Jeffrey R. Errington

Curriculum Vitae

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revised 1/2020

EDUCATION

Cornell University, Ithaca, NY

Ph.D., Chemical Engineering, August, 1999

Dissertation Title: The Development of Novel Simulation Methodologies and Intermolecular Potential Models for Real Fluids

Advisor: Professor Athanassios Z. Panagiotopoulos

University at Buffalo, Buffalo, NY

B.S., Chemical Engineering, *Summa Cum Laude*, May, 1995

PROFESSIONAL EXPERIENCE

University at Buffalo, Buffalo, NY

Associate Dean of Undergraduate Education, School of Engineering, June 2014
Professor, Chemical and Biological Engineering, September 2011
Associate Professor, Chemical and Biological Engineering, September 2006 to August 2011
Assistant Professor, Chemical and Biological Engineering, August 2001 to August 2006

Research Topics: Molecular modeling of complex fluids, investigation of phase transitions, study of interfacial phenomena, development of novel molecular simulation methods, molecular understanding of aqueous solutions, examination of the link between thermodynamic and transport properties.

Princeton University, Princeton, NJ

Post-Doctoral Research Associate, Chemical Engineering, August 1999 to August 2001

Projects: Bioprotection of Plasma Proteins in the Eradication of Viruses; Computational Investigation of Network Forming Fluids

Advisor: Professor Pablo G. Debenedetti

HONORS AND AWARDS

SUNY Chancellor's Award for Excellence in Scholarship and Creative Activities (2016)

UB Exceptional Scholar Award (Sustained Achievement), 2014

CoMSEF Impact Award, 2013

UB SEAS Faculty Excellence Award, 2008

UB Exceptional Scholar Award (Young Investigator), 2005

James D. Watson Investigator Award, 2004

National Science Foundation CAREER Award, 2003

Second Industrial Fluid Properties Simulation Challenge, first place finish for Problem 2 (Determination of Henry's law constants), 2004

PUBLICATIONS

Total Citations = 5,341; h-index = 40 (as of January 2020, per ISI)

I. Publications in Peer-Reviewed Journals

101. "Improving the efficiency of Monte Carlo simulations of ions using expanded grand canonical ensembles", H. W. Hatch, S. W. Hall, J. R. Errington, V. K. Shen, *J. Chem. Phys.* **151**, 144109 (2019).

100. "Effect of Surface Hydrophilicity on the Interfacial Properties of a Model Octane-Water-Silica System", W. J. Guo, J. R. Errington, *J. Phys. Chem. C* **123**, 19649-19658 (2019).

99. "Construction of the interface potential from a series of canonical ensemble simulations", K. Jain, A. J. Schultz, J. R. Errington, *J. Chem. Phys.* **151**, 044103 (2019).

98. "Application of the interface potential approach for studying wetting behavior within a molecular dynamics framework", K. Jain, A. J. Schultz, J. R. Errington, *J. Chem. Phys.* **150**, 204118 (2019).

97. "Effect of Carboxylic Acid on the Wetting Properties of a Model Water-Octane-Silica System", W. J. Guo, J. R. Errington, *Langmuir* **35**, 6540-6549 (2019).

96. "Using isothermal-isobaric Monte Carlo simulation to study the wetting behavior of model systems", K. Jain, K. S. Rane, J. R. Errington, *J. Chem. Phys.* **150**, 084110 (2019).

95. "Free energy and concentration of crystalline vacancies by molecular simulation", A. Purohit, A. J. Schultz, S. G. Moustafa, J. R. Errington, D. A. Kofke, *Mol. Phys.* **116**, 3027-3041 (2018).

94. "Calculation of the Saturation Properties of a Model Octane-Water System Using Monte Carlo Simulation", W. J. Guo, P. Bali, J. R. Errington, *J. Phys. Chem. B* **122**, 6260-6271 (2018).

93. "Monte Carlo Simulation Strategies to Compute the Interfacial Properties of a Model Octane-Water-Silica System", W. J. Guo, J. R. Errington, *J. Phys. Chem. C* **122**, 17309-17318 (2018).

92. "Position-dependent dynamics explain pore-averaged diffusion in strongly attractive adsorptive systems", W. P. Krekelberg, D. W. Siderius, V. K. Shen, T. M. Truskett, J. R. Errington, *Langmuir* 49, 13955-13963 (2017).

91. "Multivariable extrapolation of grand canonical free energy landscapes", N. A. Mahynski, J. R. Errington, and V. K. Shen *J. Chem. Phys.* **147**, 234111 (2017).

90. "Temperature extrapolation of multicomponent grand canonical free energy landscapes", N. A. Mahynski, J. R. Errington, and V. K. Shen *J. Chem. Phys.* **147**, 054105 (2017).

89. "Connection Between Thermodynamics and Dynamics of Simple Fluids in Pores: Impact of Fluid-Fluid Interaction Range and Fluid Solid Interaction Strength", W. P. Krekelberg, D. W. Siderius, V. K. Shen, T. M. Truskett, J. R. Errington, *J. Phys. Chem. C* **121**, 16316-16327 (2017).

88. "Predicting low-temperature free energy landscapes with flat-histogram Monte Carlo methods", N. A. Mahynski, M. A. Blanco, J. R. Errington, and V. K. Shen *J. Chem. Phys.* **146**, 074101 (2017).

87. "Multibody Interactions, Phase Behavior, and Clustering in Nanoparticle-Polyelectrolyte Mixtures", G. Pandav, V. Pryamitsyn, J. Errington, V. Ganesan, *J. Phys. Chem. B* **119**, 14536-14550 (2015).

