

Curriculum Vitae
Jana K. Shen, Ph.D.

Assistant Professor

Department of Chemistry & Biochemistry

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Employment

8/2007-present: Assistant Professor, Department of Chemistry & Biochemistry, University of Oklahoma

Education and Training

11/2003-7/2007: Postdoc research associate, The Scripps Research Institute, advisor: Professor Charles L. Brooks III

12/2003: Ph.D., Physical Chemistry, University of Minnesota, advisor: Professor Darrin M. York

7/1999: M. Sc., Theoretical Chemistry, University of Calgary, Canada, advisor: Professor Tom Ziegler

12/1995: Diplom-Chem., Bergische Universität Wuppertal, Germany, advisor: Professor Robert J. Buenker

Research Field

Computational/theoretical chemistry and biophysics

Awards and Honors

2009: Junior Faculty Research Award, College of Arts and Sciences, University of Oklahoma

2008: Junior Faculty Research Award, Office of the Vice president for Research, University of Oklahoma

2006: Poster award, Research Symposium, The Scripps Research Institute

2003: Phi Kappa Phi, University of Minnesota

2000: Louise-Dosdell Graduate Fellowship (full scholarship), University of Minnesota

1997: Nova Graduate Fellowship (full scholarship), University of Calgary, Canada

Scientific Productivity and Impact Factor

H-index of 11 (source: ISI web of science)

Corporate Consulting

2007-now: Procter & Gamble

Current Research Support

“Probing regular solution theory for mixed amphoteric/ionic surfactant systems by molecular dynamics simulations”, PI, PRF #50000-DNI6, American Chemical Society, Jan 2010-Dec 2011, \$100,000 (direct cost)

“Simulations of surfactant micelles”, PI, Procter & Gamble, Corporate Gift, Jan 2009-June 2010, \$37,000 (direct cost), renewable

New faculty start-up funds, Department of Chemistry & Biochemistry, University of Oklahoma

Peer-Reviewed Publications and Book Chapters

Manuscripts in preparation

27. **J. K. Shen**, J. A. Wallace, L. Nguyen, Y. Wang, K. Pastoor, and K. Xia, “On pK_a calculations and the dielectric response of proteins”, in preparation.

26. J. A. Wallace and **J. K. Shen**, “pH-dependent assembly of AcrAB-TolC multi-drug efflux pump”, in preparation.

25. Y. Wang, J. A. Wallace, and **J. K. Shen**, “Predicting surfactant pK_a 's in micellar environment”, in preparation.

Manuscripts to be submitted shortly

24. J. A. Wallace and **J. K. Shen**, “Origin of pH-dependent registry shift in the fibril elongation of β -amyloid (16-22)”, to be submitted.

23. **J. K. Shen**, Y. Bi, B. Shan, D. R. Raleigh, and C. L. Brooks III, “Delineating native- vs. denatured-states effects on the stability of villin headpiece subdomain HP36”, to be submitted.

Manuscripts under review

22. **J. K. Shen**, “Uncovering specific electrostatic interactions in the denatured state of proteins”, under review (2009).

Manuscripts in press

Manuscripts published

21. J. A. Wallace and **J. K. Shen**, “Predicting protein pK_a 's with continuous constant pH molecular dynamics”, *Method. Enzymol.*, 466, 455-475 (2009).

20. X. Nan, A. L. O. Campbell, D. R. Powell, **J. Khandogin**, and G. B. Richter-Addo, “A stable hyponitrite iron porphyrin”, *J. Am. Chem. Soc.*, 130, 16498-16499 (2009).

19. J. W. Wickham, J. Halye, S. Kashtanov, **J. Khandogin**, and C. V. Rice, "Revisiting magnesium chelation by teichoic acid with phosphorus solid-state NMR and theoretical calculations", *J. Phys. Chem. A*, 113, 2177-2183 (2009).
18. **J. Khandogin**, "Modeling protonation equilibria in biological macromolecules", In *Challenges and Advances in Computational Chemistry and Physics*, Springer Verlag, Chap.10, 261-284 (2009).
17. J. Qian, **J. Khandogin**, A. H. West, and P. F. Cook, "Evidence for a catalytic dyad in the active site of homocitrate synthase from *saccharomyces cerevisiae*", *Biochemistry*, 47, 6851-6858 (2008).
16. J. Chen, C. L. Brooks III, and **J. Khandogin**, "Recent advances in implicit solvent based methods for biomolecular simulations", *Curr. Opin. Struct. Biol.*, 18, 140-148 (2008).
15. **J. Khandogin** and C. L. Brooks III, "Linking folding with aggregation in Alzheimer's β -amyloid peptides", *Proc. Natl. Acad. Sci. USA*, 104, 16880-16885 (2007).
14. **J. Khandogin** and C. L. Brooks III, "Molecular simulations of pH-mediated biological processes", in *Annu. Report Comput. Chem.*, Elsevier, vol. 3, 3-11 (2007).
13. **J. Khandogin** and C. L. Brooks III, "Folding intermediate in the villin head piece domain arises from disruption of an N-terminal hydrogen-bonded network", *J. Am. Chem. Soc.*, 129, 3056-3057 (2007).
12. **J. Khandogin**, J. Chen and C. L. Brooks III, "Exploring atomistic details of pH-dependent peptide folding", *Proc. Natl. Acad. Sci. USA*, 103, 18546-18550 (2006).
11. **J. Khandogin** and C. L. Brooks III, "Toward the accurate first-principles prediction of ionization equilibria in proteins", *Biochemistry*, 45, 9363-9373 (2006). **Citation: 20+**
10. **J. Khandogin** and C. L. Brooks III, "Constant pH molecular dynamics simulation with proton tautomerism", *Biophys. J.*, 89, 141-157 (2005). **Citation: 30+**
9. **J. Khandogin**, B. A. Gregersen, W. Thiel and D. M. York, "A smooth solvation method for d-orbital semiempirical calculations of biological reactions I: implementation", *J. Phys. Chem. B*, 109, 536-556 (2005).
8. B. A. Gregersen, **J. Khandogin**, W. Thiel and D. M. York, "A smooth solvation method for d-orbital semiempirical calculations of biological reactions II: application to transphosphorylation thio effects in solution", *J. Phys. Chem. B*, 109, 9799-9809 (2005).
7. **J. Khandogin** and D. M. York, "Quantum descriptors for biological macromolecules from linear-scaling electronic structure methods", *Proteins*, 56, 724-737 (2004). **Citation: 20+**
6. **J. Khandogin**, K. Musier-Forsyth, and D. M. York, "Insights into the regioselectivity and RNA binding affinity of HIV-1 nucleocapsid protein from linear-scaling quantum methods", *J. Mol. Biol.*, 303, 993-1004 (2003). **Citation: 20+**

