

Curriculum Vitae

Collin D. Wick

Department of Chemistry
Louisiana Tech University
Ruston, LA 71270

Telephone: 318-257-2345
Email: cwick@latech.edu

EDUCATION

June 2003: Doctor of Philosophy in Physical Chemistry GPA: 3.93/4.00 for 44.66 semester course credits (only 24 credits required for Ph.D. program) University of Minnesota, Minneapolis, MN

June 1998: Bachelor of Arts in Chemistry University of Minnesota-Morris, Morris, MN

EMPLOYMENT

2007-present: Tenure-Track Assistant Professor in the Department of Chemistry at Louisiana Tech University, Ruston, LA

2004-2007: Postdoctoral Associate with Dr. Liem X. Dang Chemical Sciences Division, Pacific Northwest National Laboratory, Richland, WA

2003-2004: Postdoctoral Associate with Professor D. N. Theodorou Dept. of Chemical Engineering, National Technical University Athens, Athens, Greece

1998-2003: Research Assistant with Professor J. I. Siepmann Department of Chemistry, University of Minnesota, Minneapolis, MN Research topic: Investigating Chromatographic Retention with Monte Carlo Simulations

2001 (Sum.): Research Assistant with Professor P. T. Cummings Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN

1998-1999: Teaching Assistant for physical and analytical chemistry courses: Physical Chemistry Laboratory, Kinetics and Statistical Mechanics, Quantitative Analysis, and Instrumental Analysis, Department of Chemistry, University of Minnesota, Minneapolis, MN

1997 (Fall): Teaching Assistant for General Chemistry Laboratory, Department of Chemistry, University of Minnesota-Morris, Morris, MN

AWARDS

2004: Department of Energy Computational Science and Graduate Fellowship
Howes Scholar Award

AWARDS (continued)

2003-2004: National Science Foundation-Mathematical and Physical Sciences Distinguished International Postdoctoral Research Fellowship

2000-2003: DOE Computational Science Graduate Fellowship

2002: First Prize IBM Award in Theoretical Chemistry, administered by the Division of Physical Chemistry of the ACS

FUNDING

2008-2011: C.D. Wick, "Computational modeling and design of polymer electrolytes for lithium ion batteries," Louisiana Board of Regents, \$123,440.

2009: C.D. Wick, "Studying Ion Dissociation Rates at Aqueous-Organic Interfaces," Battelle Memorial Institute, Richland, WA, \$11,132.

2010: C.D. Wick, "Simulations Of CO₂ Capture In Ionic Liquids," Battelle Memorial Institute, Richland, WA, \$21,075.

2008-2010: 1.6 million CPU hours from the Louisiana Optical Network Initiative (LONI).

PUBLICATIONS

(1) C.D. Wick and J. I. Siepmann, 'Self-adapting fixed-endpoint configurational-bias Monte Carlo method for the regrowth of interior segments of chain molecules with strong intramolecular interactions', *Macromolecules*, **33**, 7207-7218 (2000).

(2) C.D. Wick, M.G. Martin, and J.I. Siepmann, 'Transferable potentials for phase equilibria. 4. United-atom description of linear and branched alkenes and of alkylbenzenes', *J. Phys. Chem. B*, **104**, 8008-8016 (2000).

(3) C.D. Wick, M.G. Martin, J.I. Siepmann, and M.R. Schure, 'Simulating retention in gas-liquid chromatography: Benzene, toluene, and xylene solutes,' *Intl. J. Thermophys.*, **22**, 111-122 (2001).

(4) C.J. Cramer *et al.*, 'Cooperative molecular modeling exercise—the hypersurface as classroom,' *J. Chem. Ed.*, **78**, 1202-1205 (2001).

(5) C.D. Wick, J.I. Siepmann, and M.R. Schure, 'Simulation studies of retention in isotropic and oriented liquid n-octadecane,' *J. Phys. Chem. B*, **105**, 10961-10966 (2001).

(6) C.D. Wick, J.I. Siepmann, and M.R. Schure, 'Influence of analyte overloading on retention in gas-liquid chromatography: A molecular simulation view,' *Anal. Chem.*, **74**, 37-44 (2002).

PUBLICATIONS (continued)

(7) C.D. Wick, J.I. Siepmann, and M.R. Schure, 'Temperature effects on the retention of n-alkanes and arenes in helium-squalane gas-liquid chromatography: experiment and simulation,' *J. Chromatogr. A*, **954**, 181-190 (2002).

(8) C.D. Wick, J.I. Siepmann, and M.R. Schure, 'Molecular simulation of concurrent gas-liquid interfacial adsorption and partitioning in gas-liquid chromatography,' *Anal. Chem.*, **74**, 3518-3524 (2002).

