

# Henry S. Ashbaugh

---

## RESEARCH INTERESTS

Multiscale simulation and theory of self-assembly and hierarchical organization in complex fluids including surfactant solutions, polymer melts and solutions, and biopolymer gels and networks to advance self-assembly for building tailored nanostructured materials.

## EDUCATION

**University of Delaware** - Newark, DE GPA – 3.94/4.00

PhD in Chemical Engineering (Spring '98)

Dissertation title: "The hydration of amphiphilic solutes: A theoretical and modeling perspective"

Advisors: Prof. Michael E. Paulaitis and Prof. Eric W. Kaler

**North Carolina State University** – Raleigh, NC GPA – 3.97/4.00

BS in Chemical Engineering, minor in Mathematics (Spring '92)

Summa Cum Laude

## PROFESSIONAL EXPERIENCE

**Tulane University**, New Orleans, LA (July '04 - present)

Associate Professor of Chemical and Biomolecular Engineering (June '10 – present)

Assistant Professor of Chemical and Biomolecular Engineering (July '04 – June '10)

Robert and Gayle Longmire Early Career Professorship in Chemical and Biomolecular Engineering (July '06 – June '10)

**Rensselaer Polytechnic Institute**, Troy, NY (Sept '05 – Dec. '05)

Visiting Professor of Chemical and Biological Engineering

On leave from Tulane University for one semester after Hurricane Katrina

**Los Alamos National Laboratory**, Los Alamos, NM (Aug. '01 – June '04)

Postdoctoral fellow in Theoretical Chemistry and Molecular Physics (T12) –

Supervisor: Dr. Lawrence R. Pratt. Director's fellow Oct '01- Sept. '03

**Princeton University**, Princeton, NJ (July '99 – Aug. '01)

Postdoctoral research associate in Chemical Engineering – Advisor: Prof. Robert K. Prud'homme

**Lund University**, Lund, Sweden (Mar. '98 – June '99)

Postdoctoral research associate in Physical Chemistry 1 – Advisor: Prof. Björn Lindman

**University of Delaware**, Newark, DE (Sept. '92 - Jan. '98)

Graduate research associate in Chemical Engineering – Advisors: Profs. Michael E. Paulaitis and Eric W. Kaler

**North Carolina State University**, Raleigh, NC (May '91 - Aug. '92)

Undergraduate research associate in Chemical Engineering – Advisor: Prof. H. Henry Lamb

### **ADDITIONAL TRAINING AND EXPERIENCE**

1. Summer Institute on Parallel Computing: Pittsburgh Super Computing Center, Summer '94.
2. Instructor, CHEG 112: Introduction to Chemical Engineering Analysis, Spring '96. Supervising instructor: T. W. Fraser Russell.
3. Teaching Assistant, CHEG 825: Chemical Engineering Thermodynamics, Fall '96. Supervising instructor: Norman J. Wagner.
4. National Science Foundation's Engineering Education Scholar's Workshop: Carnegie Mellon University, Summer '97.
5. Tulane Faculty Fellow Service-Learning Workshop: Tulane University, Center for Public Service, Fall '06.

### **HONORS AND AWARDS**

1. Mathematics Merit Scholarship, North Carolina State University, '87 - '88.
2. Phi Kappa Phi, '90.
3. National Science Foundation Undergraduate Research Fellowship, Center for Advanced Electronic Materials Processing, North Carolina State University, '91 - '92.
4. Summa Cum Laude, '92.
5. Pigford Fellowship, '92 - '93.
6. Dupont Fellowship, '92 - '96.
7. National Science Foundation Graduate Fellowship, '92 - '95.
8. W. R. Grace Fellowship, '93 - '96.
9. Golden Key Honor Society, '95.
10. Golden Key Honor Society Scholarship, '95.
11. Chemical Engineering Graduate Teaching Fellowship, '96.
12. University of Delaware Competitive Fellowship, '96 - '97.
13. Director's Fellowship, Los Alamos National Laboratory, '01 - '03.
14. Ralph E. Powe Award, Oak Ridge Associated Universities, '05.
15. Leon Heller Postdoctoral Publication Prize in Theoretical Physics (honorable mention), '06. Based on work reported in paper #32 in *Reviews of Modern Physics*.
16. Robert and Gayle Longmire Early Career Professorship in Chemical and Biomolecular Engineering, '06 – '10.
17. Tulane Presidential Early Career Development Award, '07 – '10.
18. National Science Foundation CAREER Award, '08.
19. Who's Who in America, '09, '10.
20. International Association for the Properties of Water and Steam Helmholtz Award, '13.
21. Inducted into Tau Beta Pi as an Eminent Engineer, '13.
22. Paper #57 selected as a 2013 Editor's Choice Article in the *Journal of Chemical Physics*.
23. Paper #58 in publications selected to appear on cover of *Langmuir*, '13.

