Lev D. Gelb

Curriculum Vitae

Address

University of Texas at Dallas
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Education

University Of Cambridge, Cambridge, United Kingdom
Ph.D. in Chemistry, 12/1995. Thesis: "Theoretical Studies of Surface Phase Transitions."
Adviser: Prof. R. M. Lynden-Bell.

Columbia University, New York City, NY
B.A. (Chemistry), *summa cum laude*, 5/1992. Cumulative G.P.A.: 4.00

Professional appointments

Associate Professor, Department of Materials Science and Engineering,
University of Texas at Dallas, 2010—present.
Affiliate Professor, Department of Chemistry, 2012—present.

Associate Professor, Department of Chemistry,
Washington University in St. Louis, 2006—2010.
Inaugural Member, Center for Materials Innovation.

Assistant Professor, Department of Chemistry,
Washington University in St. Louis 2002—2006.

Assistant Professor, Department of Chemistry and Biochemistry,
Florida State University (FSU), 1999—2002.
Associate Member, School of Computational Science and Information Technology (CSIT).

Postdoctoral Research Associate, 1999, with Prof. D. N. Beratan,
University of Pittsburgh.

Postdoctoral Research Associate, 1996—1998, with Prof. K. E. Gubbins,
Cornell University and NCSU.

Awards

NSF CAREER Award Multi-scale modeling of sol-gel materials, 2002—2006.
CISE Post-Doctoral Fellowship (at the Cornell Theory Center) NSF, 1996—1998.
NSF Graduate Fellowship National Science Foundation, 1994—1995.
Honorary Cambridge Commonwealth Trust Scholar, University of Cambridge, 1994—1995.
British Marshall Scholarship Marshall Aid Commemoration Commission, 1992—1994.
'Best Poster Prize' Molecular Liquids Conference, 1993.
Phi Beta Kappa (Junior) Columbia University, 1991.
Perkin-Elmer Corporate Scholarship Perkin Elmer, Inc., 1991.

Research interests

- New methods for free energy and phase equilibria calculations
- Data analysis and reconstruction
- Nanostructured and amorphous porous materials
- Gas adsorption, capillary phenomena and confined phase equilibria
- High-performance computing
- Potential (force-field) development and evaluation
- Nucleation
- Multiscale modeling / coarse-graining
- First-principles molecular simulations
- Liquid structure theory

Teaching experience

University of Texas at Dallas

"ENGR3341 Probability Theory and Statistics," undergraduate engineering probability. Fall 2014, Spring 2015, Fall 2015, Spring 2016, Fall 2016, Spring 2017.

"MSEN6330 Phase Transformations," Thermodynamic, kinetic, and structural aspects of metallic and ceramic phase transformations: mechanisms and rate-determining factors in solid-phase reactions; diffusion processes, nucleation theory, precipitation from solid solutions, and order-disorder phenomena. Spring 2012, Spring 2014.

"CHEM3321 Physical Chemistry I," first semester of Physical Chemistry sequence, covering core topics in thermodynamics, statistical mechanics, and chemical kinetics. Fall 2011, Fall 2013.

"CHEM3322 Physical Chemistry II," second semester of Physical Chemistry sequence, covering core topics in quantum mechanics and spectroscopy. Spring 2013.

"CHEM5314 Advanced Physical Chemistry," fundamentals of quantum mechanics as relevant for chemistry and chemical spectroscopy, including electronic structure theory as applied to molecules. Fall 2012.

"MSEN7V80 Special Topics in Materials Science and Engineering: CHEMISTRY OF MATERIALS," survey course in materials chemistry, covering the electronic structure of molecules and theories of chemical bonding, acid/base chemistry, redox and electrochemistry, reactions in the solid state, reactions at surfaces, kinetics and thermodynamics of self-assembly. Spring 2011.

"CHEM1312 General Chemistry II," second semester of a survey course covering chemical and physical equilibria, thermodynamics, electrochemistry, acids and bases, nuclear chemistry, and basic organic chemistry. Fall 2010.

Washington University

"562 Statistical Thermodynamics," physical chemistry graduate course covering equilibrium statistical thermodynamics with application to chemical systems and phase equilibria, and computational methods. Fall 2005, Fall 2006, Fall 2007, Fall 2009.

"571 Quantum Chemistry and Spectra," physical chemistry graduate course covering rigorous quantum mechanics, and electronic structure theory as applied to molecules. Spring 2005, Spring 2006, Spring 2007.

"112 General Chemistry," the second semester of a survey course for science majors and engineers, covering equilibria, thermodynamics, electrochemistry, acid/base equilibria and kinetics. Spring 2003, Spring 2004, Spring 2008, Spring 2010.

Florida State University

"1045 General Chemistry," the first semester of a survey course for science majors and engineers, covering atomic theory and structure, thermochemistry, solution chemistry, gases, and chemical bonding. Fall 2001.

"Valence Theory," a graduate course in molecular structure and chemical bonding, with emphasis on symmetry, molecular orbital methods, and a practical introduction to some computational chemistry methods. Fall 1999, Fall 2000.

"Advanced Statistical Mechanics," a graduate course in modern statistical mechanics with a focus on molecular simulation. Spring 2001, Spring 2002.

Other teaching experience

Substitute lecturer for junior-level Chemical Engineering Thermodynamics, Cornell University, 1997, and for graduate Chemical Engineering Thermodynamics, NCSU, 1998.

Supervisor, University of Cambridge, 1993—1995. (Involved weekly tutoring of several groups of two or three students, grading, and progress assessments.) Physical chemistry and statistical mechanics.

Chemistry laboratory instructor and General Chemistry grader, Columbia University, 1992.

Recitation instructor for summer-term General Chemistry course, Columbia University, 1992.

Publications

2017

55. "Structural and Transport Properties of Tertiary Ammonium Triflate Ionic Liquids: A Molecular Dynamics Study," A. Taghavi Nasrabadi and L. D. Gelb, *J. Phys. Chem. B* **121** (2017) 1908-1921.

2015

54. "Nested sampling of isobaric phase space for the direct evaluation of the isothermal-isobaric partition function of atomic systems," B. A. Wilson, L. D. Gelb and S. O. Nielsen, *J. Chem. Phys.* **143** (2015) 154108.
53. "Kinetic Monte Carlo Simulation of Electrochemical Systems," C. H. Turner, Z. Zhang, L. D. Gelb and B. I. Dunlap, in *Reviews in Computational Chemistry, Volume 28* ed. A. L. Parrill-Baker and K. B. Lipkowitz (2015) 175-204.
52. "Computational study of uniaxial deformations in silica aerogel using a coarse-grained model," C. A. Ferreiro-Rangel and L. D. Gelb, *J. Phys. Chem. B* **119** (2015) 8640-8650.
51. "Statistically Rigorous Analysis of Imaging SIMS Data in the Presence of Detector Saturation," L. D. Gelb, L. A. Bahktiari and A. V. Walker, *Surf. Interface Anal.* **47** (2015) 889-895.

2014

50. "On Including Nonlinearity in Multivariate Analysis of Imaging SIMS Data," L. D. Gelb, T. M. Milillo, and A. V. Walker, *Surf. Interface Anal.* **46** (2014) 221-225.

2013

49. "Investigation of the Bulk Modulus of Silica Aerogel using Molecular Dynamics Simulations of a Coarse-Grained Model," C. A. Ferreiro-Rangel and L. D. Gelb, *J. Phys. Chem. B* **117** (2013) 7095-7105.

