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EDUCATION

- 09/2008-present, Research Associate
Department of Bioengineering, Stanford University
- 08/2006-09/2008, Distinguished Postdoctoral Scholar
Simbios Center, Stanford University
Research Advisors: Professor Michael Levitt and Professor Vijay S. Pande
- 02/2004-07/2006, PhD in Chemical Physics
Chemistry Department, Columbia University
Research Advisor: Professor Bruce J. Berne
Thesis Title: “Theoretical and Computational Studies of Hydrophobic Effect at Large Length Scale”
- 02/2004-05/2006, Master of Philosophy
Chemistry Department, Columbia University
- 09/2001-02/2004, Master of Arts, GPA 4.1/4.0
Chemistry Department, Columbia University
- 09/1997-06/2001, Bachelor of Science (Graduate with Honor)
Department of Chemical Physics
University of Science and Technology of China (USTC)

RESEARCH EXPERIENCE

- Sep 2008 – Present, Research Associate
Aug 2006 – Sep 2008, Distinguished Postdoctoral Scholar
Simbios Center, Stanford University
Advisors: Professor Michael Levitt and Professor Vijay S. Pande

My current research focuses on understanding the thermodynamics and kinetics of the folding of proteins and small RNA molecules using all-atom simulations with explicit solvent. To obtain converged sampling I have implemented generalized ensemble algorithms such as Replica Exchange,

and Simulated Tempering on the Folding@home distributed computing environment. I have developed a more efficient scheme to determine weights for Simulated Tempering simulations and novel algorithms for the construction of Markov State Models (MSM) to study kinetics. Other projects I am working on include (1) developing a multi-scale knowledge based potential for RNA structure refinement and molecular dynamics simulations, and (2) applying computational tools to elucidate the fundamental mechanism of RNA transcription.

- Dec 01 – July 06, Research Assistant
Chemistry Dept, Columbia University
Advisor: Prof. Bruce J. Berne

My graduate research focused on understanding the hydrophobic effect in protein folding. I studied hydrophobic interactions and “dewetting” phenomena using molecular dynamics simulations for systems ranging from nano-size hydrophobic plates to proteins. I also developed the Hydrophobic-Aided Replicate Exchange method (HAREM) to enhance sampling, studied water dynamics in the solvation shell of a two-domain protein, and did molecular dynamics studies of an environmentally friendly “green” chemistry process—the extraction of organic compounds from room temperature ionic liquids using supercritical CO₂.

TEACHING EXPERIENCE

- Spring 2002, Teaching Assistant for General Chemistry Lab
Columbia University, Chemistry Dept
- Fall 2002, Teaching Assistant for Statistical Thermodynamics
Columbia University, Chemistry Dept
- Spring 2003, Teaching Assistant for General Chemistry Lab
Columbia University, Chemistry Dept

PUBLICATIONS

1. **Huang, X.**, Bowman, G. R., Bacallado, S., and Pande, V. S. “Adaptive Seeding Method: Rapid Equilibrium Sampling Initiated from Non-equilibrium Data.” *Proc. Nat. Acad. Sci. U.S.A.*, In Press, (2009)
2. Bowman, G. R., **Huang, X.**, and Pande, V. S. “Using generalized ensemble simulations and Markov state models to identify conformational states.” *Methods*, In Press, (2009)
3. Wang D., Bushnell D. A., **Huang X.**, Westover K. D., Levitt M., and Kornberg R. D. “Structural Basis of Backtracked RNA Polymerase II Ternary Complex.” *Science*, *Science*, 324, 1203-1206, (2009)
4. Kelley, N., **Huang X.**, Tamm, S., Spiess C., Frydman, J., Pande, V. S. “The Predicted Structure of the Headpiece of the Huntingtin Protein and its Implications on Huntingtin Aggregation.” *J. Mol. Bio.*, 338, 919-927, (2009)