86. "The rate of convergence of the virial series in confined systems", J. H. Yang, A. J. Schultz, J. R. Errington, and D. A. Kofke, *Mol. Phys.* **113**, 1179-1189 (2015).

85. "Understanding the influence of Coulomb and dispersion interactions on the wetting behavior of ionic liquids", K. S. Rane and J. R. Errington, *J. Chem. Phys.* **141**, 174706:1-11 (2014).

84. "Liquid-vapor phase behavior of asphaltene-like molecules", K. S. Rane, V. Kumar, S. Wierzchowski, M. Shaik, and J. R. Errington, *Ind. Eng. Chem. Res.* **53**, 17833-17842 (2014).

83. "Evaluation of the Performance of GAFF and CGenFF in the Prediction of Liquid–Vapor Saturation Properties of Naphthalene Derivatives", V. Kumar, K. S. Rane, S. Wierzchowski, M. Shaik, and J. R. Errington, *Ind. Eng. Chem. Res.* **53**, 16072–16081 (2014).

82. "Dimensionality and design of isotropic interactions that stabilize honeycomb, square, simple cubic, and diamond lattices", A. Jain, J. R. Errington, and T. M. Truskett, *Phys. Rev. X* **4**, 031049:1-8 (2014).

81. "Saturation properties of 1-alkyl-3-methylimidazolium based ionic liquids", K. S. Rane and J. R. Errington, *J. Phys. Chem. B* **118**, 8734-8743 (2014).

80. "Connection between thermodynamics and dynamics of simple fluids in highly attractive pores", W. P. Krekelberg, V. K. Shen, D. W. Siderius, T. M. Truskett, and J. R. Errington, *Langmuir* **29**, 14527-14535 (2013).

79. "Phase Behavior of Materials with Isotropic Interactions Designed by Inverse Strategies to Favor Diamond and Simple Cubic Lattice Ground States", A. Jain, J. R. Errington, and T. M. Truskett, *J. Chem. Phys.* **139**, 141102:1-4 (2013).

78. "Wetting behavior of water near nonpolar surfaces", V. Kumar and J. R. Errington, *J. Phys. Chem. C* **117**, 23017-23026 (2013).

77. "The impact of small-scale geometric roughness on wetting behavior", V. Kumar and J. R. Errington, *Langmuir* **29**, 11815-11820 (2013).

76. "Understanding wetting of immiscible liquids near a solid surface using molecular simulation", V. Kumar and J. R. Errington, *J. Chem. Phys.* **139**, 064110:1-14 (2013).

75. "Using Monte Carlo simulation to compute liquid-vapor saturation properties of ionic liquids", K. S. Rane and J. R. Errington, *J. Phys. Chem. B* **117**, 8018-8030 (2013).

74. "Application of the interface potential approach to calculate the wetting properties of a model water system", V. Kumar and J. R. Errington, *Mol. Simulat.* **39**, 1143-1152 (2013).

73. "Monte Carlo simulation strategies to compute interfacial and bulk properties of binary fluid mixtures", V. Kumar and J. R. Errington, *J. Chem. Phys.* **138**, 174112:1-14 (2013).

72. "Monte Carlo simulation methods for computing liquid-vapor saturation properties of model systems", K. S. Rane, S. Murali, and J. R. Errington, *J. Chem. Theory Comput.* **9**, 2552-2566 (2013).

71. "Predicting the relaxation time of a nanoconfined supercooled liquid", T. S. Ingebrigtsen, J. R. Errington, T. M. Truskett, and J. C. Dyre, *Phys. Rev. Lett.* **111**, 235901:1-6 (2013).

70. "Calculation of inhomogeneous-fluid cluster expansions with application to the hard-sphere/hard-wall system", J. H. Yang, A. J. Schultz, J. R. Errington, and D. A. Kofke, *J. Chem. Phys.* **138**, 134706:1-13 (2013).

69. "Inverse design of simple pairwise interactions with low-coordinated 3D lattice ground states", A. Jain, J. R. Errington, and T. M. Truskett, *Soft Matter* **9**, 3866-3870 (2013).

68. "Enhancing tracer diffusivity by tuning interparticle interactions and coordination shell structure", J. Carmer, G. Goel, M. J. Pond, J. R. Errington, and T. M. Truskett, *Soft Matter* **8**, 4083-4089 (2012).

67. "Monte Carlo simulation methods for computing the wetting and drying properties of model systems", K. S. Rane, V. Kumar, and J. R. Errington, *J. Chem. Phys.* **135**, 234102:1-13 (2011).

66. "Monte Carlo simulation strategies for computing the wetting properties of fluids at geometrically rough surfaces", V. Kumar, S. Sridhar, and J. R. Errington, *J. Chem. Phys.* **135**, 184702:1-14 (2011).

65. "Impact of surface roughness on diffusion of confined fluids", W. P. Krekelberg, V. K. Shen, J. R. Errington, and T. M. Truskett, *J. Chem. Phys.* **135**, 154502:1-9 (2011).

64. "Mapping between long-time molecular and Brownian dynamics", M. J. Pond, J. R. Errington, and T. M. Truskett, *Soft Matter* **7**, 9859-9862 (2011).

63. "Implications of the effective one-component analysis of pair correlations in colloidal fluids with polydispersity", M. J. Pond, J. R. Errington, and T. M. Truskett, *J. Chem. Phys.* **135**, 124513:1-9 (2011).

62. "Communication: Generalizing Rosenfeld's excess-entropy scaling to predict long-time diffusivity in dense fluids of Brownian particles: From hard to ultrasoft interactions", M. J. Pond, J. R. Errington, and T. M. Truskett, *J. Chem. Phys.* **134**, 081101:1-4 (2011).