48. "Optimized analysis of imaging time-of-flight SIMS data," L. D. Gelb, T. M. Milillo, and A. V. Walker, *Surf. Interface Anal.* **45** (2013) 479-482.

2012

47. "Monte Carlo strategies for first-principles simulations of elemental systems," L. D. Gelb, *Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond*, XSEDE 2012, art. no. 25, DOI: 10.1145/2335755.2335821.

46. "A Monte Carlo Simulation Study of Methane Clathrate Hydrates Confined in Slit Pores," S. N. Chakraborty and L. D. Gelb, *J. Phys. Chem. B* **116** (2012) 2183-2197.

2011

45. "Boiling point determination using adiabatic Gibbs ensemble Monte Carlo simulations: Application to metals described by embedded-atom potentials," L. D. Gelb and S. N. Chakraborty, *J. Chem. Phys.* **135** (2011) 224113.

44. "Extension of the Steele 10-4-3 potential for adsorption calculations in cylindrical, spherical, and other pore geometries," D. W. Siderius and L. D. Gelb, *J. Chem. Phys.* **135** (2011) 084703.

43. "Simulation and Modeling of Aerogels Using Atomistic and Mesoscale Methods," L. D. Gelb, in *Aerogels Handbook*, M. A. Aegerter et al. (eds.), (2011) 565-581.

2009

42. "Thermodynamic and structural properties of finely-discretized on-lattice hard-sphere fluids: virial coefficients, free energies and direct correlation functions," D. W. Siderius and L. D. Gelb, *J. Chem. Phys.* **131** (2009) 084503.

41. "Modeling amorphous porous materials and confined fluids," L. D. Gelb, *MRS Bulletin* **34** No. 8 (August 2009) pp. 553-624. (invited article.)

40. "Structure, Thermodynamics and Solubility in Tetromino Fluids," B. C. Barnes, D. W. Siderius and L. D. Gelb, *Langmuir* **25** (2009) pp. 6702-6716.

39. "Predicting Gas Adsorption in Complex Microporous and Mesoporous Materials Using a New Density Functional Theory of Finely Discretized Lattice Fluids," D. W. Siderius and L. D. Gelb, *Langmuir* **25** (2009) pp. 1296-1299.

2008

38. "Impact of Diffusion on Concentration Profiles Around Near-Critical Nuclei and Implications For Theories of Nucleation and Growth," J. Diao, R. Salazar, K. F. Kelton and L. D. Gelb, *Acta Materialia*, **56** (2008) pp. 2585-2591.

2007

37. "Simulating Silica Aerogels with a Coarse-Grained Flexible Model and Langevin Dynamics," L. D. Gelb, *J. Phys. Chem. C* **111** (2007) pp. 15792-15802.

36. "Meta-Optimization of Evolutionary Strategies for Empirical Potential Development: Application to Aqueous Silicate Systems," B. C. Barnes and L. D. Gelb, *J. Chem. Theor. Comput.* **3** (2007) pp. 1749-1764.

35. "A computational study of the reconstruction of amorphous mesoporous materials from gas adsorption isotherms and structure factors via evolutionary optimization," R. Salazar and L. D. Gelb, *Langmuir*, **23** (2007) pp. 530-541.

34. "A Molecular Dynamics Study of Laser-Assisted Cleaning: Energy Transfer Medium-Contaminant Particle Interaction," B. Unlusu, K. M. Smith, M. Y. Hussaini, L. D. Gelb and S. D. Allen, *J. Comp. Theor. Nanoscience*, **4** (2007) pp. 488-493.

2006

33. "Isothermal-isobaric Monte Carlo Simulations of Liquid Lithium using Density Functional Theory," L. D. Gelb and T. Carnahan, *Chem. Phys. Letts.*, **417** (2006) pp. 283-287.

2005

32. "Off-Lattice dynamic Monte Carlo Simulations of Aggregation in One Dimension, R. Salazar and L. D. Gelb," *Physica A*, **356** (2005) pp. 190-195.
31. "Adsorption in Controlled-Pore Glasses: Comparison of Molecular Simulations With a Mean-Field Lattice Gas Model, L. D. Gelb and R. Salazar," *Adsorption*, **11** (2005) pp. 283-288.
30. "An Investigation of Enhanced Secondary Ion Emission Under Au_n^+ (n = 1-7) Bombardment," G. Nagy, L. D. Gelb and A. V. Walker, *J. Am. Soc. Mass. Spec.* **16** (2005) pp. 733-742.
29. "Application of the Bethe-Peierls Approximation to a Lattice-Gas Model of Adsorption on Mesoporous Materials," R. Salazar and L. D. Gelb, *Phys. Rev. E* **71** (2005) art. no. 041502.

2004

28. "Molecular Dynamics Simulations of the Polymerization of Aqueous Silicic Acid and Analysis of the Effects of Concentration on Silica Polymorph Distributions, Growth Mechanisms, and Reaction Kinetics," N. Z. Rao and L. D. Gelb, *J. Phys. Chem. B*, **108** (2004) pp. 12418-12428. This research was also featured in *NCSA Access*, **17** #2, 2004.
27. "An Investigation of the Effects of the Structure of Gel Materials on Their Adsorptive Properties Using a Simple Lattice-Gas Model," L. D. Gelb and R. Salazar, *Molecular Physics* **102** (2004) pp. 1015-1030.

2003

26. "Modeling Laser-Assisted Particle Removal Using Molecular Dynamics," K. M. Smith, M. Y. Hussaini, L. D. Gelb and S. D. Allen, *App. Phys. A*, **77** (2003) pp. 877-882.
25. "Pore Size Distribution of Porous Glasses: A Test of the Independent Pore Model," S. Figueroa-Gerstenmaier, J. Bonet Avalos, L. D. Gelb, K. E. Gubbins and L. F. Vega, *Langmuir*, **19** #20 (2003) pp. 8592-8604.
24. "Molecular Modeling of Fluid-Phase Equilibria Using an Isotropic Multipolar Potential," E. A. Müller and L. D. Gelb, *Ind. Eng. Chem. Res.* **42** #17 (2003) pp. 4123-4131.
23. "Monte Carlo Simulations Using Sampling From an Approximate Potential," L. D. Gelb, *J. Chem. Phys.* (2003) **118** #17, pp. 7747-7750.

2002

22. "Dynamics of the Capillary Rise in Nanocylinders," L. D. Gelb and A. C. Hopkins, *Nano Letters*, (2002) **2** #11 pp. 1281-1285.
21. "Location of Phase Equilibria by Temperature-Quench Molecular Dynamics Simulations," L. D. Gelb and E. A. Müller, *Fluid Phase Eq.*, **203** #1-2 (2002) pp. 1-14.
20. "The Ins and Outs of Capillary Condensation in Cylindrical Pores," L. D. Gelb, *Molecular Physics*, (2002) **100** #13 pp. 2049-2057.
19. "Molecular Simulation of Capillary Phenomena in Controlled Pore Glasses," L. D. Gelb and K. E. Gubbins, in *Fundamentals of Adsorption 7*, K. Kaneko *et al*, eds., (2002) pp. 333-340.

2001

18. "Phase Equilibria of Multicomponent Systems Using Parallel Molecular Dynamics Algorithms," L. D. Gelb, M. E. Suárez and E. A. Müller, *AIChE Symposium Series* (2001) **97** #325, pp. 187-190.

