Christopher J. Fennell, Ph.D.

36 Ridgeley Rd
Smithtown, NY 11787
Tel (Cell): 415/572-0663
Email: christopher.fennell@stonybrook.edu

Laufer Center for Physical and Quantitative Biology
Stony Brook University
5252 SUNY
Stony Brook, NY 11794-5252

CURRENT POSITION

Institution: Stony Brook University, Stony Brook, NY
Title: Laufer Junior Fellow

EDUCATION

Graduate Institution: University of Notre Dame du Lac, Notre Dame, IN
Degree Obtained: Ph.D. in Chemistry **2007**

Undergraduate: Drake University, Des Moines, IA
Degree Obtained: Bachelor of Science **2001**

- Major: Chemistry
- Minors: Math & Art

RESEARCH EXPERIENCE

Laufer Junior Fellow, Laufer Center for Physical and Quantitative Biology, SUNY Stony Brook **2010-present**
Solvation studies and method development for small molecules, ions, and proteins. Phase transfer free energy calculations. Studies of protein–ligand binding affinities. Computational studies of protein folding and refinement.

Postdoctoral Researcher under Ken A. Dill, University of California, San Francisco **2006-2010**
Development of new methods for treating solvent in biological systems. Study of ion effects in molecular systems using simple analytical models.

Graduate Research Assistant under J. Daniel Gezelter, University of Notre Dame du Lac **2001-2006**
Development and study of water models for use in molecular dynamics simulation. Investigation of the phase behavior of simple molecular systems. Development and application of new techniques for the study of rigid body systems in molecular dynamics simulation.

Undergraduate Research Assistant under Robert C. Dunn, University of Kansas, REU Program **2000**
Molecular dynamics studies of lipid monolayers. Atomic force microscopy studies of monolayers and particle packing.

Undergraduate Research Assistant under Colin J. Cairns, Drake University **1999-2001**
Synthesis and analysis of thiophene based ligands and fluorescent molecules and their metal coordination complexes.

Undergraduate Research Assistant under Mark F. Vitha, Drake University **1998-1999**
Development of chemical interaction descriptors for solutes using PCA of retention times in gas chromatography.

TEACHING EXPERIENCE

Teaching Assistant For General Chemistry **2002-2003**
Organization and oversight of several tutorial/recitation sections. Entailed the development and grading of problem sets, proctoring and grading examinations, tutoring students during and outside of regular office hours, arranging review sessions, and assisting in the lecture portion of the class.

Teaching Assistant for Physical Chemistry Laboratory **2001-2002**
Setup, oversight, and modification of physical chemistry laboratory experiments for the undergraduate physical chemistry class. Additional responsibilities included grading of laboratory reports and assisting in the lecture portion of the class.

AWARDS AND HONORS

Rohm and Haas Outstanding Graduate Student Award **2006**
SGI Award for Computational Science and Visualization **2005**
Searle Fellowship **2004**
Jeremiah P. Freeman Graduate Teaching Award **2002**
Kaneb Center Outstanding Graduate Student Teacher Award **2002**

Nieuwland Fellowship **2001**
Oreon E. Scott Award - Valedictorian, *Summa Cum Laude*, Drake University **2001**
American Microchemical Society Undergraduate Research Award **2000**
Barry M. Goldwater Scholar **2000**

PROFESSIONAL MEMBERSHIPS

American Chemical Society
American Physical Society
Biophysical Society

PUBLICATIONS

T. Urbic, C. J. Fennell, and K. A. Dill, "Beyond Born: a microscopic theory of ion solvation", *Submitted*, 2011.

C. J. Fennell and K. A. Dill, "Physical Modeling of Aqueous Solvation", *J. Stat. Phys.* In Press, 2011.

C. J. Fennell, C. W. Kehoe, and K. A. Dill, "Modeling aqueous solvation with semi-explicit assembly", *Proc. Nat. Acad. Sci. USA* **108**(8), 3234–3239, 2011.

C. J. Fennell, C. Kehoe, and K. A. Dill, "Oil/Water Transfer is Partly Driven by Molecular Shape, Not Just Size", *J. Am. Chem. Soc.* **132**(1), 234–240, 2010.

