: A Poisson-Nernst-Planck approach. *J. Phys. Chem. B*, 112(2):270–275, 2008.

[3] B. Z. Lu, Y. C. Zhou, Gary A. Huber, Stephen D. Bond, Michael J. Holst, and J. Andrew McCammon. Electrodiffusion: A continuum modeling framework for biomolecular systems with realistic spatiotemporal resolution. *J. Chem. Phys.*, 127(13):135102, 2007.

[4] B. Z. Lu, X. L. Cheng, and J. A. McCammon. "New-Version-Fast-Multipole Method" Accelerated Electrostatic Calculations in Biomolecular Systems. *J. Comput. Phys.*, 226(2):1348–1366, 2007.

[5] B. Z. Lu and J. A. McCammon. Improved boundary element methods for Poisson-Boltzmann electrostatic potential and force calculations. *J. Chem. Theory. Comput.*, 3(3):1134–1142, 2007.

[6] B. Z. Lu, X. L. Cheng, J. F. Huang, and J. A. McCammon. Order N algorithm for computation of electrostatic interactions in biomolecular systems. *Proc. Natl. Acad. Sci. U. S. A.*, 103(51):19314–19319, 2006.

[7] T. J. Hou, K. Chen, W. McLaughlin, B. Z. Lu, and W. Wang. Computational analysis and prediction of the Binding Motif and Protein Interacting Partners of the Abl SH3 domain. *PLoS Computational Biology*, 2(1):e1, 2006.

[8] T. J. Hou, W. McLaughlin, B. Z. Lu, K. Chen, and W. Wang. Prediction of Binding Affinities between the Human Amphiphysin-1 SH3 Domain and Its Peptide Ligands Using Homology Modeling, Molecular dynamics and Molecular Field Analysis. *J. Proteome research*, 5(1):32–43, 2006.

[9] X. L. Cheng, B. Z. Lu, B. Grant, R. Law, and J. A. McCammon. Channel opening motion of $\alpha 7$ nicotinic acetylcholine receptor as suggested by normal mode analysis. *J. Mol. Biol.*, 355(2):310–324, 2006.

[10] M. U. Ung, B. Z. Lu*, and J. A. McCammon. E230Q mutation of the catalytic subunit of cAMP-dependent protein kinase affects local structure and the binding of peptide inhibitor. *Biopolymers*, 81(6):428–439, 2006.

[11] B. Z. Lu, D. Q. Zhang, and J. A. McCammon. Computation of electrostatic forces between solvated molecules determined by the Poisson-Boltzmann equation using a boundary element method. *J. Chem. Phys.*, 122(21):214102, 2005.

[12] B. Z. Lu, X. L. Cheng, T. J. Hou, and J. A. McCammon. Calculation of the Maxwell stress tensor and the Poisson-Boltzmann force on a solvated molecular surface using hypersingular boundary integrals. *J. Chem. Phys.*, 123(8):084904, 2005.

[13] B. Z. Lu, C. F. Wong, and J. A. McCammon. Release of ADP from the catalytic subunit of protein kinase A: A molecular dynamics simulation study. *Protein Sci.*, 14(1):159–168, 2005.

[14] B. Z. Lu and C. F. Wong. Direct calculation of entropy loss due to reduced translational and rotational motions upon molecular binding. *Biopolymers*, 79:277–285, 2005.

[15] Y. H. Yu, B. Z. Lu*, J. G. Han, and P. F. Zhang. Scoring the protein-protein docked structures based on the balance and tightness of binding. *J. Comput. Aided Mol. Des*, 18(4):251–260, 2004.

[16] J. G. Han, Z. Y. Ren, and B. Z. Lu. Geometries and stabilities of re-doped si-n (n=1-12) clusters: a density functional investigation. *J. Phys. Chem. A*, 108(23):5100–5110, 2004.

[17] B. Z. Lu, B. H. Wang, W. Z. Chen, and C. X. Wang. A new computational approach for real protein folding prediction. *Protein Eng.*, 16(9):659–663, 2003.

[18] Y. H. Yu, C. H. Li, B. Z. Lu, W. Z. Chen, and C. X. Wang. A new method to select the near-native conformations from the docked structures. *Acta Phys.-Chim. Sin. (in Chinese)*, 19(8):757–761, 2003.