## **PUBLICATIONS (PEER REVIEWED, 1700+ citations, $h = 25$ )**

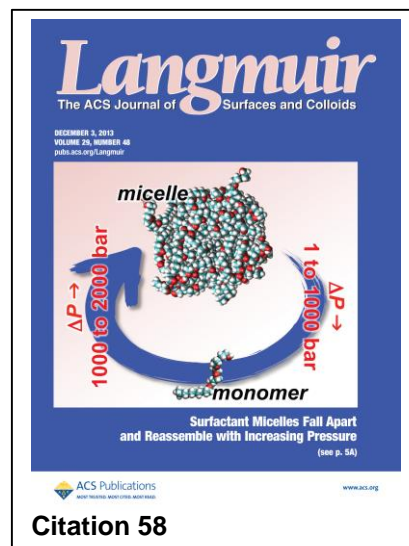
1. M. E. Paulaitis, H. S. Ashbaugh, and S. Garde "The entropy of hydration of simple hydrophobic solutes," *Biophys. Chem.*, 1994, **51**, 349-57. *Special issue on the thermodynamics of hydration.* DOI: 10.1016/0301-4622(94)00055-7. DOI: 10.1016/0301-4622(94)0005-7.
2. H. S. Ashbaugh and M. E. Paulaitis "Entropy of hydrophobic hydration: Extension to hydrophobic chains," *J. Phys. Chem.*, 1996, **100**, 1900-1913. DOI: 10.1021/jp952387b.
3. M. E. Paulaitis, S. Garde, and H. S. Ashbaugh "The hydrophobic effect," *Curr. Opin. Coll. Surf. Sci.*, 1996, **1**, 376-383. DOI: N/A.
4. H. S. Ashbaugh and R. H. Wood "Effects of long-range electrostatic potential truncation on the free energy of ionic hydration," *J. Chem. Phys.*, 1997, **106**, 8135-8139. DOI: 10.1063/1.473800.
5. H. S. Ashbaugh, S. Sakane, and R. H. Wood "Reply to comment on 'Electrostatic potentials and free energies of solvation of polar and charged molecules'," *J. Phys. Chem. B*, 1998, **102**, 3844-3845. DOI: 10.1021/jp9804852.
6. S. Sakane, H. S. Ashbaugh, and R. H. Wood "Continuum corrections to the polarization and thermodynamic properties of Ewald sum simulations for ions and ion-pairs at infinite dilution," *J. Phys. Chem. B*, 1998, **102**, 5673-5682. DOI: 10.1021/jp9808227.
7. H. S. Ashbaugh and M. E. Paulaitis "A molecular/continuum thermodynamic model of hydration," *J. Phys. Chem. B* (letter), 1998, **102**, 5029-5032. DOI: 10.1021/jp9814505.
8. H. S. Ashbaugh, M. E. Paulaitis, and E. W. Kaler "Hydration and conformational equilibria of simple hydrophobic and amphiphilic solutes," *Biophys. J.*, 1998, **75**, 755-768. DOI: N/A.
9. H. S. Ashbaugh, S. Garde, G. Hummer, E. W. Kaler, and M. E. Paulaitis "Conformational equilibria of alkanes in aqueous solution: Relationship to water structure near hydrophobic solutes," *Biophys. J.*, 1999, **77**, 645-654. DOI: N/A.
10. H. S. Ashbaugh "Influence of potential truncation on anisotropic systems," *Mol. Phys.*, 1999, **97**, 433-437. DOI: 10.1080/002689799163811.
11. H. S. Ashbaugh, E. W. Kaler, and M. E. Paulaitis "A 'universal' surface area correlation for molecular hydrophobic phenomena," *J. Am. Chem. Soc.* (communication), 1999, **121**, 9243-9244. DOI: 10.1021/ja992119h.
12. H. S. Ashbaugh, L. Piculell, and B. Lindman "Interactions of cationic/nonionic surfactant mixtures with an anionic hydrogel: Absorption equilibrium and thermodynamic modeling," *Langmuir*, 2000, **16**, 2529-2538. DOI: 10.1021/la9910778.
13. H. S. Ashbaugh "Convergence of molecular and macroscopic continuum descriptions of ion hydration," *J. Phys. Chem. B* (letter), 2000, **104**, 7235-7238. DOI: 10.1021/jp0015067.
14. H. S. Ashbaugh and B. Lindman "Swelling and structural changes of anionic hydrogel-cationic surfactant complexes induced by nonionic surfactant addition," *Macromolecules*, 2001, **34**, 1522-1525. DOI: 10.1021/ma001545g.

15. S. Garde and H. S. Ashbaugh "Temperature dependence of hydrophobic hydration and entropy convergence in an isotropic model of water," *J. Chem. Phys.* 2001, **115**, 977-982. DOI: 10.1063/1.1379576.
16. H. S. Ashbaugh and M. E. Paulaitis "Effect of solute size and solute-water attractive interactions on hydration water structure around hydrophobic solutes," *J. Am. Chem. Soc.*, 2001, **123**, 10721-10728. DOI: 10.1021/ja016324k.
17. H. S. Ashbaugh, E. W. Kaler, and M. E. Paulaitis "Conformational equilibria of polar and charged flexible polymer chains in water," *Polymer*, 2002, **43**, 559-565. DOI: 10.1016/S1089-3156(01)00010-1.
18. H. S. Ashbaugh, T. M. Truskett, and P. G. Debenedetti "A simple molecular thermodynamic theory of hydrophobic hydration," *J. Chem. Phys.* 2002, **116**, 2907-2921. DOI: 10.1063/1.1436479.
19. H. S. Ashbaugh, K. H. -R. Boon, and R. K. Prud'homme "Gelation of 'catanionic' vesicles by hydrophobically modified polyelectrolytes," *Coll. Poly. Sci.* 2002, **280**, 783-788. DOI: 10.1007/s00396-002-0702-3.
20. H. S. Ashbaugh, L. J. Fetters, D. H. Adamson, and R. K. Prud'homme "Flow improvement of waxy oils mediated by self-aggregating partially crystallizable diblock copolymers," *J. Rheology* 2002, **46**, 763-776. Selected to appear in the *Virtual Journal of Nanoscale Science and Technology*, 2002, **6**. DOI: 10.1122/1.1485280.
21. H. S. Ashbaugh, A. Radelescu, R. K. Prud'homme, D. Schwaan, D. Richter, and L. J. Fetters "Interaction of paraffin wax gels with random crystalline/amorphous hydrocarbon copolymers," *Macromolecules* 2002, **35**, 7044-7053. DOI: 10.1021/ma0204047.
22. D. Asthagiri, L. R. Pratt, and H. S. Ashbaugh "Absolute hydration free energies of ions, ion-water clusters, and quasi-chemical theory," *J. Chem. Phys.* 2003, **119**, 2702-2708. DOI: 10.1063/1.1587122.
23. L. R. Pratt and H. S. Ashbaugh "Self consistent molecular field theory for packing in classical liquids," *Phys. Rev. E* 2003, **68**, 021505-1-6. DOI: 10.1103/PhysRevE.68.021505.
24. H. S. Ashbaugh and B. A. Pethica "Alkane adsorption at the water-vapor interface," *Langmuir* 2003, **19**, 7646-7651. DOI: 10.1021/la034559z.
25. H. S. Ashbaugh, D. Asthagiri, L. R. Pratt, and S. B. Rempe "Molecular scale analysis of hydrophobic hydration of krypton in liquid water," *Biophys. Chem.* 2003, **105**, 323-338. DOI: 10.1016/S0301-4622(03)00084-X.
26. H. S. Ashbaugh, T. M. Truskett, and P. G. Debenedetti "Response to 'Comment on 'A simple molecular thermodynamic theory of hydrophobic hydration' by H.S. Ashbaugh, T. M. Truskett, P. G. Debenedetti, *J. Chem. Phys.*, 116, 2907 (2002),'", *J. Chem. Phys.* 2003, **119**, 10450-10451. DOI: 10.1063/1.1619938.
27. H. S. Ashbaugh, X. Guo, D. Schwahn, R. K. Prud'homme, D. Richter, and L. J. Fetters "Interaction of paraffin wax gels with ethylene/vinyl acetate copolymers," *Energy and Fuels* 2005, **19**, 138-144. DOI: 10.1021/ef049910i
28. H. S. Ashbaugh, H. Patel, S. K. Kumar, and S. Garde, "Mesoscale modeling of polymer melt structure: Self-consistent mapping of molecular correlations to coarse-grained potentials," *J. Chem. Phys.*, 2005, **122**, 104908. Selected to appear in the *Virtual Journal of Biological Physics Research*, 2005, **9**. DOI: 10.1063/1.1861455

