Curriculum Vitae

Collin D. Wick

Associate Dean of Research and Graduate Studies
CenturyLink Professor of Chemistry
College of Engineering and Science
PO Box 10348
Louisiana Tech University
Ruston, LA 71272

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

2022-present: Associate Dean of Research, College of Engineering and Science at Louisiana Tech University, Ruston, LA

2017-present: Associate Dean of Graduate Studies, College of Engineering and Science at Louisiana Tech University, Ruston, LA

2021-present: Professor at Louisiana Tech University, Ruston, LA

2013-2021: Associate Professor at Louisiana Tech University, Ruston, LA

2013-2017: Program Chair of Chemistry at Louisiana Tech University, Ruston, LA

2007-2013: Assistant Professor 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 and Honors

2013-present: CenturyLink Endowed Professorship

2012: College of Engineering and Science Leadership Award at Louisiana Tech University

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

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 ACS

Peer Reviewed Journal 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).

(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).

(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 H_2O-vapor and H_2O-CCl_4 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-CCl_4 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).

(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 $SrCl_2$ 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 CO_2 and SO_2 molecules binding to the air/liquid interface of 1-butyl-3-methylimidazolium tetrafluoroborate: A molecular dynamics study with polarizable potential models,' *J. Phys. Chem.B*, 114, 14965-14971 (2010) , 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.* A, 115, 5767-5773 (2011).

(39) O.T. Cummings and C.D. Wick, 'Computational study of cation influence on anion propensity for the air-water interface,' *Chem. Phys. Lett.*, 500, 41-45 (2010).

(40) 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.*, 501, 455-460 (2011).

(41) 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.*, 115, 2842-2849 (2011).

(42) L.X. Dang and C.D. Wick, Anion Effects on Interfacial Absorption of Gases in Ionic Liquids. A Molecular Dynamics Study,' *J. Phys. Chem.* B, 115, 6964-6970 (2011).

(43) C.D. Wick and O.T. Cummings, 'Understanding the factors that contribute to ion interfacial behavior,' *Chem. Phys. Lett.* 513, 4-6 (2011), Cover article.

(44) C.D. Wick, T.-M. Chang, J.A. Slocum, and O.T. Cummings, 'Computational investigation of the *n*-alkane-water interface with many- body potentials: the effect of chain length and ion distributions,' *J. Phys. Chem. C*, 116, 783-790 (2012).

(45) C.D. Wick, 'Hydronium behavior at the air-water interface with a polarizable multi-state empirical valence bond model,' *J. Phys. Chem. C*,116, 4026-4038 (2012).

(46) S.J. Keasler, S.M. Charan, C.D. Wick, I.G. Economou, and J.I. Siepmann, 'Transferable potentials for phase equilibria-united atom description of five- and six-membered cyclic alkanes and ethers,' *J. Phys. Chem. B*, 116, 11234-11246 (2012).

(47) C.D. Wick, A.J. Lee, and S.W. Rick, 'How intermolecular charge transfer influences the air-water interface,' *J. Chem. Phys.*, 137, 154701 (2012).

(48) H. Wu, O.T. Cummings, and C.D. Wick, 'Computational investigation on the effect of alumina hydration on lithium ion mobility in poly(ethylene oxide) $LiClO_4$ electrolytes,' *J. Phys. Chem. B*, 116, 14922-14932 (2012)

(49) O.T. Cummings and C.D. Wick, 'Computational study on the effect of alkyl chain length on alkane-water interfacial width,' *Chem. Phys. Lett.*, 556, 65-69 (2013).

(50) O.T. Cummings and C.D. Wick, 'Interfacial Behavior of Simple Inorganic Salts at the Air-Water Interface Investigated with a Polarizable Model with Electrostatic Damping,' *J. Chem. Phys.*, 139, 064708 (2013).

(51) C.D. Wick, 'HCl Accommodation, Dissociation, and Propensity for the Surface of Water,' *J. Phys. Chem. A*, 117, 12459-12467 (2013).

(52) V.T. Nguyen, P.T.M. Nguyen, L.X. Dang, D. Mei, C.D. Wick, and D.D. Do, 'A comparative study of the adsorption of water and methanol in zeolite BEA: a molecular simulation study', *Molecular Simulation*, 40, 1113-1124 (2014).