[19] B. Z. Lu, C. X. Wang, and B. H. Wang. A new minimization method for real protein folding prediction. *Chin. J. Chem. Phys. (in Chinese)*, 16(2):117–121, 2003.

[20] W. Y. Wang, B. Z. Lu, W. Z. Chen, and C. X. Wang. Study on the stability of insulin hexamer in solution by molecular dynamics simulations. *Acta Chim. Sin. (in Chinese)*, 60(12):2129–2134, 2002.

[21] W. Y. Wang, B. Z. Lu, W. Z. Chen, and C. X. Wang. The study on the flexibility of insulin hexamer in solution by molecular dynamics simulations. *Acta Biophysica Sinica*, (19):35–40, 2003.

[22] B. Z. Lu, W. Z. Chen, C. X. Wang, and X. J. Xu. Protein molecular dynamics with electrostatic force entirely determined by a single Poisson-Boltzmann calculation. *Proteins*, 48(3):497–504, 2002.

[23] X. H. Ma, C. H. Li, B. Z. Lu, W. Z. Chen, C. X. Wang, and X. J. Xu. Salt and pH-dependent properties of native and mutant insulin. *Chin. Sci. Bull.*, 47(6):464–466, 2002.

[24] B. Z. Lu, C. X. Wang, W. Z. Chen, S. Z. Wan, and Y. Y. Shi. A stochastic dynamics simulation study associated with hydration force and friction memory effect. *J. Phys. Chem. B*, 104(29):6877–6883, 2000.

[25] B. Z. Lu, W. Z. Chen, and C. X. Wang. The generalized Langevin dynamics associated with boundary element method. *Chinese Science Bulletin*, 45:1482–1486, 2000.

TALKS ON CONFERENCE, WORKSHOP, OR SEMINAR

"Modelling of Electrostatics and Diffusion Processes in Biological Systems", Frontiers in Science (FIS) program – Integrated Physics, Biology, Chemistry, Mathematics and Computer Science, a CTBP-CSUSM Seminar Series, California State University San Marcos, Sept. 25, 2008.

"Fully-continuum diffusion – the Poisson-Nernst-Planck model and some extensions" at the 2008 CTBP Summer School, Coarse-Grained Physical Modeling of Biological Systems: Advanced Theory and Methods, San Diego, CA, August 14, 2008.

Continuum modeling of electrodiffusion: from equlibrium to nonequilibrium states, 4/25/08, Dept. of Molecular Biology & Biochemistry, University of California at Irvine.

Informal Seminars on Mathematics and Biochemistry-Biophysics, "Boundary integral methods for electrostatics in biomolecules. Part I: An overview", 4/8/08, Spring quarter, 2008; And "Electrodiffusion", 10/2/07, Summer and Fall quarter, 2007. Department of Mathematics, UCSD.

"Electrostatics, density distribution, and diffusion - A continuum modeling frame with realistic spatiotemporal resolution" on March 7, 2007 at the Biophysical Society 51st Annual Meeting. Baltimore, Maryland, MD, March 3-7, 2007.

"Cyberinfrastructure and multiscale modeling approaches", NBCR (National Biomedical Computation Resource) Summer Institute 2006, La Jolla, California, August 7-11 August, 2006, weblink: http://nbcr.net/si/2006/contact.php (Instructor).

"Accelerating computations to order N for electrostatic interactions of biomolecular systems" on Sep. 11, 2006 at the 232nd ACS National Meeting, San Francisco, CA, September 10-14, 2006.

"Molecular Simulations of Protein Kinase A: Release of ADP from the catalytic subunit of PKA: A MD simulation study" on July 12, 2005 at ICAM Frontiers of Science Symposium: Signal Transduction and Protein Phosphorylation, UC San Diego, CA.

"A new minimization method for real protein folding prediction," presented on May. 30 at the Seventh Symposium on Life Science at Home and Abroad, Beijing, China.

"Dynamics simulation for protein-protein interaction" at Proceedings of Chinese Biomedical Engineering 2001 (CBME), Wuhan, China.