29. H. S. Ashbaugh, L. R. Pratt, M. E. Paulaitis, J. Clohery, and T. L. Beck, "Deblurred observation of the molecular structure of an oil-water interface," *J. Am. Chem. Soc.* (communication), 2005, **127**, 2808-2809. DOI: 10.1021/ja042600u
30. S. Chatterjee, H. S. Ashbaugh, and P. G. Debenedetti "Effects of nonpolar solutes on the thermodynamics response functions of aqueous mixtures," *J. Chem. Phys.*, 2005, **123**, 164503. DOI: 10.1063/1.2075127
31. H. Peng, J. Tang, J. Pang, D. Chen, L. Yang, H. S. Ashbaugh, C. J. Brinker, Z. Yang, and Y. Lu "Polydiacetylene/silica nanocomposites with tunable mesostructure and thermochromatism from diacetylenic assembling molecules," *J. Am. Chem. Soc.* (communication), 2005, **127**, 12782-12783. DOI: 10.1021/ja053966p
32. H. S. Ashbaugh and L. R. Pratt "Scaled particle theory and the length-scales of hydrophobicity," *Rev. Mod. Phys.* (colloquium), 2006, **78**, 159-178. Selected to appear in the *Virtual Journal of Nanoscale Science and Technology*, 2006, **13**. Selected to appear in the *Virtual Journal of Biological Physics Research*, 2006, **11**. Received the Leon Heller Postdoctoral Publication Prize in Theoretical Physics (honorable mention). DOI: 10.1103/RevModPhys.78.159
33. J. Pang, L. Yang, D. A. Loy, H. Peng, H. S. Ashbaugh, J. Mague, C. J. Brinker, and Y. Lu "Mesoscopically ordered organosilica and carbon-silica hybrids with uniform morphology by surfactant-assisted self-assembly of organo bis-silanetriols," *Chem. Comm.*, 2006, 1545-1547. DOI: 10.1039/B516985B
34. H. Peng, J. Tang, L. Yang, J. Pang, H. S. Ashbaugh, C. J. Brinker, Z. Yang, and Y. Lu "Responsive periodic mesoporous polydiacetylene/silica nanocomposites," *J. Am. Chem. Soc.* (communication), 2006, **128**, 5304-5305. DOI: 10.1021/ja0575732
35. H. S. Ashbaugh and M. E. Paulaitis "Monomer hydrophobicity as a mechanism for the LCST behavior of poly(ethylene oxide) in water," *Ind. Eng. Chem. Research*, 2006, **45**, 5531-5537. *Festschrift for Eduardo Glandt*. DOI: 10.1021/ie051131h
36. V. T. John, H. S. Ashbaugh, B. Mitchell, J. Prindle "From survival to renewal – Katrina and its aftermath at Tulane's Chemical and Biomolecular Engineering Department," *Chem. Eng. Ed.*, Spring 2006, **40**, 80-87 and 98. DOI: N/A.
37. A. Paliwal, D. Asthagiri, H. S. Ashbaugh, L. R. Pratt, and M. E. Paulaitis "An analysis of molecular packing and chemical association in liquid water using quasi-chemical theory," *J. Chem. Phys.*, 2006, **124**, 224502. DOI: 10.1063/1.2202350
38. J. Pang, L. Yang, B. F. McCaughey, H. Peng, H. S. Ashbaugh, C. J. Brinker, and Y. Lu "Thermochromatism and structural evolution of metastable polydiacetylenic crystals," *J. Phys. Chem. B*, 2006, **110**, 7221-7225. DOI: 10.1021/jp060309q
39. D. Asthagiri, H. S. Ashbaugh, A. Piryatinski, M. E. Paulaitis, and L. R. Pratt, "Non van der Waals' treatment of the hydrophobic solubilities of CF<sub>4</sub> and C(CH<sub>3</sub>)<sub>4</sub>," *J. Am. Chem. Soc.*, 2007, **129**, 10133-10140. DOI:10.1021/ja071037n
40. H. S. Ashbaugh and L. R. Pratt, "Contrasting non-aqueous against aqueous solvation on the basis of scaled-particle theory," *J. Phys. Chem. B*, 2007, **111**, 9330-9336. DOI: 10.1021/jp071969d
41. A. Sangwai and H. S. Ashbaugh, "Aqueous partial molar volumes from simulation and individual group contributions," *Ind. Eng. Chem. Research*, 2008, **47**, 5169 – 5174. *Festschrift for John O'Connell*. DOI:10.1021/ie071444