(53) C.D. Wick and T.-M. Chang, 'Computational observation of pockets of enhanced water concentration at the 1-octanol/water interface,' *J. Phys. Chem. B*, 28, 7785-7791 (2014).

(54) J. Jin, J.D. Miller, L.X. Dang, and C.D. Wick, 'Effect of Cu^{2+} activation on interfacial water structure at the sphalerite surface as studied by molecular dynamics simulation,' *Int. J. Miner. Process.* 145, 66-76 (2015).

(55) R. Kumar, C. Knight, C.D. Wick, and B. Chen, 'Bringing Reactivity to the Aggregation-Volume-Bias Monte Carlo Based Simulation Framework: Water Nucleation Induced by a Reactive Proton,' *J. Phys. Chem. B*, 119, 9068-9075 (2015).

(56) A.S. Hassan, A. Navulla, L. Meda, B. Ramachandran, C.D. Wick, "Molecular Mechanisms for the Lithiation of Ruthenium Oxide (RuO2) Nanoplates as Lithium-Ion Battery Anode Materials: An Experimentally Motivated Computational Study,' *J. Phys. Chem. C*, 119, 9705-9713 (2015).

(57) J. Jin, J.D. Miller, L.X. Dang, and C.D. Wick, 'Effect of surface oxidation on interfacial water structure at a pyrite (100) surface as studied by molecular dynamics simulation,' *Int. J. Miner. Process.*, 139, 64-76 (2015).

(58) A.S. Hassan, K. Moyer, B.R. Ramachandran, and C.D. Wick, 'Comparison of Storage Mechanisms in RuO_2, SnO_2, SnS_2 for Lithium-Ion Battery Anode Materials,' *J. Phys. Chem. C*, 120, 2036-2046 (2016).

(59) S.B. Ranganath, A.S. Hassan, B.R. Ramachandran, and C.D. Wick, 'Role of Metal-Lithium Oxide Interfaces in the Extra Lithium Capacity of Metal Oxide Lithium-Ion Battery Anode Materials, ' *J. Electrochem. Soc.*, 163, A2172-A2178 (2016).

(60) C.D. Wick, 'Comparing Hydroxide and Hydronium at the Instantaneous Air-Water Interface Using Polarizable Multi-State Empirical Valence Bond Models, ' *Computational and Theoretical Chemistry*, 1116 64-72 (2016). DOI: 10.1016/j.comptc.2017.01.036

(61) C.D. Wick, 'A Comparison of Sodium and Hydrogen Halides at the Air-Water Interface,' *J. Chem. Phys.*, 147, 161703 (2017).

(62) L.X. Dang, G.K. Schenter, and C.D. Wick, 'Rate Theory of Ion Pairing at the Water Liquid-Vapor Interface,' *J. Phys. Chem. C*, 121, 10018-10026 (2017).

(63) X. Zhang, B. Zhang, Y. Mu, S. Shao, C.D. Wick, B.R. Ramachandran, and W.J. Meng, 'Mechanical Failure of Metal/Ceramic Interfacial Regions Under Shear Loading,' *Acta Materialia*, 138, 224-236 (2017) DOI: 10.1016/j.actamat.2017.07.053

(64) S. Sun, B.R. Ramachandran, and C.D. Wick, 'Solid, Liquid, and Interfacial Properties of TiAl Alloys: Parameterization of a New Modified Embedded Atom Method Model,' *J. Phys*: *Condens. Matter* 30, 075002 (2018).

(65) Z.H. Swart, A.J. Ulrich, C.D. Wick, and A.D. Radadia, 'Characterizing the Local Oxidation Nanolithography on Highly Oriented Pyrolytic Graphite,' *Nanotechnology* 30, 275301 (2019).

(66) A.S.M. Miraz, S. Sun, S. Shao, W.J. Meng, B.R. Ramachandran, and C.D. Wick, 'Computational Study of Metal/Ceramic Interfacial Adhesion and Barriers to Shear Displacement,' *Comp. Mater. Sci.* 168, 104-115 (2019).

