

John M. Stubbs

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EDUCATION

- Doctor of Philosophy in Chemistry 1999–2004
Advisor: Professor J. I. Siepmann
GPA: 3.937 out of 71 course credits
Dissertation Title: Simulations of Microheterogeneous Fluids
University of Minnesota, Minneapolis, MN
- Bachelor of Arts With High Distinction in Chemistry and German 1995–1999
and a minor in Physics
GPA: 3.818 out of 236 course credits
University of Minnesota-Morris, Morris, MN

AWARDS AND HONORS

- University Faculty Scholarship Fund Mini-Grant 2007–2008
Grinnell College Faculty Scholarship Grant 2005–2006
Graduate School Dissertation Fellowship 2003–2004
National Science Foundation's Research Site for Educators in Chemistry Fellowship 2003
Frieda Martha Kunze Fellowship 2002–2003
DAAD Graduate Fellowship for Study and Research in Germany 2001–2002
Freshman Academic Scholarship 1995–1996

TEACHING EXPERIENCE

Assistant Professor, Department of Chemistry & Physics, UNE 2006–Present

Currently teaching general and physical chemistry including both lecture and laboratory.

Visiting Assistant Professor, Department of Chemistry, Grinnell College 2004–2006
Taught the year long physical chemistry course including both lecture and laboratory; currently teaching general chemistry including both lecture and laboratory.

Primary Instructor, Department of Chemistry, Drake University Fall 2003
Developed and instructed laboratory and lecture portions of a course on computational chemistry; specific responsibilities included creating lecture material, homework assignments, laboratory assignments, quizzes and exams.

Preparing Future Faculty Courses, University of Minnesota 2002–2003
Discussed effective teaching methods; taught multiple class periods; critically observed classes; created personal teaching philosophy.

Teaching Assistant, Department of Chemistry, University of Minnesota 1999–2001
For undergraduate thermodynamics and graduate statistical mechanics courses, held tutor hours; graded homework, quizzes and exams; supervised group work during class period.

Teaching Assistant, Department of Chemistry, University of Minnesota-Morris 1997–1998
Supervised undergraduate general and organic chemistry laboratories; graded laboratory results and reports; held tutor hours for student questions.

TEACHING INTERESTS

My interests are in teaching physical, general, and a special topics course on computational chemistry. For all courses, the classroom component would combine a lecture approach with active methods to effectively ensure student comprehension.

RESEARCH EXPERIENCE

Researcher, Research Director, Department of Chemistry & Physics, UNE 2006–present

Directing undergraduate research into simulations of DNA hybridization and melting transitions; developing empirical models for simulation.

Researcher, Research Director, Department of Chemistry, Grinnell College 2004–2006

Directed undergraduate research into simulations of DNA hybridization and melting transitions as well as supercritical fluid extraction systems; conducted simulations of vapor/liquid interfaces of mixtures.

Research Assistant, Department of Chemistry, University of Minnesota 1999–2004

Conducted simulations of mixtures of strongly and weakly associating fluids; fit parameters for empirical force fields; extended Monte Carlo algorithms for particle exchange; maintained research computer base, including desktop and computational machines.

Research Assistant, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum 2001–2002

Conducted simulations on the formation of the glycosidic bond; analyzed simulation results for hydrophobic diffusion in water.

Technical Aide, Basic Sciences Corporate Laboratory, 3M Corporation 1996–1999

Synthesized and analyzed micropolymer beads; modified bead surface for use in solid-phase synthesis; synthesized linking agents for bead surface modification.

RESEARCH INTERESTS

My primary interests are thermodynamic properties of DNA helix-coil transitions and the effect of oligomer surface immobilization. Additional interests are extension of existing force fields in order to calculate thermophysical properties, as well as development of new and modification of existing Monte Carlo algorithms to efficiently sample processes of interest.