(9) C.D. Wick, J.I. Siepmann, and M.R. Schure, 'Temperature dependence of transfer properties: Importance of heat capacity effects.' *J. Phys. Chem. B*, **107**, 10623-10627 (2003).

(10) C. D. Wick, J.I. Siepmann, and M.R. Schure, 'Simulation studies on the effects of mobile phase modification in liquid chromatography,' *Anal. Chem.* **76**, 2886-2892 (2004).

(11) C.D. Wick and D.N. Theodorou, 'Connectivity-altering Monte Carlo simulations of the end group effects on volumetric properties for poly(ethylene oxide),' *Macromolecules*, **37**, 7026-7033 (2004).

(12) J.-S. Lee, C.D. Wick, J.M. Stubbs, and J.I. Siepmann, 'Simulating the vapour-liquid equilibria of large cyclic alkanes,' *Mol. Phys.*, **103**, 99-104 (2005).

(13) L. Sun, C.D. Wick, J.I. Siepmann, and M.R. Schure, 'Temperature dependence of hydrogen bonding: An investigation of the retention of primary and secondary alcohols in gas-liquid chromatography,' *J. Phys. Chem. B*, **109**, 15118-15125 (2005).

(14) C.D. Wick and L.X. Dang, 'Diffusion at the liquid-vapor interface of an aqueous ionic solution utilizing a dual simulation technique,' *J. Phys. Chem. B*, **109**, 15574-15579 (2005).

(15) C.D. Wick, J.I. Siepmann, and D.N. Theodorou, 'Microscopic origins for the favorable solvation of carbonate ether copolymers in carbon dioxide,' *J. Am. Chem. Soc.*, **127**, 12338-12342 (2005).

(16) C.D. Wick and L.X. Dang, 'Investigating pressure effects on structural and dynamical properties of liquid methanol with many-body interactions,' *J. Chem. Phys.*, **123**, 184503-(1-7) (2005).

(17) C.D. Wick, J.M. Stubbs, L. Zhang, N. Rai, and J.I. Siepmann, 'Transferable potentials for phase equilibria. 7. United-atom description for amines, amides, nitriles, pyridine, and pyridine,' *J. Phys. Chem. B*, **109**, 18974-18982 (2005).

PUBLICATIONS (continued)

- (18) C.D. Wick and G.K. Schenter, 'Critical comparison of classical and quantum mechanical treatments of the phase equilibria of water,' *J. Chem. Phys.*, 124, 114505-(1-6) (2006).
- (19) C.D. and L.X. Dang, 'The distribution, structure, and dynamics of cesium and iodide ions at the H₂O-vapor and H₂O-CCl₄ interfaces,' *J. Phys. Chem. B*, 110, 6824-6831 (2006).
- (20) C.D. Wick, J.I. Siepmann, A.R. Sheth, and D.J.V. Grant, 'Monte Carlo calculations for the solid-state properties of warfarin sodium 2-propanol solvate,' *Cryst. Growth Design*, 6, 1318-1323 (2006).
- (21) C.D. Wick and L.X. Dang, 'Computational observation of enhanced solvation of the hydroxyl radical with increased NaCl concentration,' *J. Phys. Chem. B*, 110, 8917-8920 (2006), Cover article
- (22) C.D. Wick, L.X. Dang, and P. Jungwirth, 'Simulated Surface Potentials at the Vapor-Water Interface for the KCl Aqueous Electrolyte Solution,' *J. Chem. Phys.*, 125, 024706 (1-4) (2006).
- (23) C.D. Wick and L.X. Dang 'Molecule mechanism of transporting a polarizable iodide anion across the water-CCl₄ liquid/liquid interface,' *J. Chem. Phys.*, 126, 134702 (1-4) (2007).
- (24) C.D. Wick and L.X. Dang, 'Hydroxyl radical transfer between interface and bulk from transition path sampling,' *Chem. Phys. Lett.*, 444, 66-70 (2007).
- (25) C.D. Wick, I.F.W. Kuo, C.J. Mundy, and L.X. Dang, 'The effect of polarizability for the understanding of the molecular structure of aqueous interfaces,' *J. Chem. Theo. Comput.* 3, 2002-2010 (2007). Invited Review.
- (26) C.D. Wick and L.X. Dang, 'Molecular dynamics study of ion transfer and distribution at the interface of water and 1,2-dichloroethane,' *J. Phys. Chem. C*, 112, 647-649 (2008), Cover article.
- (27) C.D. Wick and L.X. Dang, 'Recent advances in understanding the transfer of polarizable ions across aqueous interfaces,' *Chem. Phys. Lett.*, 458, 1 (2008), Invited Review, Cover article.
- (28) C.D. Wick and S.S. Xantheas, 'Computational investigation of interfacial and bulk chloride and iodide first solvation shell aqueous structure,' *J. Phys. Chem. B*, 113, 4141-4146 (2008), Cover article.
- (29) C.D. Wick, 'NaCl dissociation dynamics at the air-water interface,' *J. Phys. Chem. C*, 113, 2497-2502 (2008).