61. "On the use of excess entropy scaling to describe single-molecule and collective dynamic properties of hydrocarbon isomer fluids", R. Chopra, T. M. Truskett, and J. R. Errington, *J. Phys. Chem. B* **114**, 16487–16493 (2010).

60. "Excess entropy scaling of dynamics for a confined fluid of dumbbell-shaped particles", R. Chopra, T. M. Truskett, and J. R. Errington, *Phys. Rev. E* **82**, 041201:1-10 (2010).

59. "Excess entropy scaling of dynamic quantities for fluids of dumbbell-shaped particles", R. Chopra, T. M. Truskett, and J. R. Errington, *J. Chem. Phys.* **133**, 104506:1-11 (2010).

58. "On the use of excess entropy scaling to describe the dynamic properties of water", R. Chopra, T. M. Truskett, and J. R. Errington, *J. Phys. Chem. B* **114**, 10558–10566 (2010).

57. "Nanoscale limit to the applicability of Wenzel's equation", E. M. Grzelak and J. R. Errington, *Langmuir* **26**, 13297-13304 (2010).

56. "Calculation of interfacial properties via free-energy-based molecular simulation. The influence of system size", E. M. Grzelak and J. R. Errington, *J. Chem. Phys.* **132**, 224702:1-13 (2010).

55. "Molecular Simulation Study of Anisotropic Wetting", E. M. Grzelak, V. K. Shen, and J. R. Errington, *Langmuir* **26**, 8274–8281 (2010).

54. "Generalized Rosenfeld scalings for tracer diffusivities in not-so-simple fluids: Mixtures and soft particles", W. P. Krekelberg, M. J. Pond, G. Goel, V. K. Shen, J. R. Errington, and T. M. Truskett, *Phys. Rev. E* **80**, 061205:1-13 (2009).

53. "Composition and concentration anomalies for structure and dynamics of Gaussian-core mixtures", M. J. Pond, W. P. Krekelberg, V. K. Shen, J. R. Errington, and T. M. Truskett, *J. Chem. Phys.* **131**, 161101:1-4 (2009).

52. "Available states and available space: Static properties that predict self diffusivity of confined fluids", G. Goel, W. P. Krekelberg, M. J. Pond, J. Mittal, V. K. Shen, J. R. Errington, and T. M. Truskett, *J. Stat. Mech.*, P04006:1-18 (2009).

51. "Anomalous structure and dynamics of the Gaussian-core fluid", W. P. Krekelberg, T. Kumar, J. Mittal, J. R. Errington, and T. M. Truskett, *Phys. Rev. E* **79**, 031203:1-6 (2009).

50. Response to "Comment on 'Residual multiparticle entropy does not generally change sign near freezing'" [J. Chem. Phys. 130, 037101 (2009)], W. P. Krekelberg, V. K. Shen, J. R. Errington, and T. M. Truskett, *J. Chem. Phys.* **130**, 037102:1-2 (2009).

49. "Insights into crowding effects on protein stability from a coarse-grained model", V. K. Shen, J. K. Cheung, J. R. Errington, and T. M. Truskett, *J. Biomech. Eng.* **131**, 071002:1-7 (2009).

48. "Fluid phase behavior of a model colloid-polymer mixture. Influence of polymer size and interaction strength", T. W. Rosch and J. R. Errington, *J. Chem. Phys.* **129**, 164907:1-9 (2008).

47. "The phase behavior of model confined fluids. Influence of substrate-fluid interaction strength", T. W. Rosch and J. R. Errington, *J. Phys. Chem. B* **112**, 14911-14919 (2008).

46. "Influence of substrate strength on wetting behavior", M. S. Sellers and J. R. Errington, *J. Phys. Chem. C* **112**, 12905-12913 (2008).

45. "Structure, stability, and rupture of free and supported liquid films and assemblies in molecular simulations", R. Godawat, S. Jamadagni, J. R. Errington, and S. Garde, *Ind. Eng. Chem. Res.* **47**, 3582-3590 (2008).

44. "Residual multiparticle entropy does not generally change sign near freezing", W. P. Krekelberg, V. K. Shen, J. R. Errington, and T. M. Truskett, *J. Chem. Phys.* **128**, 161101:1-3 (2008).

43. "Comparing the Use of Gibbs Ensemble and Grand-Canonical Transition-Matrix Monte Carlo to Determine Phase Equilibria", A. S. Paluch, V. K. Shen, and J. R. Errington, *Ind. Eng. Chem. Res*. **47**, 4533-4541 (2008).

42. "Layering and position-dependent diffusive dynamics of confined fluids", J. Mittal, T. M. Truskett, J. R. Errington, and G. Hummer, *Phys. Rev. Lett.* **100**, 145901:1-4 (2008).

41. "Tuning density profiles and mobility of inhomogeneous fluids", G. Goel, W. P. Krekelberg, J. R. Errington, and T. M. Truskett, *Phys. Rev. Lett.* **100**, 106001:1-4 (2008).

40. "Computation of interfacial properties via grand canonical transition matrix Monte Carlo simulation", E. M. Grzelak and J. R. Errington, *J. Chem. Phys.* **128**, 014710:1-10 (2008).

39. "Confinement, entropy, and single-particle dynamics of equilibrium hard-sphere mixtures", J. Mittal, V. K. Shen, J. R. Errington, and T. M. Truskett, *J. Chem. Phys.* **127**, 154513:1-8 (2007).

38. "Calculation of surface tension via area sampling", J. R. Errington and D. A. Kofke, *J. Chem. Phys.* **127**, 174709:1-12 (2007).