PUBLICATIONS

- [1] Stubbs, J.M.; Chen, B.; Potoff, J.J.; Siepmann, J.I. 'Monte Carlo calculations for the phase equilibria of alkanes, alcohols, water, and their mixtures,' *Fluid Phase Equil.*, **183/184**, 301-309 (2001).
- [2] Cramer, C.J.; Kormos, B.L.; Winget, P.; Audette, V.M.; Beebe, J.M.; Brauer, C.S.; Burdick, W.R.; Cochran, E.W.; Eklov, B.M.; Giese, T.J.; Jun, Y.; Kesavan, L.S.D.; Kinsinger, C.R.; Minyaev, M.E.; Rajamani, R.; Salsbury, J.S.; Stubbs, J.M.; Surek, J.T.; Thompson, J.D.; Voelz, V.A.; Wick, C.D.; Zhang, L. 'A cooperative molecular modeling exercise - The hypersurface as classroom', *J. Chem. Ed.*, **78**, 1202-1205 (2001).
- [3] Stubbs, J.M.; Siepmann, J.I. 'Aggregation in dilute solutions of 1-hexanol in *n*-hexane: A Monte Carlo simulation study,' *J. Phys. Chem. B*, **106**, 3968-3978 (2002).

- [4] Kirchner, B.; Stubbs, J.M.; Marx, D. 'Fast anomalous diffusion of small hydrophobic species in water,' *Phys. Rev. Lett.*, **89**, 215901(1-4) (2002).
- [5] Stubbs, J.M.; Marx, D. 'Glycosidic bond formation in aqueous solution: on the oxocarbenium intermediate,' *J. Am. Chem. Soc.*, **125**, 10960-10962 (2003).
- [6] Stubbs, J.M.; Siepmann, J.I. 'Binary phase behavior and aggregation of dilute methanol in supercritical carbon dioxide: A Monte Carlo simulation study' *J. Chem. Phys.*, **121**, 1525-1534 (2004).
- [7] Stubbs, J.M.; Potoff, J.J.; Siepmann, J.I. 'Transferable potentials for phase equilibria. 6. United-atom description of ethers, glycols, aldehydes and ketones', *J. Phys. Chem. B*, **108**, 17596-17605 (2004).
- [8] Lee, J.S.; Wick, C.D.; Stubbs, J.M.; Siepmann, J.I. 'Simulating the vapour-liquid equilibria of large cyclic alkanes', *Mol. Phys.*, **103**, 99-104 (2005).
- [9] Stubbs, J.M.; Marx, D. 'Aspects of glycosidic bond formation in aqueous solution: Chemical bonding and the role of water', *Chem. Eur. J.*, **11**, 2651-2659 (2005).
- [10] Stubbs, J.M.; Siepmann, J.I. 'Elucidating the vibrational spectra of hydrogen-bonded aggregates in solution: Electronic structure calculations with implicit solvent and first principles molecular dynamics simulations with explicit solvent for 1-hexanol in *n*-hexane', *J. Am. Chem. Soc.*, **127**, 4722-4729 (2005).
- [11] Wick, C.D.; Stubbs, J.M.; Rai, N.; Siepmann, J.I. 'Transferable potentials for phase equilibria. 7. Primary, secondary, and tertiary amines, nitroalkanes and nitrobenzene, nitriles, amides, pyridine and pyrimidine', *J. Phys. Chem. B*, **109**, 18974-18982 (2005).
- [12] Stubbs, J.M.; Drake-Wilhelm, D.D.; Siepmann, J.I. 'Partial molar volume and solvation structure of naphthalene in supercritical carbon dioxide: A Monte Carlo simulation study', *J. Phys. Chem. B*, **109**, 19885-19892 (2005).
- [13] Wang, S.; Stubbs, J.M.; Siepmann, J.I.; Sandler, S.I. 'Effect of conformation on sigma profiles in COSMO theories,' *J. Phys. Chem. A*, **109**, 11285-11294 (2005).
- [14] Tito, N.B; Stubbs, J.M. 'Application of a coarse-grained model for DNA to homo- and heterogeneous melting equilibria,' *Chem. Phys. Lett.*, **485**, 354-359 (2010).
- [15] Stubbs, J.M.; Siepmann, J.I. 'Comparison of the aggregation of primary, secondary and tertiary hexanol isomers in *n*-hexane,' *J. Phys. Chem. B*, in preparation.