17. "Simulations of Capillary Condensation in Porous Glasses," L. D. Gelb and K. E. Gubbins, *AIChE Symposium Series*, (2001) **97** #325, pp. 292-295.

2000

16. "Characterization of Controlled Pore Glasses: Molecular Simulations of Adsorption," L. D. Gelb and K. E. Gubbins, *Studies in Surf. Sci. Catal.*, **128** (2000) pp. 61-69.

1999

15. "Phase Separation in Confined Systems," (Review), L. D. Gelb, K. E. Gubbins, R. Radhakrishnan and M. Sliwinska-Bartkowiak, *Rep. Prog. Phys.*, **62** #12 (1999) pp. 1573-1659.

14. "Correlation Functions of Adsorbed Fluids in Porous Glass: A Computer Simulation Study," L. D. Gelb and K. E. Gubbins, *Mol. Phys.*, **96** #12 (1999) pp. 1795—1804.

13. "Phase Transitions in Pores: Experimental and Simulation Studies of Melting and Freezing," M. Sliwinska-Bartkowiak, J. Gras, R. Sikorski, R. Radhakrishnan, L. D. Gelb, and K. E. Gubbins, *Langmuir*, **15** #18 (1999) pp. 6060—6069.

12. "Pore Size Distributions in Porous Glasses: A Computer Simulation Study," L. D. Gelb and K. E. Gubbins, *Langmuir*, **15** #2 (1999) pp. 305—308.

11. "Characterization of Porous Glasses by Adsorption: Models, Simulations and Data Inversion," L. D. Gelb and K. E. Gubbins, in *Fundamentals of Adsorption 6*, ed. F. Meunier, pp. 551-556, Elsevier, Paris (1998).

10. "Liquid-Liquid Equilibria in Porous Glasses: Molecular Simulations and Experimental Results," L. D. Gelb, M. Sliwinska-Bartkowiak and K. E. Gubbins, in *Fundamentals of Adsorption 6*, ed. F. Meunier, pp. 497—502, Elsevier, Paris (1998).

1998

9. "Characterization of Porous Glasses: Simulation Models, Adsorption Isotherms, and the Brunauer-Emmett-Teller Analysis Method," L. D. Gelb and K. E. Gubbins, *Langmuir*, **14** #8 (1998) pp. 2097—2111.

1997

8. "Phase Separation for Mixtures in Well-Characterized Porous Materials: Liquid-Liquid Transitions," M. Sliwinska-Bartkowiak, R. Sikorski, S. L. Sowers, L. D. Gelb and K. E. Gubbins, *Fluid Phase Equilibria* **136** #1-2 (1997) pp. 93—109.

7. "Kinetics of Liquid-Liquid Phase Separation of a Binary Mixture in Cylindrical Pores," L. D. Gelb and K. E. Gubbins, *Phys. Rev. E*, **55** #2 (1997) pp. 1290R—1293R.

6. "Studies of Binary Liquid Mixtures in Cylindrical Pores: Phase Separation, Wetting and Finite-Size Effects from Monte Carlo Simulations," L. D. Gelb and K. E. Gubbins, *Physica A*, **244** (1997) pp. 112—123.

5. "Liquid-Liquid Phase Separation in Cylindrical Pores: Quench Molecular Dynamics and Monte Carlo Simulations," L. D. Gelb and K. E. Gubbins, *Phys. Rev. E*, **56** #3 (1997) pp. 3185—3196.

1996

4. "Decorated Lattice Models for Surface Phase Transitions," L. D. Gelb, *Molecular Physics*, **88** #6 (1996) pp. 1541—1561.

1995

3. "Surface Melting and Layering Transitions from a Lattice-Gas Model," L. D. Gelb, *Phys. Rev. B*, **50** #15 (1994) pp. 11146—11150.
2. "Effects of Atomic-Force-Microscope Tip Characteristics on Measurement of Solvation-Force Oscillations," L. D. Gelb and R. M. Lynden-Bell, *Phys. Rev. B*, **49** #3 (1994) pp. 2058—2066.

1994

1. "Force Oscillations and Liquid Structure in Simulations of an Atomic Force Microscope Tip in a Liquid," L. D. Gelb and R. M. Lynden-Bell, *Chem. Phys. Letts.*, **211**, #4,5 (1993) pp. 328—332.

Grants and contracts

Active awards and contracts

1. "Resolving Nonlinearity in Thin Film Chemical Analysis: Roughening, Matrix Effects and Chemical Damage," submitted to National Science Foundation. P.I. L. D. Gelb, Co-P.I.: A. V. Walker. $345,000, 06/01/17-05/31/20.
2. "Thermodynamics of Acid-Base Equilibria in Protic Ionic Liquids," $110,000, ACS-PRF, 09/01/15-08/31/17.
3. "REU Site: Surface Engineering for Sensing, Energy and Nanoelectronics," National Science Foundation, PI: A. V. Walker, co-PI: L. D. Gelb, DMR-1460654 $330,000, 03/01/15 - 02/28/18.
4. Unrestricted funds from Procter&Gamble to support collaborative project on colloid stability. $70,000, 2016.

Expired awards and contracts

1. Unrestricted funds from Procter&Gamble to support collaborative project on colloid stability. $25,000, 2015.
2. "REU Site: Surface Engineering for Sensing, Energy and Nanoelectronics," National Science Foundation, PI: A. V. Walker, co-PI: L. D. Gelb, $320,000, 02/01/12 - 01/31/15.
3. "CDI-Type I: Collaborative Research: Cyber-Enabled Chemical Imaging: From Terascale Data College to Chemical Knowledge," National Science Foundation, PI: A. V. Walker, Co-PI: L. D. Gelb. Total award $566,383. 2010-2014.
4. "First-principles Monte Carlo simulations of fluid phase equilibria at extreme conditions," National Science Foundation (#CHE-0718861), $381,806, 2007-2012.
5. "Collaborative Research: Cyberinfrastructure for Phase-Space Mapping – Free Energies, Phase Equilibria and Transition Paths," National Science Foundation (#CHE-0626008). Collaborative project with D. A. Kofke (PI, U. at Buffalo), S. C. Glotzer (U. Michigan), P. T. Cummings (Vanderbilt) and D. Chandler (U.C. Berkeley). Total award ∼$2.2M; Gelb subcontract $615,000. 2006-2012.
6. "Phase change materials for data storage" $19,500, Co-PI; with K. F. Kelton (WU Physics). 2009-2010.
7. "DURIP: Acquisition of a computer system for first-principles simulations of molecular solids", Army Research Office (# W911NF-07-1-0253), $157,655, 2007.
8. "Three-dimensional reconstruction of mesoporous materials from gas adsorption and structure factor data", ACS Petroleum Research Fund (#44674-AC10) $80,000, 2006-2009.
9. "Phase change materials for data storage" $25,000, Co-PI; with K. F. Kelton (WU Physics). 2008-2009.