42. H. S. Ashbaugh and H. W. Hatch, "Natively unfolded protein stability as a coil-to-globule transition in charge/hydrophobicity space," *J. Am. Chem. Soc.*, 2008, **130**, 9536–9542. DOI:10.1021/ja802124e
43. H. S. Ashbaugh and D. Asthagiri "Single ion hydration free energies from neutral pair properties: A consistent comparison between experiment and theory," *J. Chem. Phys.*, 2008, **129**, 204501. DOI: 10.1063/1.3013865
44. A. Jain and H. S. Ashbaugh "Digging a hole: Scaled-particle theory and cavity fluctuations in organic solvents," *J. Chem. Phys.*, 2008, **129**, 174505. DOI: 10.1063/1.3003577
45. H. S. Ashbaugh "Blowing bubbles in Lennard-Jonesium along the saturation curve," *J. Chem. Phys.*, 2009, **130**, 204517. DOI: 10.1063/1.3143716
46. H. S. Ashbaugh "Entropy crossover from molecular to macroscopic cavity hydration," *Chem. Phys. Lett.*, 2009, **477**, 109-111. DOI: 10.1016/j.cplett.2009.06.081
47. H. S. Ashbaugh, "Tuning the globular assembly of hydrophobic/hydrophilic heteropolymer sequences," *J. Phys. Chem. B* (letter), 2009, **113**, 14043-14046. DOI: 10.1021/jp907398r
48. H. S. Ashbaugh, N. J. Collett, H. W. Hatch, and J. A. Staton "Assessing the thermodynamic signatures of hydrophobic hydration for several common water models," *J. Chem. Phys.*, 2010, **132**, 124504. DOI: 10.1063/1.3366718
49. H. S. Ashbaugh "Ehrenfest's lottery – Time and entropy maximization," *Chem. Eng. Ed.* 2010, **44**, 229. DOI: N/A.
50. H. S. Ashbaugh and T. M. Truskett "Putting the squeeze on cavities in liquids: Quantifying pressure effects on solvation using simulations and scaled-particle theory," *J. Chem. Phys.*, 2011, **134**, 014507. Selected to appear in the *Virtual Journal of Biological Physics Research*, 2011, **21**. DOI: 10.1063/1.3510522
51. J. E. St. Dennis, Q. Meng, N. S. Pesika, G. L. McPherson, H. S. Ashbaugh, V. T. John, M. B. Dowling, S. R. Raghavan "Carbon microspheres as network nodes in novel biocompatible gel," *Soft Matter*, 2011, **7**, 4170-4173. DOI: 10.1039/c0sm01430c
52. A. Jain and H. S. Ashbaugh "Helix stabilization of poly(ethylene glycol)-peptide conjugates," *Biomacromolecules*, 2011, **12**, 2729-2734. DOI: 10.1021/bm2005017
53. H. S. Ashbaugh, L. Liu, and L. N. Surampudi "Optimization of linear and branched alkane interactions with water to simulate hydrophobic hydration," *J. Chem. Phys.*, 2011, **135**, 054510. DOI: 10.1063/1.3623267
54. M. H. Priya, H. S. Ashbaugh, and M. E. Paulaitis "Co-solvent preferential molecular interaction in aqueous solutions," *J. Phys. Chem. B*, 2011, **115**, 13633-13642. DOI: 10.1021/jp2083067
55. P. P. Wanjari, A. V. Sangwai, and H. S. Ashbaugh "Confinement induced conformational changes in *n*-alkanes sequestered within a carbon nanotube," *Phys. Chem. Chem. Phys.*, 2012, **14**, 2702-2709. DOI: 10.1039/c2cp22940d
56. J. M. Franklin, L. N. Surampudi, H. S. Ashbaugh, and D. C. Pozzo, "Numerical validation of IFT in the analysis of protein-surfactant complexes with SAXS and SANS," *Langmuir*, 2012, **28**, 12593-12600. DOI: 10.1021/la3028379

57. H. S. Ashbaugh, "Solvent cavitation under solvophobic confinement," *J. Chem. Phys.*, 2013, **139**, 064702. *Selected as a 2013 Editor's Choice Article in the Journal of Chemical Physics.* DOI: 10.1063/1.4817661
58. B. Meng and H. S. Ashbaugh, "Pressure reentrant assembly: Direct simulation of volumes of micellization," *Langmuir* (letter), 2013, **29**, 14743-14747. *Article featured on journal cover.* DOI: 10.1021/la402798f
59. M. I. Chaudhari, S. Holleran, H. S. Ashbaugh, and L. R. Pratt, "Direct numerical test of the statistical mechanical theory of hydrophobic interactions," *Proc. Nat. Acad. Sci. USA* 2013, **110**, 20557-20562. DOI: 10.1073/pnas.1312458110
60. P. P. Wanjari, B. C. Gibb, and H. S. Ashbaugh, "Simulation optimization of non-polar guest recognition by deep-cavity cavitands," *J. Chem. Phys.* 2013, **139**, 234502. DOI: 10.1063/1.4844215
61. S. M. Williams and H. S. Ashbaugh, "Nonpolar solute partial molar volume response to attractive interactions with water," *J. Chem. Phys.* 2014, **140**, 016101. DOI: 10.1063/1.4861671.
62. L. Liu, S. Parameswaran, S. M. Grayson, H. S. Ashbaugh, A. Sharma, S. W. Rick, "Molecular dynamics simulations of linear and cyclic amphiphilic polymers in aqueous and organic environments," *J. Phys. Chem. B.* 2014, **118**, 6491-6497. DOI: 10.1021/jp412184h.
63. L. N. Surampudi and H. S. Ashbaugh, "Direct evaluation of polypeptide partial molar volumes in water using molecular dynamics simulations," *J. Chem. Eng. Data* (in press). DOI: 10.1021/je5001999.
64. H. S. Ashbaugh and L. R. Pratt, "Scaled particle theory description of cylindrical solute solvation in hard sphere and Lennard-Jones solvents," *J. Stat. Phys.* (in preparation).
65. B. Meng and H. S. Ashbaugh "Effect of hydrostatic pressure on gas solubilization in micelles," *Langmuir* (in preparation).



### PUBLICATIONS (NON-PEER REVIEWED)

1. X. Guo, H. S. Ashbaugh, A. Radelescu, D. Richter, L. J. Fetters, B. A. Pethica, J. S. Huang, R. K. Prud'homme "Effect of micro-crystalline poly(ethylene-butene) on crystallization of paraffins and their mixtures from model waxy oil," *Preprints - American Chemical Society, Division of Petroleum Chemistry* 2003, **48**, 269-271. DOI: N/A.

### DISSERTATION

1. H. S. Ashbaugh, "The hydration of amphiphilic solutes: A theoretical and modeling perspective" University of Delaware, Department of Chemical Engineering, 1998.