37. "Investigation of the phase behavior of an embedded charge protein model through molecular simulation", T. W. Rosch and J. R. Errington, *J. Phys. Chem. B* **111**, 12591-12598 (2007).

36. "Relationships between self-diffusivity, packing fraction, and excess entropy in simple bulk and confined fluids" (feature article, cover), J. Mittal, J. R. Errington, and T. M. Truskett, *J. Phys. Chem. B* **111**, 10054-10063 (2007).

35. "Does confining the hard-sphere fluid between hard walls change its average properties?", J. Mittal, J. R. Errington, and T. M. Truskett, *J. Chem. Phys.* **126**, 244708:1-8 (2007).

34. "Comparative Study of the Effect of Tail Corrections on Surface Tension Determined by Molecular Simulation", V. K. Shen, R. D. Mountain, and J. R. Errington, *J. Phys. Chem. B* **111**, 6198-6207 (2007).

33. "Coarse-grained strategy for modeling protein stability in concentrated solutions III: Directional protein interactions", J. K. Cheung, V. K. Shen, J. R. Errington, and T. M. Truskett, *Biophys. J.* **92**, 4316-4324 (2007).

32. "Excess entropy-based anomalies for a water-like fluid", J. R. Errington, T. M. Truskett, and J. Mittal, *J. Chem. Phys.* **125**, 244502:1-8 (2006).

31. "Quantitative Link between Single-Particle Dynamics and Static Structure of Supercooled Liquids", J. Mittal, J. R. Errington, and T. M. Truskett, *J. Phys. Chem. B* **110**, 18147-18150 (2006).

30. "Relationship between thermodynamics and dynamics of supercooled liquids", J. Mittal, J. R. Errington, and T. M. Truskett, *J. Chem. Phys.* **125**, 076102:1-2 (2006).

29. "Using available volume to predict fluid diffusivity in random media", J. Mittal, J. R. Errington, and T. M. Truskett, *Phys. Rev. E* **74**, 040102:1-4 (2006).

28. "Nucleation and cavitation of spherical, cylindrical, and slablike droplets and bubbles in small systems", L. G. MacDowell, V. K. Shen, and J. R. Errington, *J. Chem. Phys.* **125**, 034705:1-15 (2006).

27. "Thermodynamics Predicts How Confinement Modifies the Dynamics of the Equilibrium Hard-Sphere Fluid", J. Mittal, J. R. Errington, and T. M. Truskett, *Phys. Rev. Lett.* **96**, 177804:1-4 (2006).

26. "Coarse-grained strategy for modeling protein stability in concentrated solutions II: Phase behavior", V. K. Shen, J. K. Cheung, J. R. Errington, and T. M. Truskett, *Biophys. J.* **90**, 1949-1960 (2006).

25. "Determination of Surface Tension in Binary Mixtures Using Transition-Matrix Monte Carlo", V. K. Shen and J. R. Errington, *J. Chem. Phys.* **124**, 024721:1-9 (2006).

24. "Calculation of phase coexistence properties and surface tensions of n-alkanes using grand-canonical transition-matrix Monte Carlo simulation and finite-size scaling", J. K. Singh and J. R. Errington, *J. Phys. Chem. B* **110**, 1369-1376 (2006).

23. "Prewetting boundary tensions from Monte Carlo simulation", J. R. Errington and D. W. Wilbert, *Phys. Rev. Lett.* **95**, 226107:1-4 (2005).

22. "Direct evaluation of multi-component phase equilibria using flat histogram methods", J. R. Errington and V. K. Shen, *J. Chem. Phys.* **123**, 164103:1-9 (2005).

21. "Determination of Henry's Law Constants through Transition Matrix Monte Carlo Simulation", E. C. Cichowski, T. R. Schmidt, and J. R. Errington, *Fluid Phase Equilibria* **236**, 58-65 (2005).

20. "A Computational Study of Hydration, Solution Structure, and Dynamics in Dilute Carbohydrate Solutions", S. L. Lee, P. G. Debenedetti, and J. R. Errington, *J. Chem. Phys.* **122**, 204511:1-10 (2005). Also selected to appear in *Vir. J. Bio. Phys. Res.* (June 1, 2005).

19. "Determination of fluid-phase behavior using transition-matrix Monte Carlo: Binary Lennard-Jones mixtures", V. K. Shen and J. R. Errington, *J. Chem. Phys.* **122**, 064508:1-17 (2005).

18. "Metastability and Instability in the Lennard-Jones Fluid Investigated by Transition-Matrix Monte Carlo", V. K. Shen and J. R. Errington, *J. Phys. Chem. B* **108**, 19595-19606 (2004).

17. "Calorimetric and Spectroscopic Study of Nucleic Acids at Low Hydration", S. L. Lee, P. G. Debenedetti, J. R. Errington, B. A. Pethica, and D. J. Moore, *J. Phys. Chem. B* **108**, 3098-3106 (2004).

16. "Prewetting Transitions for a Model Argon on Solid Carbon Dioxide System", J. R. Errington, *Langmuir* **20**, 3798-3804 (2004).

15. "Solid-Liquid Phase Coexistence of the Lennard-Jones System through Phase-Switch Monte Carlo Simulation", J. R. Errington, *J. Chem. Phys.* **120**, 3130-3141 (2004).

14. "Surface Tension and Vapor-Liquid Phase Coexistence of the Square-Well Fluid", J. K. Singh, D. A. Kofke, and J. R. Errington, *J. Chem. Phys.* **119**, 3405-3412 (2003).

13. "Direct Calculation of Liquid-Vapor Phase Equilibria From Transition Matrix Monte Carlo Simulation", J. R. Errington, *J. Chem. Phys.* **118**, 9915-9925 (2003).