C. J. Fennell, A. Bizjak, V. Vlachy, K. A. Dill, S. Sarupria, S. Rajamani, and S. Garde, "(Additions/Corrections) Ion pairing in molecular simulations of aqueous alkali halide solutions", *J. Phys. Chem. B* **113**(44), 14837–14838, 2009.

C. J. Fennell, A. Bizjak, V. Vlachy, and K. A. Dill, "Ion pairing in molecular simulations of aqueous alkali halide solutions", *J. Phys. Chem. B* **113**(19), 6782–6791, 2009. *– Cover article, May 14, 2009*

D. L. Mobley, A. E. Barber II, C. J. Fennell, and K. A. Dill, "Charge Asymmetries in Hydration of Polar Solutes," *J. Phys. Chem. B*, **112**(8), 2405–2414, 2008.

C. J. Fennell and J. D. Gezelter, "Is the Ewald summation still necessary? Pairwise alternatives to the accepted standard for long-range electrostatics," *J. Chem. Phys.* **124**(23), 234104*,* 2006.

C. J. Fennell and J. D. Gezelter, "Computational Free Energy Studies of a New Ice Polymorph Which Exhibits Greater Stability than Ice I_h," *J. Chem. Theory Comput.* **1**(4), 662–667, 2005.

M. A. Meineke, C. F. Vardeman II, T. Lin, C. J. Fennell, and J. D. Gezelter, "OOPSE: An Object-Oriented Parallel Simulation Engine for Molecular Dynamics," *J. Comput. Chem.* **26**(3), 252–271, 2005.

C. J. Fennell and J. D. Gezelter, "On the structural and transport properties of the soft-sticky dipole and related single point water models," *J. Chem. Phys.* **120**(19), 9175–9184, 2004.

PRESENTATIONS

240th American Chemical Society National Meeting, Boston, Massachusetts, August 2010: "Using explicit solvent implicitly," Christopher J. Fennell, Charlie Kehoe, and Ken A. Dill.

239th American Chemical Society National Meeting, San Francisoc, California, March 2010: "Rapid assessment of molecular solvation using Semi-Explicit Assembly," Christopher J. Fennell, Charlie Kehoe, and Ken A. Dill.

54th Annual Biophysical Society Meeting, San Francisco, California, February 2010: "Capturing the roles of attraction and shape in nonpolar solvation," Christopher J. Fennell, Charlie Kehoe, and Ken A. Dill.

Invited speaker, SYLICCO.09, University of California, Davis, Davis, California, July 2009: "Enhancing solvation and applying obsession in science," Christopher J. Fennell.

236th American Chemical Society National Meeting, Philadelphia, Pennsylvania, August 2008: "Ion pairing in aqueous solutions: An investigation using molecular simulations" Christopher J. Fennell, Alan Bizjak, Vojko Vlachy, and Ken A. Dill.

Invited speaker, University of Ljubljana, Slovenia, June 2007: "Current developments in solvation modeling" Christopher J. Fennell and Ken A. Dill.

Invited speaker, University of Texas at Austin, Austin, Texas, June 2006: "Is the Ewald summation still necessary? Pairwise alternatives to the accepted standard for long-range electrostatics" Christopher J. Fennell and J. Daniel Gezelter.

37th Midwest Theoretical Chemistry Conference, University of Missouri, Columbia, Missouri, June 2005: "Computational Free Energy Studies of a New Ice Polymorph Which Exhibits Greater Stability than Ice I_h" Christopher J. Fennell and J. Daniel Gezelter.

229th American Chemical Society National Meeting, San Diego, California, March 2005: "Structural and transport properties of the soft-sticky dipole (SSD) and related single point water models" Christopher J. Fennell and J. Daniel Gezelter.

35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, June 2003: "On the density maximum of the soft-sticky dipole (SSD) single point water model" Christopher J. Fennell and J. Daniel Gezelter.

Eastern Analytical Symposium, Atlantic City, New Jersey, October 2000: "Regression-Based Parameterization of Molecular Interactions via Gas Chromatography for use in Linear Solvation Energy Relationships." Christopher J. Fennell, Sarah M. Ronnebaum, Jeff D. Weckworth, and Mark F. Vitha.