(67) J. Jin, X. Wang, C.D. Wick, L.X. Dang, and J.D. Miller, 'Silica Surface States and their Wetting Characteristics,' *Surface Innovations* 8, 145-157 (2019).

(68) X. Xhang, S. Shao, A.S.M Miraz, C.D. Wick, B.R. Ramachandran, and W.J. Meng, 'Low Temperature Growth of Cu Thin Films on TiN(001) Templates: Structure and Energetics,' *Materialia* 12, 100748 (2020).

(69) A.S.M. Miraz, E. Williams, W.J. Meng, B.R. Ramachandran, and C.D. Wick, 'Improvement of Ti/TiN Interfacial Shear Strength by Doping – A First Principles Density Functional Theory Study,' *Applied Surf. Sci.* 517, 146185 (2020).

(70) S. Bhasker-Ranganath, C.D. Wick, and B.R. Ramachandran, 'Computational Insights into the Molecular Mechanisms for Chromium Passivation of Stainless-Steel Surfaces,' *Materials Today Chem.* 17, 100298 (2020).

(71) A.S.M. Miraz, N. Dhariwal, W.J. Meng, B.R. Ramachandran, and C.D. Wick, 'Development and application of interatomic potentials to study the stability and shear strength of Ti/TiN and Cu/TiN interfaces,' *Materials & Design*, 196, 109123, (2020) DOI: 10.1016/j.matdes.2020.109123.

(72) C.D. Wick, A.J. Peters, and G. Li, 'Quantifying the contributions of energy storage in a thermoset shape memory polymer with high stress recovery: A molecular dynamics study,' *Polymer*, 213, 123319, (2021) DOI: 10.1016/j.polymer.2020.123319.

(73) C. Yan, X. Feng, C.D. Wick, A.J. Peters, and G. Li, 'Machine learning assisted discovery of new thermoset shape memory polymers based on a small training set,' *Polymer*, 214, 123351, (2021) DOI: 10.1016/j.polymer.2020.123351.

(74) A.S.M. Miraz, W.J. Meng, B.R. Ramachandran, and C.D. Wick, 'Computational observation of the strengthening of Cu/TiN metal/ceramic interfaces by sub-nanometer interlayers and dopants,' *Applied Surface Sci.* 554, 149562 (2021) DOI: 10.1016/j.matdes.2021.110120.

(75) N. Dhariwal, A.S.M. Miraz, W.J. Meng, B.R. Ramachandran, and C.D. Wick, 'Impact of metal/ceramic interactions on interfacial shear strength: Study of Cr/TiN using a new modified embedded-atom potential,' *Materials & Design* 210, 110120 (2021) DOI: 10.1016/j.matdes.2021.110120.

(76) A. Shafe, C.D. Wick, A.J. Peters, and G. Li, 'Effect of atomistic fingerprints on thermomechanical properties of epoxy-diamine thermoset shape memory polymers,' *Polymer* 242, 124577 (2022) DOI: 10.1016/j.polymer.2022.124577.

(77) F. M. Sime, J. Jin, X. Wang, C.D. Wick, and J.D. Miller, "Characterization and simulation of graphite edge surfaces for the analysis of carbonaceous material separation from sulfide ores by flotation," *Minerals Engineering* 182, 107590 (2022) DOI: 10.1016/j.mineng.2022.107590.

(78) P. Nourian, C.D. Wick, G. Li, and A.J. Peters, "Correlation between cyclic topology and shape memory properties of an amine-based thermoset shape memory polymer: a coarse-grained molecular dynamics study," *Smart Materials and Structures* 31, 105014 (2022) DOI: 10.1088/1361-665X/ac8bb5.

(79) N. Dhariwal, A.S.M. Miraz, W.J. Meng, and C.D. Wick, "Strengthening the Ti/TiN interface against shear failure with Al dopants: A molecular dynamics study," *Appl. Surf. Sci.* 613, 156024 (2023). DOI:https://doi.org/10.1016/j.apsusc.2022.156024.

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).

(42) C.D. Wick, "The Importance of Polarizability and its Implementation for Understanding Aqueous Interfacial and Bulk Ion Solvation," Invited Talk, CECAM workshop, Lausanne, Switzerland (6/10).