PROFESSIONAL PRESENTATIONS

- [1] Stubbs, J.M.; Siepmann, J.I. 'Monte Carlo simulations of 1-hexanol in *n*-hexane: The formation of hydrogen-bonded clusters in *n*-hexane rich solution', 33rd Midwest Theoretical Chemistry Conference, Iowa City, IA (5/2000)
- [2] Stubbs, J.M.; Siepmann, J.I. 'Monte Carlo calculations for the aggregation of alkanols in nonpolar solvents', 2001 Midwest Thermodynamics & Statistical Mechanics Conference, East Lansing, MI (5/2001)
- [3] Stubbs, J.M. 'Monte Carlo simulations of 1-hexanol in *n*-hexane: The formation of hydrogen-bonded clusters in *n*-hexane rich solution', Theoretisch-Chemisches Seminar, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany (10/2001)
- [4] Stubbs, J.M.; Siepmann, J.I.; Wick, C.D.; Zhuravlev, N.D. 'Predicting phase equilibria using configurational-bias Monte Carlo simulations in the Gibbs ensemble', 2002 AIChE Annual Meeting, Session on 'Obtaining physical and chemical properties for process design by computational chemistry', Indianapolis, IN (11/2002)

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- [5] Stubbs, J.M.; Siepmann, J.I. ‘Aggregation of hexanol isomers in *n*-hexane’, 2003 Midwest Thermodynamics & Statistical Mechanics Conference, Columbus, OH (5/2003)
- [6] Stubbs, J.M.; Siepmann, J.I. ‘Aggregation of hexanol isomers and of 2-ethoxyethanol in *n*-hexane’, 226th ACS National Meeting, New York, NY (9/2003)
- [7] Stubbs, J.M.; Siepmann, J.I. ‘Vibrational spectra of 1-hexanol in *n*-hexane via *ab initio* molecular dynamics’, 226th ACS National Meeting, New York, NY (9/2003)
- [8] Stubbs, J.M.; Siepmann, J.I.; Wick, C.D.; Zhang, L.; Potoff, J. ‘Extension of the TraPPE force field to nitrogen functionalities’, 2003 AIChE Annual Meeting, Session on ‘Development and validation of intermolecular potential functions I’, San Francisco, CA (11/2003)
- [9] Stubbs, J.M.; Siepmann, J.I. ‘Aggregation of hexanol isomers and of 2-alkoxyethanols in *n*-hexane: Aggregation, steric hindrance, inter- and intramolecular hydrogen bonding and vibrational spectroscopy’, Poster, Tenth International Conference on Properties and Phase Equilibria for Product and Process Design, Snowbird, UT (5/2004)
- [10] Stubbs, J.M.; Siepmann, J.I. ‘Vibrational spectra of 1-hexanol in *n*-hexane using a multiscale modeling approach’, 2004 Midwest Thermodynamics & Statistical Mechanics Conference, Buffalo, NY (6/2004)
- [11] Stubbs, J.M.; Siepmann, J.I. ‘Monte Carlo simulation of water/1-butanol/2-ethoxyethanol mixtures at vapor/liquid interfaces’, Poster, 229th ACS National Meeting, San Diego, CA (3/2005)
- [12] Stubbs, J.M.; Siepmann, J.I. ‘Interfacial properties of aqueous surfactant mixtures: A Monte Carlo study’, 231st ACS National Meeting, Atlanta, GA (3/2006)
- [13] Stubbs, J.M.; Tito, N.B. ‘Modeling heterogeneous melting equilibria of surface-immobilized DNA using Monte Carlo molecular simulation’, 2009 Midwest Thermodynamics & Statistical Mechanics Conference, Detroit, MI (5/2009)
- [14] Stubbs, J.M.; Tito, N.B.; Buchanan, M.; Pedersen, R.D. ‘Predicting melting equilibria for DNA using a coarse-grained model: A Monte Carlo study’, Poster, 238th ACS National Meeting, Washington, D.C. (8/2009)

PRESENTATIONS FROM SUPERVISED RESEARCH

- [1] Pedersen, R.D.; Stubbs, J.M. ‘Molecular simulations of DNA hybridization and melting using a coarse-grained model’, Fifth Midwest Undergraduate Computational Chemistry Consortium Conference, Minneapolis, MN (7/2005)
- [2] Peters, J.F.; Stubbs, J.M. ‘Optimizing extraction of ethyl benzene from poly(ethylene glycol) using supercritical carbon dioxide, a Monte Carlo study’, Fifth Midwest Undergraduate Computational Chemistry Consortium Conference, Minneapolis, MN (7/2005)