

Dian Jiao

Sandia National Laboratories
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SUMMARY

- Computational chemist with over 7 years of interdisciplinary research experience.
- Key contributor to \$1.5 million NIH R01 project.
- Strong record of closely collaborating with experimentalists.
- Publications in top journals and presentations at international conferences.
- National award winner.

EDUCATION

Ph.D. Biomedical Engineering, *University of Texas at Austin*, December 2009

“Ion Modeling and Ligand-protein Binding Calculation with a Polarizable Force Field.”

M.S. Biomedical Engineering, *Southeast University (China)*, May 2005

“Genomic Sequence Analysis based on Features.”

B.S. Biomedical Engineering, *Southeast University (China)*, June 2002

RESEARCH EXPERIENCE

Postdoctoral Appointee, *Sandia National Laboratories*, 2009 to present

Advisor Dr. Susan Rempe, 2011 LDRD 100 award winner

CO₂ sequestration

- Estimated the pKa shift of carbonic anhydrase using QM/MM.
- Investigated catalytic mechanism of carbonic anhydrase to design CO₂ sequestering biopolymer
- Measured CO₂ solvation in liquid water with quasi-chemical theory.

Nanoparticle formation of superalloy

- Calculated redox potential of nickel ions with DFT and AIMD simulation.
- Examined superalloy growth by computing the dimerization free energies.

Graduate Research Assistant, *University of Texas at Austin*, 2005-2009

Advisor Dr. Pengyu Ren

Polypyrrole modeling for biosensor design

- Modeled polymer with molecular mechanical potential and high level QM methods.
- Explored structure and physical/chemical properties of the polymer at atomic level.

Ligand-protein binding

- Originated model for illustrating charge-charge interactions between ligand and protein.
- Achieved excellent chemical accuracy in ligand-protein binding affinity prediction with MD simulation.

ERK2 kinase drug discovery

- Virtue-screened lead candidates for extracellular signal-regulated kinase.
- Built potential lead molecule with strong binding affinity.

Metal ions and metalloprotein

- Published first polarizable force field model for divalent ions Ca²⁺ and Mg²⁺.
- Computed metal ion solvation free energies and studied solvation dynamics.

- Evaluated metal ion selectivity in EF hand protein.

Research Assistant, Southeast University, 2002-2005

Advisor Dr. Xiao Sun

Database development

- Developed Genome Feature Database System with JSP+Oracle.
- Identified similar genomic sequences based on statistical features.

TEACHING EXPERIENCE

Mentor, Sandia National Labs, Jun 2011 to present

- Trained a graduate student to do quantum mechanics calculation.

Teaching Assistant, University of Texas at Austin

Network Analysis in Biomedical Engineering, 2009 Spring

- Held weekly office hours.
- Developed problems for midterm and final exams.
- Led review sessions and presented lecture in professor's absence.

Introduction to Computing for Biomedical Engineers, 2007 Spring

- Conducted computer lab sessions.

Physiology I, 2006 Fall

- Led discussion sessions.
- Graded homeworks and exams.

PUBLICATIONS:

- **Jiao, D.**; Rempe, S. "Theoretical calculation for the pK_a of zinc-bound water in carbonic anhydrase." *Biochem.* (In prep).
- **Jiao, D.**; Rempe, S. "CO₂ solvation free energy using quasi-chemical theory". *J. Chem Phys.* 2011. 134, 224506.
- **Jiao, D.**; Leung, K.; *et al.* "First Principles Calculations of Atomic Nickel Redox Potentials and Dimerization Free Energies: A Study of Metal Nanoparticle Growth". *J. Chem. Theory Comput.* 2011. 7, 485-495.
- **Jiao, D.**; Zhang, J.; *et al.* "Binding Free Energy of Trypsin-Ligands from Explicit and Implicit Solvent Simulations with Polarizable Potential". *J. Comput. Chem.* 2009. 30, 1701-1711.
- Shi, Y.; **Jiao, D.**; *et al.* "Trypsin-ligand binding free energy calculation with AMOEBA", *EMBS Annual International Conference of the IEEE.* 2009.
- **Jiao, D.**; Golubkov, P. A.; *et al.* "Calculation of Protein-Ligand Binding Free Energy using a Polarizable Potential". *Proc. Natl. Acad. Sci. U. S. A.* 2008. 105, 6290-6295.
- Liu Z.; **Jiao D.**; *et al.* "Base-Base Correlation: A novel sequence feature and its applications". *Bioinformatics and Biomedical Engineering, ICBBE.* 2007.
- **Jiao, D.**; King, C; *et al.* "Simulation of Ca²⁺ and Mg²⁺ Solvation using Polarizable Atomic Multipole Potential", *J. Phys. Chem. B*, 2006. 110, 18553-18559.
- **Jiao, D.**; Gu, M; *et al.* "A Sequence Feature Based Searching System for Nucleotide Database." *Chinese J. Biomed. Eng.*, 2006. 25, 694-699.
- Liu, Z.; **Jiao, D.**; *et al.* "Classifying genomic sequences by sequence feature analysis", *Genomics Proteomics Bioinformatics.* 2005. 3, 201-205.
- **Jiao, D.**; Xie, J; *et al.* "Analysis of the Nuclear Location Signal of SARS-Cov Nucleoprotein." *Chinese Biomed. Engi. Annual Meeting*, 2003.

PRESENTATIONS:

- Jiao, D.; Leung, L.; Rempe, S. "Theoretical Studies of Ni Nanoparticle Growth and pK_a Shift in Carbonic Anhydrase." **Invited talk at Los Alamos National Laboratories**. Los Alamos, NM November 2011.
- Jiao, D.; Rempe, S. "Combined DFT and Continuum Calculation of pK_a s in Carbonic Anhydrase." **American Chemical Society Meeting**. Denver, CO. August, 2011.
- Jiao, D.; Leung, L.; Nenoff, T.; Rempe, S. "First Principles Calculations of Atomic Nickel Redox Potentials and Dimerization Free Energies: A Study of Metal Nanoparticle Growth." **Sandia/UNM Symposium on Nanoparticle Human Interactions**, University of New Mexico, June 2011.
- Jiao, D.; Rempe, S. "CO₂ Sequestration Study by Quasi-chemical Theory." **American Chemical Society Meeting**. Anaheim, CA. March, 2011.
- Jiao, D.; Rempe, S. "Quasi-chemical theory applied to study mechanisms of Ni nanoparticle formation and CO₂ sequestration." **Theory and Simulation of Nanoscale Materials Workshop**, Sandia National Laboratories. October, 2010.
- Jiao, D.; Rempe, S. "Quasi-chemical Theory Applied to Study Mechanisms of Ni Nanoparticle Formation and CO₂ Sequestration." **American Chemical Society Meeting**. Boston, MA. August, 2010.
- Jiao, D.; Rempe, S. "Hydration Free Energy Calculations with Quasi-chemical Theory." **Ion in Biology Workshop**, Telluride, CO. July 2010.
- Jiao, D.; Ren, P. "Calculation of protein-ligand binding free energy by a polarizable force field." **American Chemical Society Meeting**. Salt Lake City, UT. March, 2009.
- Jiao, D.; Ren, P. "Molecular Simulation of Protein-Ligand Binding Using a Polarizable Force Field." **Biomedical Engineering Society Meeting**. St. Louis, MO. September, 2008.
- Jiao, D.; Ren, P. "Ligand Binding Free Energy Simulation by a Polarizable Force Field." **Workshop on Bioinformatics, Computational Biology and Systems Biology**. Texas A&M University. February, 2008.
- Jiao, D.; Ren, P. "Ligand Binding Free Energy Simulation by a Polarizable Force Field." **Biomedical Engineering Society Meeting**. Los Angeles, CA. September, 2007.
- Jiao, D.; Ren, P. "Ligand Binding Affinity Estimated by AMOEBA polarizable force field." **Houston Society for Engineering in Medicine and Biology Annual Meeting**. February, 2007.

AWARDS

- CCG Research Excellence Award, American Chemical Society, 2009.
- Graduate School Continuing Fellowship, University of Texas at Austin, 2008.