(43) C.D. Wick, "Ions, ion pairing, and how aqueous interfaces influence them," Telluride workshop on Ions in Aqueous Solutions and Molecular Biology, Invited Talk, Telluride, CO, (07/10).

(45) C.D. Wick, "The Importance of Polarizability and its Implementation for Understanding Aqueous Interfacial and Bulk Ion Solvation," Invited Talk, PacificChem 2010, Honolulu, HI (12/10).

(46) C.D. Wick and H. Wu, “Computational Investigation of Lithium Ion Mobility in Polymer Electrolytes,” Invited Talk, 2011 ACS Spring National Meeting, Denver, CO (08/11).

(47) C.D. Wick, “How the Air-Water Interface Influences Charged Species, From Water to Ions,” Invited Talk, 2012 Mardi Gras Conference, Baton Rouge, LA (02/12).

(48) C.D. Wick, “How the Air-Water Interface Influences Charged Species, From Water to Ions,” Invited Talk, Telluride workshop on Ions in Aqueous Solutions and Molecular Biology, Telluride, CO, (07/12).

(49) C.D. Wick, “Elucidating unique behaviors at the interface of water,” Invited Talk, 2012 ACS Spring National Meeting, Philadelphia, PA (08/12).

(50) C.D. Wick, “Computational investigation of lithium transport in polymer electrolytes next to an alumina surface,” Invited Talk, 2012 Southwest American Chemical Society Regional Meeting, Baton Rouge, LA (11/12).

(51) C.D. Wick, “Computational Investigation of Ion and Acid Propensity and Dissociation at the Air-Water Interface, “ Invited Talk, 2012 AirUCI workshop, Laguna Beach, CA (02/13).

(52) C.D. Wick, “Computational Chemistry using LONI, from small *ab initio* calculations to large scale simulations for molecular systems,” Invited Talk, HPC user Symposium 2013, Baton Rouge, LA (06/13)

(53) C.D. Wick, “Ion and acid behavior at the air-water and organic-water interfaces,” Invited Talk, Telluride workshop on Ions in Aqueous Solutions and Molecular Biology, Telluride, CO, (07/14).

(54) C.D. Wick, “Polarizable Empirical Valence Bond Models for Acids and Bases at Interfaces,” Invited Talk, Advancing the Frontiers of [Bio]Chemistry with Valence Bond Approaches, Uppsala, Sweden,(06/16).

Students

Sarah Chovanec and Kathryn Nance (2009): BS students.

Hui Wu (2008-2011): PhD granted, 2 peer reviewed publications.

Oneka Cummings (2008-2013) PhD granted, in Computational analysis and modeling 5 peer reviewed publications.

Josh Slocum (2011), BS student, 1 peer reviewed publication.

David Smalley (2011), BS student in Chemistry.

David Idodo (2013-2014), MS student in Engineering, supervised research.

Suman Bhaskar (2013-2016), MS student in Engineering, co-advised with Dr. Ramachandran.

Thomas Dixon and Olayiwola Oluwatobi (2014-2015), BS students.

Ayo Hassan (2011-2015), Postdoctoral Scholar, co-advised with Dr. Ramachandran.

Shoutian Sun (2016-2018), Postdoctoral Scholar.

Shama Miraz (2016-2021), PhD student in Engineering.

Darren Bailey (2016-2017), BS student in Chemistry.

Eboni Williams (2017-2020), BS student in Chemistry

Nisha Dhariwal (2017-present), PhD student in Molec. Sci. and Tech.

Cole Allen (2018-2019), BS student in Chemistry.

Hamid Sharifi Torki (2021-present), PhD Student in Engineering.

External Funding

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

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

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

2008-present: 20.8 million CPU hours from the Louisiana Optical Network Initiative (LONI). PI

2010-2013: "Computational design of CO_2-philic hydrocarbon polymers to promote more efficient oil recovery," Petroleum Research Fund, $50,000. PI

2010-2015: "Louisiana Alliance for Simulation-Guided Materials Applications (part of the RII Track 1 award to Louisiana EPSCoR)," NSF, $20,000,000 for Louisiana, $3,600,000 for LA Tech, Senior Researcher, head of Energy Materials research thrust. Senior Investigator.