PUBLICATIONS (continued)

- (30) C.D. Wick and L.X. Dang, 'Investigating hydroxide anion interfacial activity by classical and multi-state empirical valence bond molecular dynamics simulations,' *J. Phys. Chem. A*, 113, 6356-6364 (2009), Cover article.
- (31) C.D. Wick, 'Electrostatic dampening dampens the anion propensity for the air-water interface,' *J. Chem. Phys.* 131, 084715 (2009).
- (32) X. Sun, C.D. Wick, and L.X. Dang, 'Computational studies of aqueous interfaces of SrCl₂ salt solutions,' *J. Phys. Chem. B*, 113, 13993-13997 (2009).
- (33) C.D. Wick, and L.X. Dang, 'Computational investigation of the influence of organic-aqueous interfaces on NaCl dissociation dynamics,' *J. Chem. Phys.*, 132, 044702 (2010).
- (34) H. Wu and C.D. Wick, 'Computational investigation on the role of plasticizers on ion conductivity in poly(ethylene oxide) LiTFSI electrolytes,' *Macromolecules*, 43, 3502-3510 (2010).
- (35) C.D. Wick and L.X. Dang, 'The behavior of NaOH at the air-water interface, a computational study.' *J. Chem. Phys.*, 133, 084503 (2010).
- (36) C.D. Wick, B. Chen, and K.T. Valsaraj, 'Computational investigation of the influence of surfactants on the air-water interfacial behavior of polycyclic aromatic hydrocarbons,' *J. Phys. Chem. C*, 114, 14520-14527 (2010), Cover article.
- (37) C.D. Wick, T.-M. Chang, and L.X. Dang, 'Molecular mechanism of CO₂ and SO₂ molecules binding to the air/liquid interface of 1-butyl-3-methylimidazolium tetrafluoroborate: A molecular dynamics study with polarizable potential models,' *J. Phys. Chem.*, published online, Cover article.
- (38) X. Sun, C.D. Wick, and L.X. Dang, 'Computational study of ion distributions at the air/liquid methanol interface,' *J. Phys. Chem.* published online.
- (39) O.T. Cummings and C.D. Wick, 'Computational study of cation influence on anion propensity for the air-water interface,' *Chem. Phys. Lett.*, pulished online.
- (40) X. Sun, C.D. Wick, B. McGrail, P. Thallapally, and L.X. Dang, 'Computational study of hydrocarbon adsorption in metal-organic framework Ni₂(dhtp),' *J. Phys. Chem.*, under review.
- (41) X. Sun, C.D. Wick, B. McGrail, P. Thallapally, and L.X. Dang, 'Molecular mechanism of hydrocarbons binding to the metal-organic framework,' *Chem. Phys. Lett.*, under review.

PRESENTATIONS

2000-2007: Lead presenter in 35 presentations.

(36) C.D. Wick, "Computational Study of Interfacial Reaction Dynamics and Basicity," 2008 ACS Spring National Meeting, New Orleans, LA (4/08).

(37) C.D. Wick, "Monte Carlo simulations for phase equilibria: Polymer solubility and quantum effects," Invited Talk, 2008 ACS Spring National Meeting, New Orleans, LA (4/08).

(38) C.D. Wick, "Computational study of environmentally important interfaces," 17th Current Trends in Computational Chemistry Conference, Jackson, MS (10/08).

(39) C.D. Wick, "Importance of polarizability for understanding aqueous interfaces and bulk ion solvation," 2009 ACS Spring National Meeting, Salt Lake City, Utah, (03/09).

(40) C.D. Wick, "Using computers to discover strange behavior at water surfaces," Invited Talk, Louisiana State University, Baton Rouge, LA, (12/09).

(41) H. Wu and C.D. Wick, "Computational investigation of lithium ion mobility in polymer electrolytes," 17th annual Mardi Gras Conference, Baton Rouge, LA, (2/10).

STUDENTS

PhD: Hui Wu (2008-): 1 peer reviewed publication (34) and 1 presentation (41)
Oneka Cummings (2008-) 1 peer reviewed publication (39)