### CONTRIBUTED PRESENTATIONS (listing only personally given presentations)

1. "Investigations into the molecular origin of the hydrophobic effect," Mid-Atlantic Thermodynamics Conference: Princeton University, Princeton, NJ, October '94.

2. "A thermodynamic model of the hydration of hydrophobic solutes: A molecular approach," American Institute of Chemical Engineers Annual Meeting, Miami, FL, November '95.
3. "Conformational equilibrium of amphiphilic chains in water," Mid-Atlantic Thermodynamics Conference: Johns Hopkins University, Baltimore, MD, March '96.
4. "Conformational equilibrium of amphiphilic chains in water," (poster) The Royal Society of Chemistry: Faraday Discussion No.103, Sheffield University, Sheffield, UK, April '96.
5. "Conformational equilibrium of nonionic surfactants in water," American Institute of Chemical Engineers Annual Meeting, Chicago, IL, November '96.
6. "Conformational equilibrium of 1,2-dimethoxyethane in aqueous solution," Center for Molecular and Engineering Thermodynamics Research Review, University of Delaware, Newark, DE, June '97.
7. "Conformational equilibrium of 1,2-dimethoxyethane in aqueous solution," American Institute of Chemical Engineers Annual Meeting, Los Angeles, CA November '97.
8. "The hydration of amphiphilic solutes: A theoretical and modeling perspective," Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, February '98.
9. "The hydration of amphiphilic solutes: A theoretical and modeling perspective," Physical Chemistry 1, Lund University, Lund, Sweden, April '98.
10. "Interaction of cationic/nonionic surfactant mixtures with an anionic hydrogel," Center for Amphiphilic Polymers Research Review, Halmstad, Sweden, April '99.
11. "Interaction of cationic/nonionic surfactant mixtures with an anionic hydrogel," American Institute of Chemical Engineers Annual Meeting, Dallas, TX, November '99.
12. "Hydrophobic effects on microscopic and mesoscopic length scales," American Institute of Chemical Engineers Annual Meeting, Dallas, TX, November '99.
13. "The theory of ion solvation," Department of Chemical Engineering, Rensselaer Polytechnic Institute, Troy, NY, April '00.
14. "Hydrophobic effects on microscopic and mesoscopic length scales," American Institute of Chemical Engineers Annual Meeting, Los Angeles, CA, November '00.
15. "Convergence of molecular and macroscopic continuum dielectric descriptions of hydration," American Institute of Chemical Engineers Annual Meeting, Los Angeles, CA, November '00.
16. "Water: A stage for self-assembly," Rutgers University, Department of Chemistry, Piscataway, NJ, April '01.
17. "Rheology of self-assembled crude oil wax crystal modifiers," 75th Colloids and Surface Science ACS Symposium, Pittsburgh, PA, June '01.
18. "Convergence of molecular and macroscopic continuum descriptions of hydrophobic hydration," 75th Colloids and Surface Science ACS Symposium, Pittsburgh, PA, June '01.
19. "Hydrophobic effects on microscopic and mesoscopic length scales," American Institute of Chemical Engineers Annual Meeting, Reno, NV, November '01.
20. "Rheology of self-assembled crude oil wax crystal modifiers," American Institute of Chemical Engineers Annual Meeting, Reno, NV, November '01.



21. "A simple molecular thermodynamic theory of hydrophobic hydration," American Institute of Chemical Engineers Annual Meeting, Reno, NV, November '01.
22. "Effects of solute size, shape, and attractive interactions on hydrophobic hydration," American Chemical Society National Meeting, Boston, MA, August '02.
23. "Effects of solute size, shape, and attractive interactions on hydrophobic hydration," American Institute of Chemical Engineers Annual Meeting, Indianapolis, IN, November '02.
24. "Coarse graining of atomistic simulations of polymeric melts to access long length and time scales," American Institute of Chemical Engineers Annual Meeting, Indianapolis, IN, November '02.
25. "Coarse graining of atomistic simulations of polymeric melts to access long length and time scales," Fifteenth Symposium on Thermophysical Properties, Boulder, CO, June '03.
26. "Effects of solute size, shape, and attractive interactions on hydrophobic hydration," Fifteenth Symposium on Thermophysical Properties, Boulder, CO, June '03.
27. "Coarse graining of atomistic simulations of polymeric melts to access long length and time scales," American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, Nov. '03.
28. "Competing roles of chain conformation and monomer hydration on the cloud point of poly(ethylene oxide) in water," American Institute of Chemical Engineers Annual Meeting, Austin, TX, Nov. '04.
29. "Probing the stability of natively unfolded proteins," American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, Nov. '06.
30. "Stability Of natively unfolded proteins as a coil/globule transition in charge/hydrophobic space," American Institute of Chemical Engineers Annual Meeting, Salt Lake City, UT, Nov. '07.
31. "Disentangling the stability of natively unfolded proteins," 82nd Colloids and Surface Science ACS Symposium, Raleigh, NC, June, '08.
32. "Stability of natively unfolded proteins as a coil/globule transition in charge/hydrophobic space," American Chemical Society National Meeting, Philadelphia, PA, Aug. '08.
33. "Conformational stability of templated protein sequences," American Institute of Chemical Engineers Annual Meeting, Philadelphia, PA, Nov. '08.
34. "Alcohol effects on trans nuclear membrane transport," American Institute of Chemical Engineers Annual Meeting, Nashville, TN, Nov. '09.
35. "Blowing bubbles in Lennard-Jonesium," American Institute of Chemical Engineers Annual Meeting, Nashville, TN, Nov. '09.
36. "Helix stabilization of poly(ethylene glycol)-peptide conjugates," American Institute of Chemical Engineers Annual Meeting, Salt Lake City, UT, Nov. '10.
37. "Solvent cavitation under solvophobic confinement," ACS 2013 Colloid and Surface Science Symposium, Riverside, CA, Jun. '13.
38. "Solvent cavitation under solvophobic confinement," American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, Nov. '13.
39. "Solvent cavitation under solvophobic confinement," ACS 2014 Colloid and Surface Science Symposium, Philadelphia, PA, Jun. '13.
40. "Effect of pressure on micellar assemblies," ACS 2014 Colloid and Surface Science

- Symposium, Philadelphia, PA, Jun. '13.
41. "Solvent cavitation under solvophobic confinement," American Institute of Chemical Engineers Annual Meeting, Atlanta, GA, Nov. '14.
  42. "Effect of pressure on micellar assemblies," American Institute of Chemical Engineers Annual Meeting, Atlanta, GA, Nov. '14.