10. "CRIF: Purchase of a Resource for Computational Chemistry", National Science Foundation (#CHE-0443511), $132,558, 2005-2008 (Co-PI with J. Ackerman (Dept. Chair) and several "major users", but primary author.)
11. "Multi-Scale Modeling of Sol-Gel Materials", National Science Foundation CAREER Award $433,900, 2002-2006.
12. "Nucleation Control", WU Center for Materials Innovation, $15,000 collaborative project with K. F. Kelton (PI) and others, 2005. (Total award: $60,000.)
13. "Materials for Hydrogen Storage", WU Center for Materials Innovation, $11,500, PI, collaborative project, 2005.
14. "Parallel molecular simulations of nano-scale bubble formation and collapse dynamics", Research Corporation (Research Innovation Award) $34,000, for 2001-2002.
15. "Computational Modeling of Nanoporous Silica Xerogels", First-year Assistant Professor Award of $10,000, from the FSU Council on Research and Creativity. 2000.
16. "Generation of computer graphics of silica aerogels," Cabot Corporation, 2/2003, $8,000.
17. "GOALI: Mechanisms and Optimization of Laser Assisted Particle Removal," National Science Foundation, 2003, $250,627. S. D. Allen (PI), M. Y. Hussaini (Co-PI) and L. D. Gelb (Co-PI).

Conference presentations and seminars

(Presenter's name underlined)

2016

1. Molecular simulations of ammonium-based protic ionic liquids, A. Taghavi Nasrabadi and L. D. Gelb, 2016 ACS Southwestern Regional Meeting, Galveston, TX.
2. Molecular simulations of ammonium-based protic ionic liquids, A. Taghavi Nasrabadi and L. D. Gelb, 2016 AIChE Annual Meeting, San Francisco, CA.
3. Relationships Between Structure and Permeability in Colloidal Networks, L. D. Gelb, A. M. Mertz, M. S. Ingber, A. L. Graham and A. Redondo, AIChE 2016 Annual Meeting. San Francisco, CA.
4. Relationships Between Structure and Permeability in Colloidal Networks, L. D. Gelb, A. M. Mertz, M. S. Ingber, A. L. Graham and A. Redondo, 90th ACS Colloid and Surface Science Symposium, Cambridge, MA.

2015

1. A. L. Graham, A. Mertz, M. Ingber, A. Redondo and L. D. Gelb "Numerical Computation of Permeability in Unstable Colloidal Gels," ACS Colloid and Surface Science Symposium, Pittsburgh, PA.
2. L. D. Gelb and A. V. Walker "Statistically Rigorous Analysis of Imaging SIMS Data in the Presence of Detector Saturation," SIMS XX, Seattle, WA.
3. A. Mertz, L. D. Gelb, A. L. Graham, A. Redondo and M. Ingber "Permeability in Fractal Aggregates: Application to Unstable Colloidal Gels," AIChE Fall Meeting, Salt Lake City, UT.
4. A. Mertz, L. D. Gelb, A. L. Graham, A. Redondo and M. Ingber "Permeability in Fractal Aggregates: Application to Unstable Colloidal Gels," Society of Rheology Annual Meeting, Baltimore, MD.

2014

1. L. D. Gelb and C. Ferreiro-Rangel, "Computational Mechanics of Aerogels," Ninth Liblice Conference on the Statistical Mechanics of Liquids, Czech Republic. (Invited talk.)
2. C. Ferreiro-Rangel and L. D. Gelb, "Computational Mechanics of Aerogels and aggregation-based nanocomposite materials," ACS 2014 Fall Meeting, San Francisco, CA.
3. A. M. Mertz, M. S. Ingber, A. Graham, A. Redondo, L. D. Gelb, "Numerical Computation of Permeability in Unstable Colloidal Gels," Society of Rheology (SOR) 2014.
4. A. M. Mertz, L. D. Gelb, A. Redondo, M. S. Ingber, A. Graham, "Numerical Computation of Permeability in Unstable Colloidal Gels," AIChE Annual Meeting, Atlanta, GA.
5. L. D. Gelb, "Analysis of Imaging Mass Spectrometry Data," UT-Dallas Computational Science Seminar series (4/4/14.)

2013

1. A. V. Walker, T. Milillo, and L. D. Gelb, "Optimized Analysis of Imaging TOF SIMS Data," 19th International Conference on Secondary Ion Mass Spectrometry (SIMS 19), Jeju, Korea.
2. L. D. Gelb and C. Ferreiro-Rangel, "Computational Mechanics of Aerogels and Aggregation-Based Nanocomposite Materials," AIChE Annual Meeting, San Francisco, CA.
3. L. D. Gelb and Y. Wang, "On the Location of Phase Boundaries in Alloys Using Multi-Phase and Multi-Cell Simulation," AIChE Annual Meeting, San Francisco, CA.
4. L. D. Gelb and C. Ferreiro-Rangel, "Computational Mechanics of Aerogels and Aggregation-Based Nanocomposite Materials," Southwest Regional Meeting of the ACS, Waco, TX. (Invited talk.)
5. L. D. Gelb and C. Ferreiro-Rangel, "Computational Mechanics of Aerogels and Aggregation-Based Nanocomposite Materials," Texas Materials Modeling Network meeting, Houston, TX. (Invited talk.)

2012

1. D. Zhang, Y. Wang and L. D. Gelb, "Towards Alloy Phase Diagrams from Embedded-Atom Model Simulations," Foundations of Molecular Modeling and Simulations 2012, Portland, OR (Poster.)
2. L. Gelb, "Monte Carlo strategies for first-principles simulations of elemental systems," XSEDE12 (1st Conference of the Extreme Science and Engineering Discovery Environment), Chicago, IL.
3. L. Gelb, S. N. Chakraborty, Y. Wang and D. Zhang, "Phase boundaries and mixing thermodynamics in model atomic systems," NIST Workshop on Atomistic Simulations for Industrial Needs, Gaithersburg, MD.
4. D. Zhang and L. D. Gelb, "Liquid-vapor and liquid-liquid phase equilibria in binary alloys with modified quantum-corrected Sutton-Chen potentials," AIChE Annual Meeting, Pittsburgh, PA.
5. C. Ferreiro-Rangel and L. D. Gelb, "Simulating the Mechanical Properties of Silica Aerogels using a Coarse-Grained Flexible Model," AIChE Annual Meeting, Pittsburgh, PA.

2011

1. L. D. Gelb, "Coarse-Grained Modeling of Aerogels and The Effects of Material Compliance on Capillary Phenomena," University of North Texas Department of Materials Science and Engineering, Denton, TX.
2. A. V. Walker, T. Milillo, and L. D. Gelb, "Optimized Analysis of Imaging TOF SIMS Data," 18th International Conference on Secondary Ion Mass Spectrometry (SIMS 18), Riva del Garda, Italy.
3. L. D. Gelb and S. N. Chakraborty, "Reliability of Embedded-Atom Potentials for Boiling Points of Metals," AIChE Annual Meeting, Minneapolis, MN.
4. L. D. Gelb, "First principles Monte Carlo simulations of elemental fluid phase equilibria," AIChE Annual Meeting, Minneapolis, MN.

2010

1. B. C. Barnes and L. D. Gelb, "Structure and Thermodynamics of Polyomino Fluids and Crystals," Midwest Thermodynamics and Statistical Mechanics Conference, Notre Dame, IN.
2. S. Nath Chakraborty and L. D. Gelb, "Estimating the free energy of auto-dissociation in the Revised Central Force model of water using Molecular Dynamics simulations," Midwest Thermodynamics and Statistical Mechanics Conference, Notre Dame, IN.