COLLABORATING PRESENTATIONS

SAMPL3 Workshop, Stanford, California, August 2011: "Semi-Explicit Assembly: Fast Physics Make Better Solutions" Charles Kehoe, Christopher Fennell, Ken Dill.

54th Annual Biophysical Society Meeting, San Francisco, California, February 2010: "A new Semi-Explicit solvation model: Fast physics for better results" Charles Kehoe, Christopher Fennell, Ken Dill.

236th American Chemical Society National Meeting, Philadelphia, Pennsylvania, August 2008: "Ions, polar solvation, and ligand binding to proteins" Ken A. Dill, David L. Mobley, and Christopher J. Fennell.

235th American Chemical Society National Meeting, New Orleans, Louisiana, September 2007: "Insights on aqueous solvation from alchemical free energy calcualtions" David L. Mobley, Alan Barber II, John D. Chodera, Christopher J. Fennell, and Ken A. Dill.

37th Midwest Theoretical Chemistry Conference, University of Missouri, Columbia, Missouri, June 2005: "Spherical Harmonic Approximate Potential Energy Surfaces (SHAPES) as Coarse-Grained Models for Rigid Molecules." Christopher J. Fennell, Kyle Daily, and J. Daniel Gezelter.

229th American Chemical Society National Meeting, San Diego, California, March 2005: "Computational free energy studies of a new ice polymorph which exhibits greater stability than ice I_h," Christopher J. Fennell and J. Daniel Gezelter.

Federation of Analytical Chemistry and Spectroscopy Societies, Detroit, Michigan, October 2001, Special Session: New Investigators in Analytical Science: Innovative Leaders in the New Millennium: "Chemically Distinct Solute Parameters for Linear Solvation Energy Relationships." Mark F. Vitha, Joshua Sandquist, Kali Mulville, Sarah Ronnebaum, Benjamin Richards, Christopher Fennell, and Lisa Stalheim.

Eastern Analytical Symposium, Atlantic City, New Jersey, October, 2000: "A New Set of Chemically Distinct Solute Parameters for Use in LSERs." Sarah M. Ronnebaum, Christopher J. Fennell, Josh Sandquist, Kali Mulville, Jeff D. Weckwerth, and Mark F. Vitha.

XXIX Scientific Meeting of the Group of Chromatography and Related Techniques, Universidad de Alcalá, Alcalá de Henares, Spain, July 2000: "Study of the Retention in Micellar Liquid Chromatography on a C-8 Column Using Linear Solvation Energy Relationships." M.A. Garcia, Mark F. Vitha, Christopher J. Fennell, Sarah Ronnebaum, and M.L. Marina.

DEVELOPED SOFTWARE

The Chemical Touch: Lite Edition (iPhone and iPod touch application) **December, 2008**

The Chemical Touch (iPhone and iPod touch application) **August, 2008**

The Periodic Table (Mac OS X widget) – Featured Widget at www.apple.com, Feb. 20, 2007 **July, 2005**

OpenMD: An Object-Oriented Parallel Simulation Engine for Molecular Dynamics. **July, 2004**

REVIEWER FOR

Journal of the American Chemical Society
Journal of Chemical Physics
Journal of Physical Chemistry B
Journal of Physical Chemistry Letters
Journal of Chemical Theory and Computation
Journal of Physics: Condensed Matter
Journal of Computer-Aided Molecular Design

REFERENCES

Ken A. Dill
Professor and Director
Laufer Center for Physical & Quantitative Biology
Stony Brook University
Stony Brook, NY 11794-5252
tel: (631) 632-4124
fax: (631) 632-4125
email: dill@laufercenter.org

J. Daniel Gezelter
Associate Professor of Chemistry
Director of Graduate Admissions
Department of Chemistry and Biochemistry
251 Nieuwland Science Hall
University of Notre Dame
Notre Dame, IN 46556-5670
tel: (574) 631-7595
email: gezelter@nd.edu

Dennis C. Jacobs
Provost & Vice President for Academic Affairs
500 El Camino Real
204 Walsh Admin. Building
Santa Clara University
Santa Clara, CA 95053-0460
tel: (408) 554-4533
fax: (408) 551-6074
email: dcjacobs@scu.edu