### **INVITED PRESENTATIONS**

1. "Water: A stage for self-assembly," Los Alamos National Laboratory, May. '01.
2. "Water: A stage for self-assembly," Washington University, Department of Chemical Engineering, St. Louis, MO February '02.
3. "From Ångstroms to objects: Building bridges between micro and macro length scales," University of Cincinnati, Department of Chemistry, Cincinnati, OH, December '03.
4. "From Ångstroms to objects: Building bridges between micro and macro length scales," Sandia National Laboratory, Albuquerque, NM, January '04.
5. "From Ångstroms to objects: Building bridges between micro and macro length scales," Tufts University, Department of Chemical Engineering, Boston, MA, January '04.
6. "From Ångstroms to objects: Building bridges between micro and macro length scales," Auburn University, Department of Chemical Engineering, Auburn, AL, February '04.
7. "From Ångstroms to objects: Building bridges between micro and macro length scales," University of South Florida, Department of Chemical Engineering, Tampa, FL, February '04.
8. "From Ångstroms to objects: Building bridges between micro and macro length scales," Tulane University, Department of Chemical Engineering, New Orleans, LA, March '04.
9. "From Ångstroms to objects: Building bridges between micro and macro length scales," Arizona State University, Department of Chemical Engineering, Tempe, AZ, March '04.
10. "From Ångstroms to objects: Building bridges between micro and macro length scales," Tulane University, Center for Computational Science, New Orleans, LA, December, '04.
11. "From Ångstroms to objects: Building bridges between micro and macro length scales," Rensselaer Polytechnic Institute, Department of Chemical Engineering, Troy, NY, October, '05.
12. "From Ångstroms to objects: Building bridges between micro and macro length scales," University of Massachusetts, Department of Chemical Engineering, Amherst, MA, November, '05.
13. "From Ångstroms to objects: Building bridges between micro and macro length scales," Hamilton College, Department of Chemistry, Clinton, NY, November, '05.
14. "The scales of hydrophobic hydration," American Chemical Society Southwest Regional Meeting special session "Hydrophobicity," Houston, TX, October '06.
15. "From Ångstroms to objects: Building bridges between micro and macro length scales," University of New Orleans, Department of Chemistry, New Orleans, LA, October, '06.

16. "Scaled-particle theory and the length-scales of hydrophobicity," Leon Heller Postdoctoral Publication Prize P/T Colloquium, Los Alamos National Laboratory, Los Alamos, NM, December, '06.
17. "Disentangling the stability and function of natively unfolded proteins," University of Pennsylvania, Department of Chemical Engineering, Philadelphia, PA, October, '07.
18. "Disentangling the stability and function of natively unfolded proteins," Purdue University, Department of Chemistry, West Lafayette, IN, November, '07.
19. "Scaled particle theory and the length-scales of hydrophobicity," APS March Meeting special session "Hydrophobicity," New Orleans, LA, March, '08.
20. "Disentangling the stability of natively unfolded proteins," Joint ACS/AIChE special session "Thermodynamics in Chemical Engineering: Prospects and Perspectives," New Orleans, LA, April, '08.
21. "Disentangling the stability and function of natively unfolded proteins," University of Maryland, Institute for Physical Science and Technology Brown Bag Lunch, College Park, MD, May, '08.
22. "Disentangling the stability of natively unfolded proteins," NaTex Annual Meeting, Dallas, TX, May, '08.
23. "Disentangling the stability of natively unfolded proteins," The Johns Hopkins University, Department of Chemical and Biomolecular Engineering, Baltimore, MD, October, '08.
24. "Disentangling the stability and function of natively unfolded proteins," Vanderbilt University, Department of Chemical Engineering, Nashville, TN, March, '09.
25. "Disentangling the stability and function of natively unfolded proteins," Sandia National Laboratory, Livermore, CA, April, '09.
26. "Disentangling the stability and function of natively unfolded proteins," Yale University, Department of Chemical Engineering, New Haven, CT, October, '09.
27. "Disentangling the stability and function of natively unfolded proteins," University of Houston, Department of Chemical Engineering, Houston, TX, February, '10.
28. "Disentangling the stability and function of natively unfolded proteins," Washington University, Computational Biology, Molecular Engineering, and Biophysics Seminar Series, Saint Louis, MO, March, '10.
29. "Stability of natively unfolded proteins as a coil/globule transition in charge/hydrophobicity space," 18<sup>th</sup> Annual Texas Protein Folders Meeting, Navasota, TX, April, '10.
30. "Disentangling the stability and function of natively unfolded proteins," University of Notre Dame, Department of Chemical and Biomolecular Engineering, Notre Dame, IN, April, '10.
31. "Disentangling the stability and function of natively unfolded proteins," Louisiana State University, Department of Chemical Engineering, Baton Rouge, LA, October, '10.
32. "Disentangling the stability and function of natively unfolded proteins," University of Delaware, Department of Chemical and Engineering, Newark, DE, October, '10.
33. "Helix stabilization of poly(ethylene glycol)-peptide conjugates," American Chemical Society Southwest Regional Meeting, New Orleans, LA, December '10.
34. "Disentangling the stability and function of natively unfolded proteins," Louisiana State University, Department of Mechanical Engineering, Baton Rouge, LA, March,

- '11.
35. "Blowing bubbles in solution," ACS National Meeting, San Diego, CA, March '12.
  36. "Who's afraid of the hydrophobic effect?," U. Texas at Austin, Molecular Biophysics group seminar, Austin, TX, April, '12.
  37. "Who's afraid of the hydrophobic effect?," U. C. Riverside, Department of Chemical and Environmental Engineering, Riverside, CA, May, '13.
  38. "Who's afraid of the hydrophobic effect?," 2013 IAPWS Helmholtz Award Lecture, 16<sup>th</sup> International Conference on the Properties of Water and Steam, University of Greenwich, London, UK, Sept. '13.
  39. "Polymer induced helical folding," Invited talk in Thermodynamics of Biomolecular Folding and Assembly session, American Institute of Chemical Engineers Annual Meeting, San Francisco, CA, Nov. '13.
  40. "Who's afraid of the hydrophobic effect?," Syracuse University, Department of Biomedical and Chemical Engineering, Syracuse, NY, Nov., '13.
  41. "Who's afraid of the hydrophobic effect?," Clemson University, Department of Chemical Engineering, Clemson, SC, Mar. '14.
  42. "Who's afraid of the hydrophobic effect?," Lehigh University, Department of Chemical Engineering, Bethlehem, PA, Apr. '14.
  43. "Adventures in hydrophobicity," 14<sup>th</sup> Southern School on Computational Chemistry and Materials Science Conference, Jackson State University, Jackson, MS, July '14.
  44. "Adventures in hydrophobicity," Mississippi State University, Department of Chemical Engineering, Starkville, MS, Jan. '15.

