

# *Curriculum Vitae*

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*

- 2006-present **Computation and Informatics in Biology and Medicine Postdoctoral Trainee**  
Development and application of computational approaches for the investigation of diffuse X-ray scattering in biological molecules.  
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 quantum mechanics and molecular mechanics (QM/MM) methods for simulating biological systems. Please see publications for details.  
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.

## *Teaching Experience*

- 2005 Teaching Assistant. CHEM 562, Fall. *Quantum Chemistry*. University of Wisconsin
- 2002 Teaching Assistant. CHEM 104, Spring. *General Chemistry*. University of Wisconsin
- 2001 Teaching Assistant. CHEM 103, Fall. *General Chemistry*. University of Wisconsin
- 1999 Teaching Assistant. CHEM 244, Fall. *Organic Chemistry Lab*. Vassar College

## *Technical Skills*

**Computer Operating Systems:** Linux (Red Hat, Fedora), Mac OSX, Windows XP  
**Programming Languages:** Fortran, Perl, Unix Shells  
**Computational chemistry programs:** CHARMM and Gaussian-03.

## *Honors and Awards*

- 2000 **Department honors in biochemistry** Vassar College.
- 1998 **Scholar Athlete Award.** Division III swimming, Vassar College.

## Publications

- Riccardi D, Cui Q, “pK<sub>a</sub> analysis for the zinc-bound water in Human Carbonic Anhydrase II: benchmark for “multi-scale” QM/MM simulations and mechanistic implications”, *J. Phys. Chem. A*, **111**, 5703 (2007), Special Section: DFTB Symposium
- Riccardi D, König 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, König 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<sub>a</sub> 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
- Range K, Riccardi D, Cui Q, Elstner M, York DM, “Benchmark calculations of proton affinities and gas-phase basicities of molecules important in the study of biological phosphoryl transfer”, *Phys. Chem. Chem. Phys.*, **7**, 3070 (2005)
- Schaefer P, Riccardi D, and Cui Q, “Reliable treatment of electrostatics in combined QM/MM simulation of macromolecules”, *J. Chem. Phys.*, **123**, 014905 (2005)
- Riccardi D, Li GH, Cui Q, “Importance of van der Waals interactions in QM/MM Simulations”, *J. Phys. Chem. B*, **108**, 6467 (2004)
- Grabowski P, Riccardi D, Gomez MA, Asthagiri D, Pratt LR, “Quasi-chemical theory and the standard free energy of H<sup>+</sup>(aq)”, *J. Phys. Chem. A*, **106**, 9145 (2002)
- Sachdev KG, Lei CC, Riccardi D, “Semi-Aqueous Solvent-Based Method of Cleaning Rosin Flux Residue”, Patent 6,800,141

## Presentations

- 2007 Riccardi D, Phillips GN Jr., “Calculating the diffuse X-ray Scattering from biomolecular crystals”, poster at the August meeting of ACS in Boston, MA
- 2007 Riccardi D, Phillips GN Jr., “Motions of biological molecules in crystals and their diffuse scattering”, poster at the annual meeting of ACA in Salt Lake City, UT
- 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
- 2006 Riccardi D, König P, Cui Q, “Proton and hydroxide transfer in carbonic anhydrase: insights from QM/MM reaction path and potential of mean force analyses”, poster at 32nd Steenbock Symposium, Madison, WI
- 2005 Riccardi D, “Ensembles of long-ranged proton transfers in carbonic anhydrase II. ”, Biophysics Super Group Seminar, University of Wisconsin-Madison
- 2004 Riccardi D, “Long-range proton transport in carbonic anhydrase”, Physical Chemistry Student Seminar, University of Wisconsin-Madison
- 2004 Riccardi D, Ghosh N, Cui Q, “Long-range proton transport in carbonic anhydrase”, poster at the August meeting of ACS in Philadelphia, PA

- 2004 Schaefer PS, Riccardi D, Cui Q, "QM/MM approach to treating long-range electrostatics", poster at the August meeting of ACS in Philadelphia, PA
- 2003 Riccardi D and Cui Q, "How important are van der Waals parameters in hybrid QM/MM simulations?", poster at the September Meeting of ACS in New York, NY
- 2001 Grabowski P, Riccardi D, Gomez MA, Pratt LR, "Calculation of the Solvation Free Energy of a Proton in Water", poster at the March meeting of APS in Seattle, WA