5. Yao, Y., Sun, J., **Huang, X.**, Bowman, G. R., Singh, G., Lesnick, M., Guibas, L. J., Pande, V. S., Carlsson, G. "Topological Methods for Exploring Low-density States on Biomolecular Folding Pathways", *J. Chem. Phys.*, 130, 144115, (2009)
6. Bowman, G. R., **Huang, X.**, Yao, Y., Sun, J., Carlsson, G., Guibas, L. J., Pande V. S. "Structural Insight into RNA Hairpin Folding Intermediates." *J. Am. Chem. Soc.*, 130, 9676–9678, 2008
7. **Huang, X.**, Bowman, G. R., and Pande, V. S. "Convergence of Folding Free Energy Landscapes Via Application of Enhanced Sampling Methods in a Distributed Computing Environment." *J. Chem. Phys.*, 128, 205106, 2008
8. Hu, Z., **Huang, X.**, Annapureddy, H. V. R., and Margulis C. J. "Molecular Dynamics Study of the Temperature-Dependent Optical Kerr Effect Spectra and Intermolecular Dynamics of Room Temperature Ionic Liquid 1-Methoxyethylpyridinium Dicyanoamide." *J. Phys. Chem. B*, 112, 7837–7849, 2008
9. **Huang, X.**, Hagen, M., Kim, B., Friesner, R. A., Zhou, R and Berne, B. J. "Replica Exchange with Solute Tempering: Efficiency in Large Scale Systems." *J. Phys. Chem. B*, 111, 5405-5410, 2007
10. Hua, L., **Huang, X.**, Liu, P., Zhou, R. and Berne, B. J. "Nanoscale Dewetting Transition in Protein Complex Folding." *J. Phys. Chem. B*, 111, 9069-9077, 2007
6. Liu, P., **Huang, X.**, Zhou, R., Berne, B. J. "Hydrophobic Aided Replica Exchange: an Efficient Algorithm for Protein Folding in Explicit Solvent." *J. Phys. Chem. B*, 110, 19018-19022, 2006
7. Hua, L., **Huang, X.**, Zhou, R., Berne, B. J. "Dynamics of Water Confined in the Interdomain Region of a Multi-domain Protein." *J. Phys. Chem. B*, 110, 8, 3704-3711, 2006
8. **Huang, X.**, Margulis, C. J., Li, Y., Berne, B. J. "Why is the Partial Molar Volume of CO₂ So Small When Dissolved in a Room Temperature Ionic Liquid? Structure and Dynamics of CO₂ Dissolved in [Bmim+][PF₆-]." *J. Am. Chem. Soc.*, 127, 50, 17842-17851, 2005
9. **Huang, X.**, Zhou, R., Berne, B. J. "Drying and Hydrophobic Collapse of Paraffin-like Plates." *J. Phys. Chem. B*, 109, 3546 –3552, 2005
10. Liu, P., **Huang, X.**, Zhou, R., Berne, B. J. "Observation of a Dewetting Transition in the Collapse of the Melittin Tetramer." *Nature*, 437, 159-162, 2005
11. **Huang, X.**, Margulis, C.J., Berne, B.J. "Comment on "Do Molecules as Small as Neopentane Induce a Hydrophobic Response Similar to that of Large Hydrophobic Surfaces?" - Reply " *J. Phys. Chem. B*, 108, 9373-9374, 2004
12. Zhou, R., **Huang, X.**, Margulis, C. J., Berne, B. J. "Hydrophobic Collapse in Multidomain Protein Folding " *Science*, 305, 1605-1609, 2004

13. **Huang, X.**, Margulis, C. J., Berne, B. J. "Do Molecules as Small as Neopentane Induce a Hydrophobic Response Similar to that of Large Hydrophobic Surfaces?" *J. Phys. Chem. B*, 107, 11742-11748, 2003
14. **Huang, X.**, Margulis, C. J., Berne, B. J. "Dewetting-induced Collapse of Hydrophobic Particles." *Proc. Nat. Acad. Sci. U.S.A.*, 100, 11953-11958, 2003
15. **Huang, X.**, Yao Y., Sun J., Bowman G.R., Guibas L., and Carlsson G. and Pande V.S. "Constructing Multi-resolution Markov State Models(MSMs) to elucidate RNA hairpin folding mechanisms", *The Pacific Symposium on Biocomputing 2010*, Submitted
16. Sun J, Yao Y, **Huang, X.**, Pande V.S., Carlsson G. and Guibas L., "A Fast Geometric Clustering Method on Conformation Space of Biomolecules", *J. Phys. Chem. B.*, Submitted, (2009)
17. Young T., Hua L., **Huang, X.**, Abel R., Friesner R., Berne B.J., "Dewetting Transitions in Protein Cavities", *Proteins.*, Submitted, (2009)