3. L. D. Gelb, "Phase transitions, thermodynamics and solubility in polyomino fluids," 8th Liblice Conference on Statistical Mechanics, Brno, Czech Republic. (Invited talk.)
4. L. D. Gelb, "Computational Studies of Capillary Phenomena: The Effects of Aerogel Compliance on Adsorptive Behavior," Fundamentals of Adsorption 10, Awaji, Japan.
5. D. W. Siderius and L. D. Gelb, "Modeling Adsorption in Complex Structures: Use of Finely-Discretized Lattice-Gas DFT to Study the Effects of Pore Shape and Surface Roughness on Adsorption of Simple Gases," Fundamentals of Adsorption 10, Awaji, Japan.

2009

1. B. C. Barnes, D. W. Siderius and L. D. Gelb, "Structure, Thermodynamics, and Solubility in Polyomino Fluids," AIChE Annual Meeting, Nashville, TN.
2. D. W. Siderius and L. D. Gelb, "Modeling Adsorption in Complex Structures: Use of Finely-Discretized Lattice-Gas DFT to Study the Effects of Pore Length, Shape and Surface Roughness on Adsorption of Simple Gases," AIChE Annual Meeting, Nashville, TN.
3. D. W. Siderius and L. D. Gelb, "Characterization of Microporous Adsorbents: A Lattice DFT Study of the 'Surface Area' of Metal-Organic Frameworks," AIChE Annual Meeting, Nashville, TN.
4. L. D. Gelb, "Computational Studies of Capillary Phenomena: The Effects of Aerogel Compliance on Adsorptive Behavior," Missouri University of Science and Technology, Rolla, MO.
5. L. D. Gelb, "Structure, Thermodynamics, and Solubility in Polyomino Fluids," Thermodynamics 2009, London, U.K. (Invited (plenary) talk.)
6. L. D. Gelb, "Computational Studies of Capillary Phenomena: The Effects of Aerogel Compliance on Adsorptive Behavior," Foundations of Molecular Modeling and Simulation (FOMMS) 2009, Semiahmoo, WA. (Invited talk.)
7. D. W. Siderius and L. D. Gelb, "Modeling Adsorption in Complex Structures: Use of a Recent Lattice-Gas DFT to Study the Effect of Pore Length, Shape, and Surface Roughness on Adsorption of Simple Gases," Fifth International Workshop on Characterization of Porous Materials, New Brunswick, NJ.
8. L. D. Gelb, "Computational studies of gas adsorption and capillary phenomena: fundamental insights and characterization tools from molecular simulations, lattice models, and density functional theory", Louisiana State University, Baton Rouge, LA.

2008

1. S. N. Chakraborty and L. D. Gelb, "Molecular Simulation of Clathrate Hydrates In Porous Media", AIChE Annual Meeting, Philadelphia, PA.
2. B. C. Barnes and L. D. Gelb, "Structural and Thermodynamic Properties of a Seven-Component on-Lattice Fluid Model", AIChE Annual Meeting, Philadelphia, PA.
3. L. D. Gelb, "Computational Studies of Gas Adsorption In Aerogels: The Effects of Gel Flexibility on Adsorptive Behavior", AIChE Annual Meeting, Philadelphia, PA.
4. D. W. Siderius and L. D. Gelb, "A High-Resolution Lattice Model for Adsorption: Weighted Density Functional Theory for Lattice Fluids and Application to Adsorption In Porous Materials", AIChE Annual Meeting, Philadelphia, PA.
5. B. C. Barnes and L. D. Gelb, "Atomistic Charge-Transfer Potentials for Silica and Aqueous Silicates", AIChE Annual Meeting, Philadelphia, PA.
6. L. D. Gelb, "First Principles Monte Carlo Simulations of Elemental Fluid Phase Equilibria", AIChE Annual Meeting, Philadelphia, PA.
7. L. D. Gelb, "Computational Modeling of Sol-Gel Materials," Truman State University, Kirksville, MO.

8. L. D. Gelb, "First-principles Monte Carlo simulations of fluid phase equilibria at extreme conditions," ACS Fall Meeting, Philadelphia, PA.
9. L. D. Gelb, "Computational studies of adsorption in aerogels: the effects of gel flexibility of adsorptive behavior," American Conference on Theoretical Chemistry, Evanston, IL. (Poster.)
10. S. Chakraborty and L. D. Gelb, "Clathrate Hydrates in Porous Media," American Conference on Theoretical Chemistry, Evanston, IL. (Poster.)
11. B. C. Barnes and L. D. Gelb, "Atomistic Charge-Transfer Potentials for Silicon Dioxide," American Conference on Theoretical Chemistry, Evanston, IL. (Poster.)
12. D. W. Siderius and L. D. Gelb, "Improved lattice models for adsorption: applications to characterization and capillary phenomena," Characterization of Porous Solids (COPS) VIII, Edinburgh, UK.
13. L. D. Gelb, "Computational Modeling of Sol-Gel Materials," Louisiana State University, Baton Rouge, LA.
14. L. D. Gelb, "Computational Modeling of Sol-Gel Materials," The University of Memphis, Memphis, TN.
15. L. D. Gelb, "Applications of lattice gas models to confined fluids: phase equilibria, stochastic reconstructions and adsorption in compliant materials," Advances in the Properties of Confined Fluids: From Superfluids to Oil Reservoirs, Abingdon, UK. (Invited talk.)

2007

1. L. D. Gelb, "Simulating Silica Aerogels With A Coarse-Grained Flexible Model and Langevin Dynamics," AIChE Fall Meeting, Salt Lake City, UT.
2. B. C. Barnes and L. D. Gelb, "Development and Evaluation of Reactive Potentials using Evolutionary Strategies and Molecular Dynamics Simulations" AIChE Fall Meeting, Salt Lake City, UT.
3. B. C. Barnes and L. D. Gelb, "Development and Evaluation of Reactive Potentials using Evolutionary Strategies and Molecular Dynamics Simulations" Midwest Thermodynamics Meeting, Ames, IA.
4. L. D. Gelb, "Coarse-grained Modeling of Sol-gel Materials," Midwest Thermodynamics Meeting, Ames, IA (Invited talk.)

2006

1. L. D. Gelb and R. Salazar, "Three-Dimensional Reconstruction of Mesoporous Materials From Structure Factor and Gas Adsorption Data," AIChE Fall Meeting, San Francisco, CA.
2. L. D. Gelb and T. Carnahan, "*Ab initio* Monte Carlo simulation of fluid phase equilibria at extreme conditions," AIChE Fall Meeting, San Francisco, CA. (Poster.)
3. L. D. Gelb and T. Carnahan, "*Ab initio* Monte Carlo simulation of fluid phase equilibria at extreme conditions," Thermo 2006, Boulder, CO.
4. L. D. Gelb and T. Carnahan, "*Ab initio* Monte Carlo simulation of fluid phase equilibria at extreme conditions," CCCC6, Vancouver, Canada (poster).
5. L. D. Gelb, "Computer simulations of capillary phenomena and the structure of porous materials," University of Missouri, Columbia, MO. (Invited talk.)
6. L. D. Gelb, "Computer simulations of capillary phenomena and the structure of porous materials," University of Kentucky, Lexington, KY. (Invited talk.)

2005

1. L. D. Gelb, "Computer simulations of capillary phenomena and the structure of porous materials," WU (Chemical Engineering). (Invited talk.)