5. **J. Khandogin** and D. M. York, "Quantum mechanical characterization of nucleic acids in solution: a linear-scaling study of charge fluctuations in DNA and RNA", *J. Phys. Chem. B.*, 106, 7693-7703 (2002).
4. **J. Khandogin**, A. Hu, and D. M. York, "Electronic structure properties of solvated biomolecules: a quantum approach for macromolecular characterization", *J. Comput. Chem.*, 21, 1562-1571 (2000).
3. **J. Khandogin** and T. Ziegler, "A simple relativistic correction to the nuclear spin-spin coupling constant", *J. Phys. Chem. A*, 104, 113-120 (2000). **Citation: 20+**
2. **J. Khandogin** and T. Ziegler, "Density functional study of nuclear magnetic resonance spin-spin coupling constants", *Spectrochimica Acta A*, special issue: Theoretical spectroscopy: State of the Science, 55, 607-624 (1999). **Citation: 30+**
1. **Y. Khandogin**, A.B. Alexeyev, H.-P. Liebermann, G. Hirsh, and R.J. Buenker, "Ab Initio relativistic CI calculations of the spectroscopic constants and transition probabilities for the low-lying states of the BiOH/HBiO isomers", *J. Mol. Spectrosc.*, 186, 22-33 (1997).

Invited Seminars (after August 2007)

10. Telluride Workshop on Proteins in Cellular Environment, July 18-24, 2010, Telluride, CO
9. Telluride Workshop on Enhanced Sampling Techniques, June 14-18, 2010, Telluride, CO
8. Workshop CBSB10 - From Computational Biophysics to Systems Biology, June 6-8, 2010, Traverse City, MI
7. "Effects of specific denatured-state interactions on the stability of proteins", 23rd Annual Gibbs Conference in Biothermodynamics, Oct 3-6, 2009, Carbondale, IL
6. "Electrostatic determinants of tertiary structure in amyloid fibrils", 238th ACS National meeting, Aug 16-20, 2009, Washington, DC
5. "Constant pH molecular dynamics", Molecular Simulation and Structure Prediction using Amber, CHARMM and MMTSB Tool Set, Aug 4-7, 2009, La Jolla, CA
4. "De novo prediction of protein pK_a values", Telluride Workshop on Protein Electrostatics, July 6-10, 2009, Telluride, CO
3. "Constant pH molecular dynamics", Procter & Gamble, Sept 8, 2008, Cincinnati, Ohio
2. "Electrostatic interactions in the unfolded states of proteins", Gordon Research Conference on Computational Chemistry, July 27-Aug 1, 2008, South Hadley, MA
1. "Linking folding with aggregation in beta amyloid peptides", Gordon Research Conference on Protein Folding Dynamics, Jan 6-11, 2008, Ventura, CA

Teaching Experience

2010 Fall: Quantum Chemistry (CHEM 5213)
2009 Fall: Statistical Mechanics (CHEM 5123)
2009 Spring: Computational Chemistry and Biophysics (CHEM 6670)
2008 Fall: Quantum Chemistry (CHEM 5213)
2008 Spring: Computational Chemistry and Biophysics (CHEM 6670)

Students Advising

PhD students: Jason Wallace and Yuhang (Steven) Wang
Master students: Adam Campbell (joint with Richter-Addo group), graduated May 2009
Undergraduate students: Ross Evans, Alim Ramji

Professional Experience

Summer School/Workshop Teaching

Instructor, Molecular Simulation and Structure Prediction using Amber, CHARMM and MMTSB Tool Set, Aug 4-7, 2009, University of California, La Jolla, CA

Conference Organization

Session chair, Symposium on "Molecular Basis of Protein Aggregation and Amyloid Formation", 38th ACS National meeting, Aug 16-20, 2009, Washington, DC

Journal reviews

Biophysical Journal; FEBS Letters; Frontiers of Interdisciplinary Research in the Life Sciences; Journal of Biological Inorganic Chemistry; Journal of Biomolecular Structure and Dynamics; Journal of Computational Chemistry; Journal of Molecular Graphics and Modeling; Proteins: Structure, function, and Bioinformatics; BBA - Proteins and Proteomics

Proposal reviews

National science foundation

Professional Affiliations

American Chemistry Society; Biophysical Society