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YUHUI CHENG, Ph.D.

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EDUCATION AND TRAINING

- Postdoctoral Fellow**, Computational Chemistry and Biology, June, 2007-present
 National Biomedical Computation Resource, University of California, San Diego La Jolla, CA
- Ph.D. in Physical Chemistry**, June, 2007. Advisors: Prof. James Andrew McCammon
 University of California, San Diego La Jolla, CA
- B.S. in Chemical Physics**, July, 2002.
 University of Science & Technology of China Hefei, P. R. China

RESEARCH EXPERIENCE

University of California, San Diego La Jolla, CA

2007-present: **Postdoctoral Fellow** with Prof. Michael J. Holst and James Andrew McCammon

2002-2007: **Research Assistant** with Prof. James Andrew McCammon

Invent the continuum modeling and coarse-grained Brownian dynamics (CGBD) package SMOL for multiscale biological reaction coupled diffusion studies. (<http://mccammon.ucsd.edu/smol/>)

- Developing the C++ software package SMOL with finite element method for computational chemistry and neuroscience, for example: ACh diffusion in a single AChE cluster, APS²⁻ channeling in sulfate activating complexes, synaptic transmission and drug-induced modification of ionic conductance in neuromuscular junction, Ca²⁺ diffusion in cardiovascular t-tubule in the normal and failing rodent heart.
- Programming the state-in-the-art CGBD code for simulating electrostatic effect in synaptic transmission.
- Coding the tool chain for tetrahedral mesh generation, optimization and refinement and visualization of continuum modeling output with TetGen, OpenDX, GMV, etc.

Accomplish enzyme-ligand interaction and reaction mechanism prediction project.

- Exploring the nature of agonist/antagonist interactions in wild-type and mutated mouse and human acetylcholinesterase (AChE) with molecular docking approach combined with sophisticated binding free energy post-processing techniques; structure-based identification of new ligands specifically targeting the AChE using virtual screening; and accurate binding free energy calculations with QM/MM-FEP and thermodynamic integration approaches;
- Understanding the relation between the phosphorylation and conformation changes in the wild protein kinase A and its mutants with various computational approaches, such as: evolutionary profile analysis, homology modeling, molecular dynamics and QM/MM approaches.
- Investigating Group I Intron cleavage reaction mechanism and role of divalent metal ion Mg²⁺ with ab initio pseudo-bond QM/MM approach.

University of Science and Technology of China Hefei, P. R. China

2001 – 2002: **Undergraduate Research Assistant** in Biomass Clean Energy Laboratory.

- Applying quantum chemistry on different organic molecules to explore various chemical and physiological properties. The project concentrates on visualizing and drawing 3-D target molecules, analyzing the energy profile of bond breaking/forming and pi-cation interactions, and comparing various functioning groups, anions or cations.

TECHNICAL EXPERTISE

Languages C, C++, Perl/C-shell, Tcl/Tk, Python, Fortran, XML

Software Insight II, Sybyl, Autodock, VMD, PyMOL, NAMD, Amber, CHARMm, Gaussian 98 and 03, ab initio QM/MM, Molden, Chimera, OpenDX, GMV, Geomview, NetGen, TetGen, Data Display Debugger, Concurrent Versions System, Finite Element Tool Kit, Matlab, APBS.

Systems Windows 2000, XP, Linux CentOS, UNIX, Mac OS X

HONORS AND AWARDS

- Travel Awards: The Pacific Symposium on Biocomputing 2009
- Travel Awards: IXth Interational Meeting on Cholinesterase 2007
- Travel Awards: ICAM Workshop, St. Louis, 2005
- Excellent Student Awards: University of Science and Technology of China, 2002