2. L. D. Gelb and R. Salazar, "Three-Dimensional Reconstruction of Mesoporous Materials From Structure Factor and Gas Adsorption Data," AIChE Fall Meeting, Cincinnati, OH.
3. R. Salazar and L. D. Gelb, "Off-lattice Dynamic Monte Carlo Simulations of Aggregation and Gelation," AIChE Fall Meeting, Cincinnati, OH.
4. L. D. Gelb, "Coarse-grained Modeling of Sol-gel Materials," AIChE Fall Meeting, Cincinnati, OH.
5. J. Diao, R. Salazar, K. F. Kelton and L. D. Gelb, "Effect of Diffusion on Precipitate Nucleation and Growth," AIChE Fall Meeting, Cincinnati, OH.
6. L. D. Gelb, "Computer Simulation of Capillary Phenomena and the Structure of Porous Materials," Western Kentucky University, Bowling Green, KY.
7. L. D. Gelb and T. Carnahan, "Monte Carlo simulation of phase equilibria using DFT potentials," 2005 American Conference on Theoretical Chemistry, Los Angeles, CA. (Poster.)
8. J. Diao, L. D. Gelb, R. Salazar, and K. F. Kelton, "Effect of Diffusion on Precipitate Nucleation and Growth," 2005 Midwest Thermodynamics and Statistical Mechanics Conference, Purdue University, West Lafayette, IN.
9. R. Salazar, L. D. Gelb, "Off-lattice Dynamic Monte Carlo simulations of aggregation and gelation," 2005 Midwest Thermodynamics and Statistical Mechanics Conference, Purdue University, West Lafayette, IN.
10. R. Salazar, L. D. Gelb, "Three-dimensional reconstruction of mesoporous materials from structure factor and gas adsorption data," Characterization of Porous Solids 7, Aix-en-Provence, France.
11. L. D. Gelb, "Computational studies of sol-gel processing and capillary phenomena," Department of Chemistry, University of Minnesota, Minneapolis, MN.
12. L. D. Gelb, "Multiscale modeling of sol-gel materials and capillary phenomena," Department of Chemistry, Boston University, Boston, MA.
13. L. D. Gelb, "Multiscale modeling of sol-gel materials and capillary phenomena," Department of Chemistry, Kansas State University, Manhattan, KS.

2004

1. R. Salazar, L. D. Gelb, "Off-lattice Dynamic Monte Carlo simulations of aggregation and gelation," XIV Conference on Nonequilibrium Statistical Mechanics and Nonlinear Physics (MEDYFINOL04) La Serena, Chile.
2. L. D. Gelb, R. Salazar and N. Z. Rao, "Multiscale simulations of capillary phenomena and material structure in sol-gel materials," Symposium on Atomistic Simulation, Queen's University, Belfast, UK. (Invited talk.)
3. L. D. Gelb, R. Salazar and N. Z. Rao, "Molecular scale and coarse-grained modeling of xerogels and aerogels", ACS Midwest Annual Meeting, Manhattan, KS. (Invited talk.)
4. R. Salazar, L. D. Gelb, "Capillary phenomena in porous materials: modeling adsorption using lattice gases in the mean-field and Bethe-Peierls approximations," 28th Int'l Workshop on Condensed Matter Theories, at Washington University in St. Louis. (Invited talk.)
5. L. D. Gelb, R. Salazar and N. Z. Rao, "Multiscale simulations of capillary phenomena and material structure in sol-gel materials," University College, Dublin, Ireland.
6. R. Salazar and L. D. Gelb, "Adsorption in sol-gel materials and porous glasses: molecular simulations and mean-field lattice-gas results," Fundamentals of Adsorption 8, Sedona, AZ.
7. R. Salazar, N. Z. Rao, B. C. Barnes, and L. D. Gelb, "Modeling capillary phenomena in porous glasses and sol-gel materials," Gordon Research Conference on Computational Chemistry, Plymouth, NH. (Poster.)

8. R. Salazar and L. D. Gelb, "Capillary phenomena in sol-gel materials: modeling adsorption using lattice gases in the mean-field and Bethe-Peierls approximations," AIChE Annual Meeting, Austin, TX.
9. L. D. Gelb and T. Carnahan, "Towards Monte Carlo simulations using *ab initio* potentials," AIChE Annual Meeting, Austin, TX.

2003

1. J. J. Glennon and L. D. Gelb "Dynamics of the capillary rise in nanocylinders and structured nanopores," ACS Spring Meeting, New Orleans, LA. (Poster.)
2. N. Z. Rao and L. D. Gelb, "Molecular simulation of porous silica materials," ACS Spring Meeting, New Orleans, LA. (Poster.)
3. N. Z. Rao and L. D. Gelb, "Multiscale modeling of xerogels and aerogels," ACS Spring Meeting, New Orleans, LA.
4. L. D. Gelb and N. Z. Rao, "Multiscale modeling of xerogels and aerogels," CERC-3 Young Chemists' Workshop, Göteborg, Sweden.
5. L. D. Gelb and N. Z. Rao, "Multiscale modeling of xerogels and aerogels," Southeastern Theoretical Chemistry Association (SETCA) Meeting, Clemson, SC. (Invited talk.)
6. B. C. Barnes and L. D. Gelb, "Potential Development for Sol-Gel Modeling," CCP5 Methods in Molecular Simulation Summer School, London, UK. (Poster.)
7. L. D. Gelb and N. Z. Rao, "Monte Carlo simulations using sampling from an approximate potential," AIChE Fall Meeting, San Francisco, CA.
8. L. D. Gelb, N. Z. Rao and R. Salazar, "Adsorption and desorption in aerogels and xerogels," AIChE Fall Meeting, San Francisco, CA.
9. L. D. Gelb, N. Z. Rao and B. C. Barnes, "Reactive potentials for water/silicate systems," AIChE Fall Meeting, San Francisco, CA.
10. L. D. Gelb, "Modeling of aerogels, xerogels and gas adsorption," presentation to Ackerman group, Washington University, St. Louis, MO.

2002

1. L. D. Gelb "Simulations of Gel Drying Using a Coarse-Grained Model," AIChE Fall Meeting, Indianapolis, IN.
2. L. D. Gelb "Capillary Phenomena in Porous Glasses," AIChE Fall Meeting, Indianapolis, IN.
3. L. D. Gelb "Computer simulation as a virtual laboratory: looking at liquids in nanoscale spaces," Central Missouri State University, Warrensburg, MO.
4. L. D. Gelb "Capillary phenomena in porous glasses: a study using molecular simulation," Quantachrome, Inc., Boynton Beach, FL.
5. L. D. Gelb "Capillary phenomena in porous glasses: a study using molecular simulation," Department of Chemistry, Washington University, St. Louis, MO.
6. L. D. Gelb "Capillary condensation in porous glasses: A microscopic view using molecular simulation," CSIT Seminar, FSU, Tallahassee, FL.
7. L. D. Gelb "Capillary phenomena in porous glasses: a study using molecular simulation," MARTECH Colloquium, FSU, Tallahassee, FL.

2001

1. L. D. Gelb, "Capillary Phenomena in Controlled Pore Glasses: Molecular Simulations and The Effects of Pore Connectivity," Hahn-Meitner Institute, Berlin, Germany.
2. L. D. Gelb and Erich A. Müller, "Phase Equilibria Using Temperature Quench Molecular Dynamics," AIChE Fall Meeting, Reno, NV.