12. "Evaluating Surface Tension Using Grand-Canonical Transition-Matrix Monte Carlo Simulation and Finite-Size Scaling", J. R. Errington, *Phys. Rev. E* **67**, 012102:1-4 (2003).

11. "Quantification of Order in the Lennard-Jones System", J. R. Errington, P. G. Debenedetti, and S. Torquato, *J. Chem. Phys.* **118**, 2256-2263 (2003).

10. "Cooperative Origin of Low-Density Domains in Liquid Water", J. R. Errington, P. G. Debenedetti, and S. Torquato, *Phys. Rev. Lett.* **89**, 215503:1-4 (2002).

9. "Relationship between Structural Order and the Anomalies of Liquid Water", J. R. Errington and P. G. Debenedetti, *Nature* **409**, 318-321 (2001).

8. "Molecular Simulation of Phase Equilibria for Water – *n*-Butane and Water – *n*-Hexane Mixtures", G. C. Boulougouris, J. R. Errington, I. G. Economou, A. Z. Panagiotopoulos and D. N. Theodorou, *J. Phys. Chem. B* **104**, 4958-4963 (1999).

7. "Molecular Simulation of Phase Equilibria for Mixtures of Polar and Non-Polar Components", J. J. Potoff, J. R. Errington and A. Z. Panagiotopoulos, *Mol. Phys.* **97**, 1073-1083 (1999).

6. "New Intermolecular Potential Models for Benzene and Cyclohexane", J. R. Errington and A. Z. Panagiotopoulos, *J. Chem. Phys.* **111**, 9731-9738 (1999).

5. "A New intermolecular Potential Model for the *n*-Alkane Homologous Series", J. R. Errington and A. Z. Panagiotopoulos, *J. Phys. Chem. B* **103**, 6314-6322 (1999).

4. "Molecular Simulation of Phase Equilibria for Water-Methane and Water-Ethane Mixtures", J. R. Errington, G. C. Boulougouris, I. G. Economou, A. Z. Panagiotopoulos and D. N. Theodorou, *J. Phys. Chem. B* **102**, 8865-8873 (1998).

3. "A Fixed Point Charge Model for Water Optimized to the Vapor-Liquid Coexistence Properties", J. R. Errington and A. Z. Panagiotopoulos, *J. Phys. Chem. B* **102**, 7470-7475 (1998).

2. "Phase Coexistence and Critical Properties of the Modified Buckingham Exponential-6 Potential from Hamiltonian Scaling Grand Canonical Monte Carlo", J. R. Errington and A. Z. Panagiotopoulos, *J. Chem. Phys.* **109**, 1093-1100 (1998).

1. "Monte Carlo Simulation of High-Pressure Phase Equilibria in Aqueous Systems", J. R. Errington, K. Kiyohara, K. E. Gubbins and A. Z. Panagiotopoulos, *Fluid Phase Equil.* **150**, 33-40 (1998).

II. Invited Review Articles and Book Chapters

2. "Concentration and crowding effects on protein stability from a coarse-grained model", J. K. Cheung, V. K. Shen, J. R. Errington, and T. M. Truskett, in *Statistical Mechanics of Cellular Systems and Processes*, M. H. Zaman, ed. Cambridge University Press, Cambridge pp. 1-25 (2009).

1. "Computing free volume, structural order, and entropy of liquids and glasses", J. Mittal, W. P. Krekelberg, J. R. Errington, and T. M. Truskett, *Reviews in Computational Chemistry* **25**, 125-158 (2007).

INVITED PRESENTATIONS

40. "Understanding the wetting behavior of octane-water-silica systems using Monte Carlo simulation", Department of Chemical and Biomolecular Engineering Seminar, Ohio University, March 2019.

39. "Understanding the wetting behavior of octane-water-silica systems using Monte Carlo simulation", 2017 Midwest Regional Meeting, University of Kansas, October 2017.

38. "Understanding the Interfacial Properties of Hydrocarbon-Water-Rock Systems Using Monte Carlo Simulation", Department of Biomedical and Chemical Engineering, Syracuse University, March 2017.

37. "Using the interface potential approach to determine oil/water interfacial tensions", AIChE Annual Meeting, Salt Lake City, UT, November 2015.

36. "Using Molecular Simulation to Examine the Sequestration of Carbon Dioxide in Saline Aquifers", Conference on Foundations of Molecular Modeling and Simulation (FOMMS), Mount Hood, OR, July 2015.

35. "Using molecular simulation to understand the bulk and interfacial behavior of ionic liquids", Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA, February 2015.

34. "Using Monte Carlo simulations to study the interfacial behavior of ionic liquids", Thermodynamics at the Nanoscale Session, AIChE Annual Meeting, Atlanta, GA, November 2014.

33. "Using molecular simulation to understand the bulk and interfacial behavior of ionic liquids", Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA, November 2014.

32. "Using Monte Carlo simulation to compute liquid-vapor saturation properties of realistic models of room temperature ionic liquids", Physical Chemistry of Ionic Liquids Section, 248th ACS Spring National Meeting, San Francisco, CA, August 2014.

31. "Using molecular simulation to understand wetting behavior", Wetting Phenomena Section, MMT-2014 Conference, Ariel, Israel, July 2014 (canceled).

30. "Using molecular simulation to understand interfacial phenomena", CoMSEF Plenary Session, AIChE Annual Meeting, San Francisco, CA, November 2013.

29. "Molecular simulation study of wetting and drying behavior", ACS Colloid and Surface Science Symposium, Riverside, CA, June 2013.