PRESENTATIONS

Invited Talks

1. USA-Mexico Workshop in Biological Chemistry, Mexico City, Mexico, March 2009
2. Departmental Seminar, Department of Biochemistry and Molecular Biophysics, Washington University, St. Louis, MO, March 9, 2009
3. Computational Molecular Biophysics Seminar, Department of Biochemistry and Molecular Biophysics, University of Tennessee, Knoxville, TN, Feb 25, 2009
4. Theoretical Chemistry Seminar, Department of Chemistry, Hong Kong University of Science and Technology, Hong Kong, Feb 16, 2009
5. Departmental Colloquium, Department of Physics, Chinese University of Hong Kong, Hong Kong, Feb 6, 2009
6. Departmental Seminar, Department of Physics, Chinese University of Hong Kong, Hong Kong, Feb 5, 2009
7. Physical Chemistry Seminar, Department of Chemistry, Syracuse University, Syracuse, NY, Jan 29, 2009
8. Biophysics and Biophysical Chemistry Seminar, School of Medicine, Johns Hopkins University, Jan 21, 2009
9. Physical Chemistry Seminar, Department of Chemistry, Wayne State University, Detroit, MI, Jan 12, 2009

10. Theoretical Chemistry Seminar, Department of Chemistry, University of California, Merced, Merced, CA, Dec 12, 2008
11. Departmental Seminar, Department of Systems and Computational Biology, Albert Einstein College of Medicine, Bronx, NY, Nov 24, 2008
12. All Hands Meeting (AHM) for the NIH Roadmap National Centers for Biomedical Computing (NCBC), Bethesda, Maryland, Aug 2008.
13. Telluride Science Research Center workshop Algorithmic Development on Enhanced Sampling, Telluride, CO, July 2008.
14. Simbios Seminar, NIH center for Biomedical Computation at Stanford University. Stanford, CA, May 2008.
15. 235th ACS National Meeting, New Orleans, LA, April 2008
16. Simbios Seminar, NIH center for Biomedical Computation at Stanford University. Stanford, CA, May 2007.

Contributed talks:

1. Bay Area RNA Meeting, San Francisco, CA, Jun 2008
2. 235th ACS National Meeting, New Orleans, Apr 2008.

Selected poster presentations:

1. **Huang, X.**, Bowman, G. R., Bacallado, S., and Pande, V. S. "Adaptive Seeding Method". Molecular Kinetics 2009, Berlin, Germany, May 2009
2. **Huang X**, Wang D, Weiss D, Bushnell DA, Kornberg RD, Levitt M, "Computational Studies to Elucidate the Role of a Critical Histidine Residue in Transcription Elongation", 2008 Transcriptional Regulation by Chromatin and RNA Polymerase II, Lake Tahoe, CA, Oct, 2008
3. **Huang, X.**, Bowman, G.R., Pande, V.S. "Convergence of folding free energy landscapes via application of enhanced sampling methods", Gordon Research Conference on Protein Folding Dynamics, Ventura, CA, Jan 2008
4. **Huang, X.**, "Exploring the folding free energy landscape of a helical peptide via serial replica exchange method", BCATS, 2006, Stanford, CA, Oct 2006.
5. **Huang, X.**, Li Y., Margulis, C.J., Berne, B.J. "A molecular dynamics simulation study of structure and dynamics of CO₂ dissolved in a room temperature ionic liquid", 231st ACS National Meeting, Atlanta, GA, March 2006

6. **Huang, X.**, Liu, P, Zhou, R, Berne, B.J., “Hydrophobic-aided replica exchange: An efficient algorithm for sampling biological systems in explicit solvent”, 231st ACS National Meeting, Atlanta, GA, March 2006. (CCG Excellence Award Winner Poster)
7. **Huang, X.**, Margulis, C.J., Zhou, R, Berne, B.J., “Drying and hydrophobic collapse in the multi-domain protein and protein oligomers”, 230th ACS National Meeting, Washington, DC, August 2005.

AWARDS & FELLOWSHIP

- CCG Excellence Award, American Chemical Society, COMP Division. (Atlanta, 2006)
- Faculty Fellowship, Columbia University 2001-2003
2004-2006
- Blanche R. and David Kasindorf Fellowship in Physical Chemistry, Columbia University 2003-2004
- Scholarships for excellent students, USTC 2000
- Duohui He Fellowship, USTC 1998
- Zhongzhi Zhang Fellowship, USTC 1997

PROGRAM COMMITTEES

- Organize committee. 9th Annual Symposium of Biomedical Computing at Stanford, Stanford, CA, Oct, 2008
- Session co-chair. Multi-resolution Modeling of Biological Macromolecules Session, Pacific Symposium on Biocomputin, Big Island, Hawaii, Jan, 2010

Editorial Activities

Server as the reviewer for:

- Journal of Molecular Biology
- Nucleic Acid Research
- Plos Computational Biology
- RNA