#### **PATENTS**

1. H.S. Ashbaugh, R. K. Prud'homme, and D. H. Adamson "Amphoteric stabilization of crude petroleum," United States Patent 6,566,454 (filed 6/5/01, granted 5/20/03).

#### **POST-DOCTORAL RESEARCHERS SUPERVISED**

1. Dr. Lu Yang (Ph.D. Rensselaer Polytechnic Institute), January, '05 – September, '06. "Simulation of complex materials." Present: Research staff at Applied Materials.

#### **GRADUATE STUDENTS SUPERVISED**

*Ph.D.*

1. Lalit Surampudi, Spr '10 – Present.
2. Bin Meng, Fall '11 – Present.
3. J. Wes Barnett (B.S. Miss State U), Fall '12 – Present.
4. Alexander Saltzmann (B.S. Yale), Fall '13 – Present.
5. Kun Chao, Fall '13 – Present.

#### **GRADUATE ALUMNI**

*Ph.D.*

1. Ashish Sangwai (B.S. UICT), Fall '05 – Sum. '10. Dissertation title: "Investigation of solvent-mediated molecular interactions driving self-assembly." Present: Intel, Portland, OR.

2. Amit Jain (B.S. LIT, M.S. UICT), Fall '05 – Sum. '10. Dissertation title: “Solvent and biomolecular interactions guiding assembly and recognition.” Present: Fluid Flow and Assurance Engineer for Shell India Markets Private Limited, Bangalore, India.
3. Piyush Wanjari (B.S. LIT), Fall '08 – Fall '12. Dissertation title: “Investigation of solvent-mediated host-guest interactions and conformational changes in n-alkanes trapped under hydrophobic confinement.” Present: Post-doc, Sanofi Aventis, Paris, France.
4. Pradeep Venkataraman (co-advised with Vijay John, B.S. IIT Madras), Fall '06 – Fall '12. Dissertation title: “Investigation of molecular hydrophobicity for energy and environmental applications: Simulation and experiments.” Present: Post-doc, Department of Chemical Engineering, Rice University, Houston, TX.
5. Lixin Liu, Fall '09 – Sum. '14. Dissertation title: “Molecular dynamics simulation studies of tailored nanostructured polymers.” Present: Honeywell, Shanghai, China.

### **THESIS COMMITTEE SERVICE**

#### *Ph.D.*

1. Rong Kou – advisor Prof. Yunfeng Lu, Summer '06.
2. Hongmei Luo - advisor Prof. Yunfeng Lu, Summer '06.
3. Huisheng Peng – advisor Prof. Yunfeng Lu, Summer '06.
4. Zhiwang Wu – advisor Prof. Yunfeng Lu, Summer '06.
5. Andrew Heinz – advisor Prof. Brian Mitchel, Summer '08.
6. Luigi Verdoni – advisor Prof. Brian Mitchel, Spring '12.
7. Mangesh Chaudhari – advisor Prof. Lawrence Pratt, Spring '13.
8. Brooke Peadon – advisor Wayne Reed (physics), Summer '14.

#### *M.S.*

1. Kyriakos Vistas – advisor Prof. Kyriakos Papadopoulos, Spring '08.
2. Christopher Day – advisor Prof. Vijay John, Summer '08.

### **UNDERGRADUATE STUDENTS SUPERVISED**

1. Asani Phillips – NSF-REU student, Princeton University, Summer '00. “Viscosification of surfactant vesicles using hydrophobically modified polymers.”
2. Preetesh Kantak – Work study student, Princeton University, Fall '00. “Phase behavior of semifluorinated alkane surfactants in organic media.”
3. Eric Altoonean – Work study student, Princeton University, Spring '01. “Synthesis of pH sensitive polymeric emulsifiers.”
4. Kathleen Boon – Senior thesis research student, Princeton University, Fall '00 – Spring '01. “Viscosification of surfactant vesicles using hydrophobically modified polymers.”
5. Jessika Pazool – NSF-REU student, Princeton University, Summer '01. “Emulsion formulation for organic and silicon based oils.”
6. Jonathan Bakke – Tulane University, Fall '04 – Spring '05. “Thermodynamics of a confined van der Waals fluid.” Present: Global product manager at Applied Materials after completing Ph.D. in Chemical Engineering at Stanford University in 2011.

7. Harold Hatch – Tulane University, Spring '06 – Spring '08. “Coil-globule transitions in heteropolymer models of proteins.” – supported by the Provost’s Fund for Faculty/Undergraduate Engagement. Present: NRC post-doctoral researcher at NIST after completing Ph.D. in Chemical Engineering at Princeton University in 2013.
8. Jennifer Staton – Tulane University, Spring '08 – Spring '10. “Simulations of hydrophobic hydration.” Present: Product development engineer at Generson IGS after completing MS in Chemical Engineering at the University of California Davis in 2013.
9. Nicholas Collett – Tulane University, Spring '08 – Spring '10. “Simulations of hydrophobic hydration.” Present: Process engineer at Star Engineering Services Inc.
10. Christina Oerter – LA-SiGMA REU student from University of Colorado, Summer '11.
11. Steven Williams – Tulane University, Spring '11 – Spring '13. “Thermal expansion of aqueous solutes.” Present: graduate student in Chemical Engineering at Rice University.
13. Ian Terry – Tulane University, Spring '11. “Thermal expansion of aqueous solutes.” Present: Physics teacher at YES Prep Public Schools.
14. Ellie Rodebeck – LA-SiGMA REU student (w/Anne Robinson) from Tulane University, Summer '12.
15. Nicholas Altieri – Tulane University, Summer '12. “Effect of pressure on micellar assembly.” Present: graduate student in Chemical Engineering at UCLA
16. Christa Cook – LA-SiGMA REU student from Louisiana State University, Summer '13.
17. Tuan Tran – Tulane University, Spring '12 - present. “Ionic liquids as assembly media.”
18. Katie Weiss – LA-SiGMA REU student from Alfred University, Summer '14.