SELECTED PUBLICATIONS

1. **Yuhui Cheng**, Anushka Michailova, Zeyun Yu, Michael J. Holst and J. Andrew McCammon, "Effects of 3D t-tubule anatomy on Ca^{2+} signaling in rodent ventricular myocytes with inhibited sarcoplasmic reticulum", in preparation.
2. **Yuhui Cheng**, Chia-en Chang, Zeyun Yu, Yongjie Zhang, Meihao Sun, Thomas S. Leyh, Michael J. Holst and J. Andrew McCammon, "Diffusional Channeling in the Sulfate Activating Complex: Combined Continuum Modeling and Coarse-grained Brownian Dynamics Studies", *Biophys. J.* 2008, 95: 4659-4667.
3. **Yuhui Cheng**, Xiaolin Cheng, Zoran Radić and J. Andrew McCammon, "Acetylcholinesterase: Mechanisms of Covalent Inhibition of Wild-type and H447I Mutant Determined by Computational Analyses" *J. Am. Chem. Soc.*, 2007, 129: 6562-6570.
4. **Yuhui Cheng**, Jason K. Suen, Deqiang Zhang, Stephen D. Bond, Yongjie Zhang, Yuhua Song, Nathan A. Baker, Chandrajit L. Bajaj, Michael J. Holst, and J. Andrew McCammon, "Finite Element Analysis of the Time-Dependent Smoluchowski Equation for Acetylcholinesterase Reaction Rate Calculations", *Biophys. J.*, 2007, 92: 3397-3406
5. **Yuhui Cheng**, Jason K. Suen, Zoran Radić, Stephen D. Bond, Michael J. Holst and J. Andrew McCammon, "Continuum Simulations of Acetylcholine Diffusion with Reaction-determined Boundaries in Neuromuscular Junction Models", *Biophys. Chem.*, 2007, 127: 129-139.
6. Sanjib Senapati, **Yuhui Cheng**, and J. Andrew McCammon, "Why is the syn isomer of TZ2PA6 the sole product of "click chemistry" in the acetylcholinesterase environment", *J. Med. Chem.* 2006, 49: 6222-6230.
7. **Yuhui Cheng**, Yingkai Zhang, and J. Andrew McCammon, "How does activation loop phosphorylation modulate catalytic activity in the cAMP-dependent protein kinase: A Theoretical Study", *Protein Science.* 2006, 15: 672-683.
8. **Yuhui Cheng**, Yingkai Zhang, and J. Andrew McCammon, "How Does the cAMP-Dependent Protein Kinase Catalyze the Phosphorylation Reaction: an ab initio QM/MM Study", *J. Am. Chem. Soc.* 2005, 127: 1553-1562.
9. **Yuhui Cheng**, Yao Fu, Lei Liu, Qing-Xiang Guo, "Substituent effects on the hydrogen bonding between 4-substituted phenols and HF, H₂O, NH₃", *Chinese Journal of Chemistry*, 2003, 21: 1433-1439
10. **Yuhui Cheng**, Lei Liu, Yao Fu, Rong Chen, Xiao-Song Li, Qing-Xiang Guo, "Counterion effects on the cation-pi interaction between alkaline earth cations and benzene", *J. Phys. Chem. A*, 2002, 106: 11215-11220.
11. **Yuhui Cheng**, Xing Zhao, Ke-Sheng Song, Lei Liu, Qingxiang Guo, "Remote substituent effects on bond dissociation energies of para-substituted aromatic silanes", *J. Org. Chem.*, 2002, 67: 6638-6645.
12. **Yuhui Cheng**, Ying Fang, Xing Zhao, Lei Liu, Qing-Xiang Guo, "A theoretical study of the substituent effects on the P-X (X = H, F, Cl) bond dissociation energies in para- and meta-substituted aromatic phosphines", *Bull. Chem. Soc. Jpn.*, 2002, 75: 1715-1722.
13. Lei Liu, **Yuhui Cheng**, Yao Fu, Rong Chen, Qing-Xiang Guo, "The Nonpolar Resonance Effects and the Non-Hammett Behaviors", *J Chem Inf Comput Sci.*, 2002, 42: 1164-1170.
14. Ke-Sheng Song, **Yuhui Cheng**, Yao Fu, Lei Liu, Xiao-Song Li, Qing-Xiang Guo, "Radical stabilization energies of substituted XNH • radicals", *J. Phys. Chem. A*, 2002, 106: 6651-6658.
15. **Yuhui Cheng**, Lei Liu, Ke-Sheng Song, Qing-Xiang Guo, "A theoretical study on the homolytic dissociation energies of H-N⁺ bonds", *J. Chem. Soc. Perkin Trans. II*, 2002, 2: 1406-1411