28. "Using molecular simulation to compute interfacial properties", NIST Workshop on Atomistic Simulations for Industrial Needs, Gaithersburg, MD, September 2012.

27. "Molecular Simulation Approach for Computing Liquid-Vapor Saturation Properties", International Conference on Chemical Thermodynamics, Buzios, Brazil, August 2012.

26. "Understanding the Wetting Behavior of Fluids at Heterogeneous Surfaces", Eighteenth Symposium on Thermophysical Properties, Boulder, CO, June 2012.

25. "Molecular Simulation Approach for Computing Liquid-Vapor Saturation Properties", Eighteenth Symposium on Thermophysical Properties, Boulder, CO, June 2012.

24. "Calculating the excess entropy", Viscous liquids and the glass transition X Workshop, Roskilde University, Roskilde, Denmark, June 2012.

23. "Using molecular simulation to understand wetting of chemically and geometrically heterogeneous surfaces", Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, March 2012.

22. "Using molecular simulation to understand wetting of chemically and geometrically heterogeneous surfaces", Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN, March 2012.

21. "Interface potential based approach to computing the wetting properties of fluids at heterogeneous surfaces via molecular simulation", Cecam Workshop, Lausanne, Switzerland, September 2011.

20. "Molecular simulation study of wetting of octane on surfaces with nanoscale re-entrant features", 66th Calorimetry Conference (CALCON 2011), Oahu, HI, June 2011.

19. "Using molecular simulation to understand wetting at rough surfaces", Department of Chemical Engineering, Colorado School of Mines, Golden, CO, March 2010.

18. "Using molecular simulation to understand wetting at rough surfaces", Department of Chemical Engineering, Princeton University, Princeton, NJ, September 2009.

17. "Using molecular simulation to understand wetting at rough surfaces", Department of Chemical Engineering, Case Western Reserve University, Cleveland, OH, September 2009.

16. "Using molecular simulation to understand wetting at rough surfaces", 64th Calorimetry Conference (CALCON 2009), Santa Fe, NM, June 2009.

15. "Molecular simulation study of confined liquid crystalline systems", Seventeenth Symposium on Thermophysical Properties, Boulder, CO, June 2009.

14. "Using molecular simulation to understand wetting behavior", 237th ACS National Meeting and Exposition, Salt Lake City, UT, March 2009.

13. "Using molecular simulation to understand wetting at rough surfaces", Department of Chemical and Biomolecular Engineering, Tulane University, New Orleans, LA, March 2009.

12. "Using molecular simulation to investigate wetting phase behavior", AIChE Spring Meeting, New Orleans, LA, April 2008.

11. "Investigating the phase behavior of fluids in the vicinity of a surface", AIChE Annual Meeting, Salt Lake City, UT, November 2007.

10. "Computational studies of the behavior of fluids at surfaces", Chemical and Biomolecular Engineering Department, Cornell University, Ithaca, NY, October 2006.

9. "Understanding the surface phase behavior of fluids", Sixteenth Symposium on Thermophysical Properties, Boulder, CO, August 2006.

8. "Investigation of fluid phase behavior for a variety of systems using transition-matrix Monte Carlo simulation", China/USA/Japan Joint Chemical Engineering Conference, Beijing, China, October 2005.

7. "Understanding the surface phase behavior of fluids", Chemical Engineering Department, University of Texas at Austin, Austin, TX, September 2005.

6. "Investigation of fluid phase behavior for a variety of systems using transition-matrix Monte Carlo simulation", The First China - USA Workshop on Chemical Engineering, Beijing, China, August 2005.

5. "Computational Investigation of Prewetting Transitions", National Institute of Standards and Technology, Gaithersburg, MD, March 2004.

4. "The Stabilization of Labile Biological Molecules in Amorphous Solids", Department of Pharmaceutical Sciences, University at Buffalo, Buffalo, NY, February 2004.

3. "Direct Calculation of Liquid-Vapor Phase Equilibria from Transition Matrix Monte Carlo Simulation", Midwest Thermodynamics and Statistical Mechanics Conference, Columbus, OH, May 2003.

2. "The Phase Behavior of the Lennard-Jones and Mercedes-Benz models from Phase Switch Monte Carlo", Cecam Workshop, Lyon, France, May 2003.

1. "Relationship Between Structural Order and the Anomalies of Liquid Water", Complex Materials Seminar, Princeton University, Princeton, NJ; February 2001.

RESEARCH GRANTS

I. Funded

18. National Science Foundation: "HDR DSC: Collaborative Research: Connecting the Dots"; Amount: $747,947; Term of Award: 10/1/19 – 9/30/22; Role: PI; JRE share: 20%.

17. National Science Foundation: "Development of Molecular Simulation Methods to Compute Phase and Interfacial Properties of Complex Fluids"; Amount: $394,422; Term of Award: 6/1/19 – 5/31/22; Role: PI; JRE share: 90%.

16. National Science Foundation: "Molecular Simulation Study of Rock-Water-Oil Systems"; Amount: $300,000; Term of Award: 11/1/17 – 10/31/20; Role: PI; JRE share: 100%.

15. New York State Center for Clean Water Technology: "Rational Development of Robust Membranes for Nitrate Removal from Wastewater"; Amount: $33,000; Term of Award: 9/1/17 – 8/31/18; Role: Co-PI; JRE share: 50%.

14. National Science Foundation: "Development and Application of Molecular Simulation Methods to Compute Bulk and Interfacial Properties of Ionic Liquids"; Amount: $405,000; Term of Award: 6/1/14 – 5/31/17 (no-cost extension to 5/31/18); Role: PI; JRE share: 100%.