#### **ADDITIONAL ACTIVITIES**

1. Chair, “Self-assembly in solution,” American Institute of Chemical Engineers Annual Fall Meeting - '01, '02, '03.
2. Chair, “Thermodynamics at the nanoscale,” American Institute of Chemical Engineers Annual Fall Meeting – '04, '09, '10, '11.
3. Chair, “Multiscale modeling of thermodynamic and mesoscale properties,” American Institute of Chemical Engineers Annual Fall Meeting – '04, '05.
4. Chair, “Self and directed nanoscale assembly,” American Institute of Chemical Engineers Annual Fall Meeting – '04, '05, '06.
5. Chair, “Computational studies of self-assembly,” American Institute of Chemical Engineers Annual Fall Meeting – '05, '07, '08, '09, '13.
6. Chair, “Thermodynamics and phase behavior,” American Institute of Chemical Engineers Annual Fall Meeting – '06.
7. Chair, “Thermodynamics and phase equilibria,” American Institute of Chemical Engineers Spring Meeting – '08.
8. American Institute of Chemical Engineers Area 1a Programming Committee, '13 – '16.

9. Symposium Organizer w/ Lawrence Pratt (LANL), "Hydrophobicity," American Chemical Society Southwest Regional Meeting, Houston, TX – Fall '06.
10. Symposium Organizer w/ Dor Ben-Amotz (Purdue), "Water Mediated Interactions," American Chemical Society National Meeting, Philadelphia, PA – Aug. '08.
11. Symposium Organizer w/ Bill Swope (IBM Almaden) and Steve Rick (UNO), "Functional Polymers: Connecting Modeling and Experiment," American Chemical Society National Meeting, Boston, MA – Aug. '15.
12. Leader of Science Driver 3 – Biomolecular Materials in the Louisiana Alliance for Simulation Guided Materials Applications (LA-SiGMA), '10 – '15.
13. Member NSF Reverse Site Visit review team for LA-SiGMA, '11.
14. Journal Reviewer (ongoing): *AIChE Journal*; *Biophysical Journal*; *Canadian Journal of Chemistry*; *Fluid Phase Equilibria*; *Fuel*; *Industrial and Engineering Chemistry Research*; *Journal of Physical Chemistry B*; *Journal of Chemical Physics*; *Journal of the American Chemical Society*; *Langmuir*; *Journal of Polymer Science Part B: Polymer Physics*; *Crystal Growth and Design*; *Journal of Physical Chemistry Letters*; *Physical Review Letters*; *Proceedings of the National Academy of Science USA*; *Proteins: Structure, Function, and Bioinformatics*; *Soft Matter*; *Chemical Communications*, *Entropy*, *Cellulose*.
15. External Proposal Reviewer: U. S. Civilian Research and Development Foundation (2004); National Science Foundation (CHE – 2007); American Chemical Society Petroleum Research Fund (Type B – 2007, Doctoral New Investigator – 2010, New Directions – 2012, 2014); Department of Energy (Advanced Scientific Computing Research – 2010), Oak Ridge Associated Universities - NASA Postdoctoral Program (2013).
16. Panel Proposal Reviewer: National Science Foundation (CBET – 2006, 2008, 2009, 2010, 2011), (CBET-CAREER – 2008).
17. Book Proposal Reviewer: World Scientific Publishing/Imperial College Press (2009).

### **COURSES TAUGHT (Instructor Evaluation in Parentheses from 1 (Worst) to 5 (Best))**

1. CENG 212/2120 - "Chemical engineering thermodynamics I" (Spring 2006 (2.60), Fall 2006 (3.30), Fall 2007 (4.78), Spring 2013 (4.31)).
2. CENG 311/3110 – "Chemical engineering thermodynamics II" (Fall 2008 (4.54), Fall 2009 (4.79), Fall 2010 (4.44), Fall 2011 (4.90)).
3. CENG 3390 – "Transport II" (Fall 2012 (4.33), Fall 2013 (3.9)).
3. CENG 4905/4925 – "Chemistry and engineering science in the community/Independent study," a service learning course (Spring 2007 (N/A), Spring 2008 (N/A), Spring 2009 (N/A), Spring 2010 (N/A), Spring 2011 (N/A), Spring 2012 (N/A), Spring 2013 (N/A), Spring 2014 (N/A)).
4. CENG 611 – "Thermodynamics and the properties of matter" (Spring 2007 (4.64), Spring 2008 (4.50), Spring 2010 (5.00)).
5. CENG 752 - "Applied statistical thermodynamics" (Spring 2005 (4.40), Summer/Lagniappe 2006 (N/A), Spring 2011 (4.67)).
6. CENG 792 – Special Topics: Computational Biophysics (Spring 2012 (4.25)).

### **UNIVERSITY SERVICE**

1. CBE Departmental Seminar Committee (2004 – 2011)
2. CBE Departmental Graduate Committee (2004 – 2014, Chair (2010 – 2011))
3. CBE Faculty Representative to the Library (2004 – present)
4. CBE Faculty Recruiting Committee (2005 – 2007, 2012-present (Chair)). Successfully recruited Assistant Profs. Noshir Pesika and Julie Albert.
5. CBE Department Chair Recruiting Committee (2010 – 2011). Successfully recruited Prof. Anne Robinson.
6. SSE Representative to the Center for Public Service Executive Committee (2009 – 2012)
7. SSE Representative to the Tulane University Graduate Advisory Council (2011 – 2014)
8. Member CBE Graduate Qualifying Exam Committee (2005, 2010 (Chair), 2013 (Chair))
9. Chair of CBE Entergy Chair Recruiting Committee (2012 - 2014). Successfully recruited Prof. Daniel Shantz.