2015-2020: "Consortium for Innovation in Manufacturing and Materials (part of the RII Track 1 award to Louisiana EPSCoR)," NSF, $20,000,000 for Louisiana. Senior Investigator.

2017: "HC/HPLC Equipment for Chemistry Research," LA Board of Regents, $85,220, Co-PI.

2018-2021: "Increasing Diversity in Doctoral Populations at Louisiana Tech University," LA Board of Regents $120,000, co-PI.

2019-2022: "Increasing Diversity in Doctoral Populations at Louisiana Tech University," LA Board of Regents $120,000, co-PI.

2020-2023: "Increasing Diversity in Doctoral Populations at Louisiana Tech University," LA Board of Regents $120,000, co-PI.

2021-2024: "Increasing Diversity in Doctoral Populations at Louisiana Tech University," LA Board of Regents $60,000, co-PI.

2022-2025: "Increasing Diversity in Doctoral Populations at Louisiana Tech University," LA Board of Regents $60,000, co-PI.

2021: "Rick and Lisa Shirley Endowed Graduate Student Scholarships Matching Funds," LA Board of Regents $120,000, co-PI.

2023-2026: "Increasing Diversity in Doctoral Populations at Louisiana Tech University," LA Board of Regents $60,000, co-PI.

2020-2025: "Louisiana Materials Design Alliance (LAMDA)," NSF, $20,000,000 for Louisiana, Senior Investigator.

Administrative Positions, Duties, and Highlights

2013-2017: Program Chair of Chemistry. I was responsible for the Undergraduate Chemistry Program, including setting the curriculum, class schedule, assuring accreditation with SACS, and ACS Certification of all degrees. In addition, I was responsible for overseeing student advising, was significantly involved in faculty hiring (chairing the hiring committees), and made efforts to improve student experience, retention, and recruitment. A notable accomplishment during my time as program chair was an increase in the number of undergraduate majors, increasing from 39 the Fall of 2013 to 102 students in the Fall of 2017 (an increase of 160%). During this same period,

the College of Engineering and Science increased by 33%. Moreover, the student affiliate of the ACS tripled in size, was finally recognized by the National ACS, and became much more active in the community. Part of the increased enrollment was due to changing the Biochemistry track from that used primarily for pre-professional majors into a very popular degree program in itself, outpacing the 'traditional' Chemistry track by more than double.

2017-present: Associate Dean of Graduate Studies for the College of Engineering and Science. I am in responsible for all graduate programs in the College of Engineering and Science, which includes four PhD programs (with numbers of students averaging 130), and seven MS programs (with an average of approximately 200 students). These include two MS programs that can be taken online. Additionally, two graduate certificates can be earned, a six-sigma black belt, and a data science certificate in which I wrote the proposal that was approved by the state. The position requires that I manage multiple budgets, including the graduate student assistantship budget, the student worker budget, and the graduate scholarship budget, all for the entire college. These are used to cover all teaching assistantship duties, faculty and staff support, and research assistant support for new faculty on startup assistance. The budgets total approximately 1.5 million dollars. I am responsible for maintaining SACS accreditation for the MSE in Engineering program specifically, and have oversight on all graduate program coordinators, including them keeping up with accreditation. I approve all theses and dissertations, student plans of study, curriculum changes, and course additions and changes. I have written a proposal for a new doctoral program in Engineering and Technology management, which is waiting for final approval by the Louisiana Board of Regents. This program will be designed for students to be able to earn a doctoral degree while on campus, but is also designed to cater to adults who are working a regular job, and can be earned remotely.

2022-present: Associate Dean of Research for the College of Engineering and Science. In this position, I facilitate faculty professional development to improve research productivity, help them navigate the grant writing and submission processes, and bring together groups of faculty members into teams to go after larger grant proposals. This includes leading and helping bring in workshops for proposal writing, improving the dissemination of research outputs, and the grant submission process. I review proposal submissions, suggesting improvements, and work as a liaison with the Office of Sponsored Projects and sometimes Program Managers. Additionally, I oversee and supervise the directors for the five research centers in the college, including the Institute for Micromanufacturing, Trenchless Technology Center, Integrated STEM Education Research Center, Center for Biomedical Engineering and Rehabilitation Science, and the Center for Applied Physics Science.

References will be made available upon request.