3. L. D. Gelb, "The Surface Tension of Lennard-Jones Fluids: Implications for Adsorption Calculations," AIChE Fall Meeting, Reno, NV.
4. L. D. Gelb, "Network Connectivity and Its Effect on Capillary Phenomena," AIChE Fall Meeting, Reno, NV.
5. L. D. Gelb, "Capillary Phenomena in Controlled-Pore Glasses: Molecular Simulations and the Effects of Pore Connectivity," University of Florida Physical Chemistry Colloquium, Gainesville, FL.
6. L. D. Gelb, "Capillary Condensation in Porous Glass: A Microscopic View Using Molecular Simulations," Phase Transitions In Complex Confined Systems (CECAM/ESF), Lyon, France.
7. L. D. Gelb and K. E. Gubbins, "Molecular simulation of capillary phenomena in controlled pore glasses," Fundamentals of Adsorption 7, Nagasaki, Japan.
8. L. D. Gelb, "Computer Simulation as a Virtual Laboratory: Studies of Porous Glass and Capillary Phenomena," Southern University A&M, Baton Rouge, LA.

2000

1. L. D. Gelb, "Simulation Studies of Adsorption in Mesoporous Silica Materials," AIChE Fall Meeting, Los Angeles, CA.
2. L. D. Gelb, "Molecular Simulation of Capillary Phenomena in Porous Glasses," Pennsylvania State University, Physical Chemistry Colloquium, State College, PA.
3. S. F. Gerstenmaier, L. F. Vega, F. J. Blas, L. D. Gelb, and K. E. Gubbins, "Pore Size Distribution Analysis of Model Porous Glasses by Molecular Simulation and Density Functional Theory," AIChE Fall Meeting, Los Angeles, CA.
4. L. D. Gelb, M. E. Suárez and E. A. Müller, "Phase Equilibria of Multicomponent Systems Using Parallel Molecular Dynamics Algorithms," Foundations of Molecular Modeling and Simulation, Keystone, CO.
5. L. D. Gelb and K. E. Gubbins, "Simulations of Capillary Condensation in Porous Glasses," Foundations of Molecular Modeling and Simulation, Keystone, CO.
6. L. D. Gelb and K. E. Gubbins, "Simulations of Capillary Condensation in Porous Glasses," CCP5 Annual General Meeting, University of Surrey, U.K.
7. L. D. Gelb and D. N. Beratan, "Electrostatic Interactions in ATP Synthase: Implications for the Catalytic Mechanism," ACS Spring Meeting, San Francisco, CA.

1999

1. L. D. Gelb and K. E. Gubbins, "Characterization of Controlled Pore Glasses: Molecular Simulations of Adsorption and Capillary Condensation," Characterization of Porous Solids 5, Heidelberg, Germany.
2. M. Sliwinska-Bartkowiak, L. D. Gelb, R. Radhakrishnan and K. E. Gubbins, "Phase transitions in Pores: Molecular Simulations and Experimental Results," ACS Spring Meeting, Anaheim, CA.
3. K. E. Gubbins and L. D. Gelb, "Molecular modeling of Adsorption in Amorphous Nano-Porous Materials," ACS Spring Meeting, Anaheim, CA.

pre-1999

1. L. D. Gelb and K. E. Gubbins, "Adsorption in Porous Glasses: Realistic Models," AIChE Fall Meeting, Miami, FL. 1998
2. L. D. Gelb and K. E. Gubbins, "Thermodynamics of Fluids Confined in Porous Glasses: A Simulation Study," 5th Liblice Conference on the Statistical Mechanics of Liquids, Železná Ruda, Czech Republic. 1998.

3. L. D. Gelb and K. E. Gubbins, "Characterization of Porous Glasses by Adsorption: Models, Simulations, and Data Inversion," Fundamentals of Adsorption 6, Giens, France. 1998.
4. L. D. Gelb, M. Sliwinska-Bartkowiak and K. E. Gubbins, "Liquid-liquid Equilibria in Porous Glasses: Molecular Simulation and Experimental Results," Fundamentals of Adsorption 6, Giens, France. 1998.
5. L. D. Gelb and K. E. Gubbins, "Characterization of Porous Glasses by Simulation: Models, Adsorption Isotherms, and Data Inversion," Royal Society of Chemistry, Autumn Meeting — Structured Fluids, University of Durham, U.K. 1997.
6. L. D. Gelb and K. E. Gubbins, "Binary Liquid Mixtures in Nanoporous Materials: Phase Separation Kinetics, Wetting and Equilibrium Properties from Numerical Simulation," ACS Spring Meeting, San Francisco. 1997.
7. M. Sliwinska-Bartkowiak, L. D. Gelb, S. Sowers and K. E. Gubbins, "Molecular Simulation of Fluids in Pores: Adsorption and Phase Transitions," 14th IUPAC Conference on Chemical Thermodynamics, Osaka, Japan. 1996.
8. L. D. Gelb and K. E. Gubbins, "Phase Equilibria in Porous Materials," International Symposium on Nanopore Fluid Chemistry, Chiba, Japan. 1996.
9. L. D. Gelb and K. E. Gubbins, "Phase Equilibria in Porous Materials," International Workshop on Molecular Simulation and its Application, Keimyung University, Korea. 1996.
10. L. D. Gelb and K. E. Gubbins, "Phase Coexistence and Immiscibility of Liquid Mixtures in Porous Materials," 3rd EPS Liquid Matter Conference University of East Anglia, U.K. 1996.
11. L. D. Gelb and R. M. Lynden-Bell, "Decorated Lattice Models for Surface Phase Transitions," EMLG: Structure and Order in Liquids, Blankenberge, Belgium. 1995.
12. L. D. Gelb and R. M. Lynden-Bell, *(title unavailable)* RSC Autumn Meeting — Simulation of Molecular Materials, University of Sheffield, U.K. 1995.
13. L. D. Gelb and R. M. Lynden-Bell, "Force Oscillations and Liquid Structure in Simulations of an Atomic Force Microscope Tip in a Liquid," European Molecular Liquids Group: Computer Simulations and Experiments, University of Kent, Canterbury. 1993.

Committee assignments and other service activities

Extra-university

1. AIChE/COMSEF Liason Director (2013-2015).
2. AIChE/COMSEF Impact Award Selection Committee (2014), Graduate Student Award judge (2013,2015), Conference Presentation Award Committee (2015).
3. Member, Scientific Committee for *Fundamentals of Adsorption 13* (2013).
4. Member, Scientific Committee for *Fundamentals of Adsorption 10* (2010).
5. ACS national award committee member, 2007-2009.

