Demian Riccardi

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Education

2001-2006 Ph.D., Department of Chemistry, University of Wisconsin-Madison,
Dissertation: Computational investigations of long-range proton transfer: Method validation and application.
Advisor: Dr. Qiang Cui.

1996-2000 B.A., Biochemistry, Vassar College, Poughkeepsie, NY.

Research Experience

2011-Present **Postdoctoral Fellow**
Application of quantum chemical methods to understand mercury speciation and transformation in the biosphere. Development and application of mixed quantum mechanics and molecular mechanics (QM/MM) methods for simulating mercury chemistry.
Group Leader: Dr. Jeremy C. Smith

2006-2010 **Computation and Informatics in Biology and Medicine Postdoctoral Trainee**
Development and application of computational approaches for the investigation of correlated motions in biological crystals and the effects of these motions on X-ray diffraction. Built Fortran 95 toolkit for carrying out normal mode analysis with elastic network models using various boundary conditions including the Born Von Karman treatment of lattice modes.
Mentor: Dr. George N. Phillips, Jr.; Secondary Mentor: Dr. Qiang Cui.
University of Wisconsin-Madison

2001-2006 **Doctoral Research.** Involved in the development and application of mixed QM/MM methods for simulating biological systems. Extensive experience with free energy calculations of pK_as and long-range proton transfers.
Advisor: Dr. Qiang Cui. University of Wisconsin-Madison

2000-2001 **Cooperative Student.** Multidisciplinary research towards the development of environmentally friendly cleaning processes for microchip interconnect manufacturing.
Advisor: Dr. Krishna Sachdev (Late); Manager: Dr. James Humenik.
International Business Machines, East Fishkill, NY.

1999-2001 **Research Assistant.** Application of quasi-chemical theory to computing the solvation free energy of a proton in water.
Advisor: Dr. Maria Gomez. Department of Chemistry, Vassar College.

1999 **Summer Intern.** Functional screening of novel human genes in Xenopus laevis frogs.
Advisor: Dr. Lakshmi Amaravadi. Millenium Pharmaceuticals, Cambridge, MA.

Honors and Awards

2006 **CIBM Postdoctoral Fellowship.** University of Wisconsin-Madison.
2000 **Department honors in biochemistry.** Vassar College.
1998 **Scholar Athlete Award.** Division III swimming, Vassar College.

Select Publications

Riccardi D, Guo HB, Parks JM, Gu B, Summers AO, Miller SM, Liang L, Smith JC "Why mercury prefers thiols" (submitted)

Riccardi D, Guo HB, Parks JM, Gu B, Liang L, Smith JC "Cluster-continuum calculations of hydration free energies of anions and group 12 divalent cations" *J Chem Theor Comp*, **9**, 555 (2013)

Riccardi D, Cui Q, Phillips Jr. GN, "Evaluating elastic network models of crystalline biological molecules with temperature factors, correlated motions, and diffuse X-ray scattering", *Biophys J*, **99**, 2616 (2010)

Riccardi D, Yang S, Cui Q, "Proton transfer function of Carbonic Anhydrase: Insights from QM/MM simulations", *BBA. Proteins and Proteomics*, **1804**, 342 (2010)

Riccardi D, Cui Q, Phillips Jr. GN, "Application of elastic network models to proteins in the crystalline state", *Biophys. J.*, **96**, 464 (2009)

Riccardi D, Koenig P, Guo H, Cui Q, "Proton transfer in Carbonic Anhydrase is controlled by electrostatics rather than the orientation of the acceptor group", *Biochem.*, **47**, 2369 (2008)

Riccardi D, Konig P, Yu H, Prat-Resina X, Elstner M, Frauenheim T, Cui Q, " 'Proton holes' in long-range proton transfers in solution and enzymes", *J. Am. Chem. Soc.*, **128**, 16302 (2006)

Riccardi D, Schaefer P,Yang Y, Yu H, Ghosh N, Prat-Resina X, Konig P, Li G, Xu D, Guo H, Elstner M, and Cui Q, "Development of effective QM/MM methods for complex biophysical processes", *J. Phys. Chem. B*, **110**, 6458 (2006), Feature Article

Riccardi D, Schaefer P, Cui Q, "pK_a calculations in solution and proteins with QM/MM free energy perturbation simulations: A quantitative test of QM/MM protocols", *J. Phys. Chem. B*, **109**, 17715 (2005), Featured on the journal cover

Select Presentations

2012 Riccardi D, "Carving up biomolecular objects to understand how mercury causes so much trouble", talk at Yet Another Perl Conference : North America (YAPC::NA) in Madison, WI

2010 Riccardi D, Cui Q, Phillips GN Jr., "Computational models of crystalline protein dynamics", poster at the annual meeting of ACA in Chicago, IL

2007 Riccardi D, König P, Cui Q, " 'Proton holes' in long-range proton transfers in solution and enzymes", presentation at the March meeting of ACS in Chicago, IL

2006 Riccardi D, "Transferring protons over long distances with computers", Chemistry Department Seminar, Vassar College, Poughkeepsie, NY

2004 Riccardi D, Ghosh N, Cui Q, "Long-range proton transport in carbonic anhydrase", poster at the August meeting of ACS in Philedelphia, PA