13. National Science Foundation: "Molecular Simulation Study of Interfacial Phenomena Related to Geological CO2 Storage"; Amount: $307,674; Term of Award: 6/1/13 – 5/31/16 (no-cost extension to 5/31/17); Role: PI; JRE share: 100%.

12. Shell International Exploration and Production Inc.: "Liquid-vapor phase coexistence properties of asphaltenes"; Amount: $136,471; Term of Award: 6/15/12 – 1/31/14; Role: PI; JRE share: 100%.

11. Petroleum Research Fund: "Understanding Interfacial Phenomena Related to Enhanced Oil Recovery"; Amount: $100,000; Term of Award: 1/1/12 – 8/31/14; Role: PI; JRE share: 100%.

10. National Science Foundation: "Development of Molecular Simulation Methods to Compute Interfacial Properties of Electrolytes"; Amount: $337,420; Term of Award: 9/15/10 – 8/31/13; Role: PI; JRE share: 100%.

9. National Science Foundation: "Molecular Simulation Study of Wetting at Rough Surfaces"; Amount: $200,001; Term of Award: 9/1/08 – 8/31/10 (no-cost extension to 8/31/11); Role: PI; JRE share: 100%.

8. National Science Foundation RET Supplement: "CAREER: Connecting structural order to thermodynamic and kinetic properties of aqueous solutions: a research and education program"; Amount: $19,945; Role: PI; JRE share: 25%.

7. National Science Foundation RET Supplement: "CAREER: Connecting structural order to thermodynamic and kinetic properties of aqueous solutions: a research and education program"; Amount: $10,000; Role: PI; JRE share: 100%.

6. Petroleum Research Fund: "Investigation of the Effect of Substrate Molecular Roughness on Surface Phase Behavior"; Amount: $80,000; Term of Award: 8/1/05 – 8/31/07; Role: PI; JRE share: 100%.

5. New York State Office of Science, Technology and Academic Research, J. D. Watson Investigator Program: "Novel approaches to the stabilization of biotherapeutic agents"; Amount: $200,000; Term of Award: 11/1/04 – 10/31/06; Role: PI; JRE share: 100%.

4. National Science Foundation: "2004 Midwest Thermodynamics and Statistical Mechanics Meeting"; Amount: $7,100; Term of Award: 5/1/04 – 4/30/05; Role: PI; JRE share: 50%.

3. National Science Foundation REU Supplement: "CAREER: Connecting structural order to thermodynamic and kinetic properties of aqueous solutions: a research and education program"; Amount: $5,150; Role: PI; JRE share: 100%.

2. National Science Foundation CAREER Program: "CAREER: Connecting structural order to thermodynamic and kinetic properties of aqueous solutions: a research and education program"; Amount: $406,555; Term of Award: 2/1/03 – 1/31/08; Role: PI; JRE share: 100%.

1. Petroleum Research Fund: "Understanding the Relationship between Structural Order and the Kinetic and Thermodynamic Properties of Ions in Aqueous Solutions"; Amount: $35,000; Term of Award: 9/1/02 – 8/31/04; Role: PI; JRE share: 100%.

II. Pending

1. National Science Foundation: "REU Site: Design of materials guided by experiment and computation"; Amount: $381,595; Role: PI.

TEACHING EXPERIENCE

I. Formal Courses

Instructor, CE 525, Advanced Chemical Engineering Thermodynamics, University at Buffalo

- Have full responsibility for required, three-credit, graduate-level course in advanced chemical engineering thermodynamics and introductory statistical mechanics.
- Typical enrollment of 30 students.
- Instructor from 2003 to present (Fall semester).

Instructor, EAS 198, UB Seminar-The Places You Will Go, University at Buffalo

- Serve as a member of a team that of instructors that deliver the course. Another faculty member, Jennifer Zirnheld, serves as the course coordinator.
- Typical enrollment of 28 students.
- Instructor Fall 2016, 2017, 2018, 2019.

Instructor, EAS 204 (now MAE 204), Thermodynamics I, University at Buffalo

- Had full responsibility for required, three-credit, undergraduate-level course in engineering thermodynamics.
- Typical enrollment of 220 students.
- Instructor during the Fall semester from 2001 to 2006.
- Restructured the course recitation sections.

Co-Instructor, CE 410 (formerly CE 412), Molecular Modeling, University at Buffalo

- Developed a new elective course at the senior undergraduate level with Prof. David A. Kofke.
- Enrollment of 5 to 10 students.
- Instructor Spring 2004, Spring 2005, Fall 2007.

Instructor, CE 457/527, Colloid and Surface Phenomena, University at Buffalo

- Served as the instructor for our elective, three-credit, dual-listed undergraduate/graduate-level course in colloid and surface phenomena.
- Typical enrollment of 10 undergraduate and 10 graduate students.
- Instructor Spring 2006, Fall 2008.

Instructor, CE 498, Undergraduate Research and Creative Activity, University at Buffalo

- Serve as the instructor for our elective, one-credit, lecture section of CE 498. Each student that participates in undergraduate research is required to participate in this one-credit lecture-based class.
- Topics addressed include the role of research in science and engineering, tools for inquiry, dissemination of results, and performing research.
- The course leads students towards the preparation of a journal-style written report and an oral presentation of their research findings.
- Typical enrollment of 10 students.
- Instructor from Fall 2009 to Spring 2014.

Advisor, EAS 496, Engineering Co-Op, University at Buffalo

- Advisor for students participating in an elective, two-credit, undergraduate-level industrial Co-Op.
- Enrollment of 4 to 10 students.
- Summer semester from 2005 to 2008.

Advisor, CE 496 (formerly CE 406 XXX), CBE Internship/practicum, University at Buffalo

- Advisor for students participating in an elective, three-credit, undergraduate-level industrial internship.
- Enrollment of 0 to 2 students.
- Fall and Spring semester from 2001 to 2006.

II. Student Advisement

Ph.D. Graduates

Thomas Rosch, Ph.D. conferred September 2008
Eric Grzelak, Ph.D. conferred September 2009
Ravi Chopra, Ph.D. conferred September 2010
Vaibhaw Kumar, Ph.D. conferred September 2013
Kaustubh Rane, Ph.D. conferred September 2014

Jung Ho Yang, Ph.D. conferred February 2015
Wenjing Guo, Ph.D. conferred September 2017
Adam Rall, Ph.D. conferred September 2018
Karnesh Jain, Ph.D. conferred September 2018

M.S. Graduates

Lu Liu, M.S. conferred June 2004
Eric Cichowski, M.S. conferred February 2007
Wai Keong Choong, M.S. conferred September 2007
Shyam Sridhar, M.S. conferred June 2011
Aravindh Nadha, M.S. conferred February 2012
Sabharish Murali, M.S. conferred September 2012
Prannay Bali, M.S. conferred September 2015
Meng Wang, M.S. conferred September 2015
Haihua Yan, M.S. conferred September 2017

M.Eng. Graduates

Chiau Funn Ma, M.Eng. conferred September 2006
Yi Luan, M.Eng. conferred September 2009
Suman Samantray, M.Eng. conferred September 2015

Former Undergraduate Research Students

Conor Kellner, Timothy Buchanan, Yunong Cao, Marina Gadkary, Justin Patton, Andrew Paluch, Barry Van Tassell, Do Yeh Jeong, Man Tsz Yau, Ravi Chopra, Michael Sellers, Nathaniel Ives, Wai Keong Choong, David Wilbert, Eric Cichowski, Todd Schmidt, and Folarin Erogbogbo

Current Ph.D. Students

Yiqi Chen, started September 2015
Xiaoyu Liang, started September 2015
Gaurab Sarkar, started September 2019

Current M.S. Students

Krishna Vaka, started September 2016

Current M.Eng. Students

None

Current Undergraduate Research Students

None

PROFESSIONAL ACTIVITIES

I. Professional Society Memberships

Member: American Institute of Chemical Engineers, American Chemical Society, American Association for the Advancement of Science, Tau Beta Pi

II. Peer Review

Journal Review: Physical Review Letters, Physical Review, Journal of Chemical Physics, Journal of Physical Chemistry, Langmuir, Industrial & Engineering Chemistry Research, Molecular Physics, Fluid Phase Equilibria, Theoretical Chemistry Accounts, Journal of Supercritical Fluids, Journal of Statistical Physics, Soft Matter

Proposal Panel Review: National Science Foundation, National Institutes of Health

Proposal ad hoc Review: National Science Foundation, the Petroleum Research Fund

III. Professional Service and Symposia Organization

Trustee: Computer Aids for Chemical Engineering (CACHE) Corporation, 2014-present.

Past-Chair: Computational Molecular Science and Engineering Forum, American Institute of Chemical Engineers (AIChE), 2018-2020.

Chair: Computational Molecular Science and Engineering Forum, American Institute of Chemical Engineers (AIChE), 2016-2018.

Vice-Chair: Computational Molecular Science and Engineering Forum, American Institute of Chemical Engineers (AIChE), 2014-2016.

Liaison Director: Computational Molecular Science and Engineering Forum, American Institute of Chemical Engineers (AIChE), 2008-2010.

Programming Committee Member: Area 1a (Thermodynamics and Transport Properties), American Institute of Chemical Engineers (AIChE), 2003-2009.

Conference Programming Chair: Organizer of the Area 1a sessions for the 2005 AIChE Spring Meeting in Atlanta, GA.

Conference Organization: Co-organizer of the 2004 Midwest Thermodynamics and Statistical Mechanics Conference held in Buffalo, NY (with D. A. Kofke).

Session Chair: Chair/Vice-Chair of the following sessions at AIChE Annual meetings: Advances in Protein Structure, Function, and Stability, 2002; Thermodynamic Properties and Phase Behavior I, 2003; Molecular Modeling Methods I: Recent advances in Molecular Dynamics, 2004; Nanoscale Systems: Water in Inhomogeneous Environments, 2005; Development of Intermolecular Potential Models, 2006; Mesoscale and Nanoscale Thermodynamics II, 2006; Thermodynamics under Confinement, 2007. Chair of sessions at the 15th (2003), 16th (2006), 17th (2009), and 18th (2012) Symposium on Thermophysical Properties.

UNIVERSITY SERVICE

Chemical and Biological Engineering Undergraduate Committee

- Member since 2002
- Interim Director of Undergraduate Studies, August 2004 – January 2005
- Director of Undergraduate Studies, January 2006 – July 2014
- Director of ABET Accreditation, January 2006 – July 2014

Graduate Research Open House Organizing Committee

- Member from 2001 to 2005
- Joined other chemical and biological engineering assistant professors in organizing an annual symposium that enables other UB departments and local industries to view the research activities in our department. The event also provides graduate students an opportunity to present their research through a poster presentation.

Middle States Accreditation

- Co-chair of Working Team 6: *Assessment: Institutional Effectiveness and Assessment of Student Learning Outcomes*.
- Member of Middle States Steering Committee.

School of Engineering and Applied Sciences Grievance Committee

- Served on a panel during the Spring semester of 2005.

Freshman Engineering Mentor

- Member of mentoring program from 2001-2011, 2014-present.