University of Texas at Dallas

1. Associate Head, Department of Materials Science and Engineering (from 2016)
2. Graduate Director, Department of Materials Science and Engineering (from 2016)
3. UTD University Senator (from 2011)
4. *ad hoc* tenure and promotion committee member (2013 and 2014)
5. Member, UTD Senate Committee on Educational Policy (CEP) (from 2011)
6. Member, UTD University Sustainability Committee (from 2015)

7. MSEN Curriculum Committee (2010; Chair from 2011-2016)
8. MSEN Graduate Recruitment and Admissions Committee (2010-2014)
9. MSEN Graduate Admissions Committee (2014-2016)
10. MSEN Undergraduate Nano Committee (2014-2016)
11. MSEN Personnel Review Committee (2011-2013)
12. MSEN Website Development Committee (2010-2014)
13. Dissertation/Thesis/Advisory Committees: Udayana Ranathunga Jayasekara (Chemistry), Tyson Bartlett (MSEN), Sudarshan Narayan (MSEN), Abraham Vega (MSEN), Tatiana Peixoto (MSEN), Gautam Gaddemane (MSEN), Sadeq Malakooti (ME), Joshua Sisk (Chemistry), Mahesh Bhatt (Chemistry), Amir Nasrabadi (Chemistry), Blake Wilson (Chemistry), Ashley Ellsworth (Chemistry), Jing Yang (MSEN), Bo Fu (MSEN)

Washington University

1. Arts & Sciences Curriculum Implementation Committee, 2009-2010 acad. year.
2. Condensed Matter Theory (Dept. of Physics) search committee, 2003-2004, 2006-2007 and 2008-2009 acad. years.
3. Inorganic Chemistry Faculty Search committee, 2007-2008 acad. year.
4. University Chancellor's Fellowship award committee, 2007-2010.
5. Undergraduate curriculum committee, 2007-2009.
6. Computational Biochemistry (Dept. of Biochemistry) search committee, 2006-2007 acad. year.
7. Arts and Sciences Curriculum Committee, 2005-2006 acad. year.
8. Physical Chemistry Faculty Search committee, 2004-2005 acad. year.
9. University Marshall Scholar endorsement committee, 2003-2010.
10. University mock-interviewer for Rhodes scholar candidates, 2003.
11. Chair, Departmental seminar committee, 2006-2010.
12. Chair, Departmental web-site oversight committee, 2003-2009.
    Redesigned the Departmental website in August and September of 2003. Summer 2005, supervised an undergraduate (J. M. Engle) in transferring the site to a modern content management system.
13. CSPC (Center for Scientific Parallel Computing) Oversight Committee, 2004-2008.
14. Graduate Admissions/Recruitment Committees, 2002-2010.
15. Research Computing Committee, 2003-2010. Also maintained Computational Chemistry facility (16-node system) obtained via CRIF grant, above.
16. Assisted with 2004 graduate brochure revision.
17. Developed and maintained the *Center for Materials Innovation* web-site, 2004-2009.
18. Dissertation committees: D. Zhou (as reader), C. Hogan (Chemical Engineering), A. Vitalis (Computational Biology), B. Olsen (Computational Biology), J. Xiang (Computational Biology), Jeff Anderson (Chemistry), M. Wyczalkowski (Computational Biology).
19. "Materials for Energy Applications" thrust area coordinator, *Center for Materials Innovation*, 2005-2007.

Florida State University

1. Capital Resources and Space Committee, 2001-2002.
2. Laboratory and Computer Facility Committee, 2001-2002.
3. Public Relations Committee, 2000-2002.
4. "Computational Science and Information Technology / Center Of Excellence" faculty search committee, 2001-2002.
5. Departmental representative on CSIT Computational Science Committee, 2001-2002.
6. Departmental representative on Supercomputer Users Group Committee, 2001-2002.
7. Biochemistry Seminar Series Committee, 2001-2002.
8. Organized weekly Physical Chemistry Seminar series for the 2000-2001 and 2001-2002 academic years. Invited approx. ten speakers from outside the University during this period, and six to eight from other departments at FSU.
9. Maintainer of the Physical Chemistry Division and Chemical Physics Program web-sites, 1999-2002.
10. Installed and maintained a 9-node workstation cluster as a Department-wide computational chemistry resource, 2001-2002.
11. Member of four graduate thesis committees and one undergraduate Honors' thesis committee.

Review work (1999-2015)

Papers: 113, for:

J. Phys. Chem. B, C	Langmuir	Mol. Phys.
Chem. Phys. Letts.	J. Chem. Phys.	Mol. Sim.
Adsorption	J. Am. Chem. Soc.	Phys. Rev. E
Phys. Rev. Letts.	J. Comp. Chem.	Chem. Mat.
Chem. Eng. Comm.	J. Chem. Theor. Comp.	Comp. Mat. Sci.
Env. Prog.	Microp. and Mesop. Mater.	Fluid Phase Eq.
Int. J. Hydrogen Energy	SIAM J. Sci. Comp.	Theor. Chem. Accts.
Model. Sim. Mat. Sci. Eng.	Ind. & Eng. Chem. Res.	AIChE J.
Conference proceedings volumes.		

Proposals: 42, for NSF, DOE, CRDF, ACS (PRF), Research Corp, LA Board of Regents, NSERC (Canada), NASA/EPSCoR, Netherlands Organisation for Scientific Research (NWO).

Panel reviews: 1, for NSF (CBET Division).

Books: 2, for *Springer* and *Acad. Press*.

Tenure evaluations: 4.

Conference sessions chaired/organized

1. Effects of Confinement on Molecular Properties (chair), AIChE Annual Meeting, San Francisco, CA. 2016.
2. Effects of Confinement on Molecular Properties (chair), AIChE Annual Meeting, Salt Lake City, UT. 2015.
3. Effects of Confinement on Molecular Properties (chair), AIChE Annual Meeting, Atlanta, GA. 2014.

4. Effects of Confinement on Molecular Properties (co-chair),
   AIChE Annual Meeting, San Francisco, CA. 2013.
5. First-Principles Simulation of Condensed Phases (co-chair),
   AIChE Annual Meeting, Salt Lake City, UT. 2011.
6. First-Principles Simulation of Condensed Phases (co-chair),
   AIChE Annual Meeting, Salt Lake City, UT. 2010.
7. First-Principles Simulation of Condensed Phases: Bulk (chair),
   First-Principles Simulation of Condensed Phases: Surfaces (chair),
   AIChE Annual Meeting, Nashville, TN. 2009.
8. First-Principles Simulations (chair, Sessions I and II),
   AIChE Annual Meeting, Philadelphia, PA. 2008.
9. First-Principles Simulations of Condensed Phases (chair),
   AIChE Annual Meeting, Salt Lake City, UT. 2007.
10. Keith Gubbins 70th Birthday Celebration II (chair),
    AIChE Annual Meeting, Salt Lake City, UT. 2007.
11. Hydrogen storage, (vice-chair),
    AIChE Annual Meeting, San Francisco, CA. 2006.
12. Best practices in Electronic Structure Calculations (vice-chair),
    AIChE Annual Meeting, San Francisco, CA. 2006.
13. Frontiers in Nanoscience and Technology (chair),
    AIChE Annual Meeting, Austin, TX. 2004.
14. Recent Advances in Molecular Simulation: Monte Carlo Methods (co-chair),
    AIChE Annual Meeting, Austin, TX. 2004.
15. Frontiers in Nanoscience and Technology (co-chair),
    AIChE Annual Meeting, San Francisco, CA. 2003.
16. Molecular Modeling and Design of Nanostructured Adsorbents (chair),
    AIChE Annual Meeting, Indianapolis, IN. 2002.
17. Poster Session - Fundamentals of Adsorption and Ion Exchange (co-chair),
    AIChE Annual Meeting, Reno, NV. 2001.
18. Physical Chemistry Session (chair), Florida ACS Annual Meeting, Orlando, FL. 2001.
19. Physical Chemistry Session (chair), Florida ACS Annual Meeting, Orlando, FL. 2000.

Research associates and students supervised

Postdoctoral associates

1. Carlos Ferreiro, 11/2011 — 11/2013.
2. Dongsheng Zhang, 10/2011 — 2/2014.
3. Tammy Milillo, 3/2011 — 8/2013.
4. Subhashis Biswas: 2/2009 — 5/2009.
5. Daniel Siderius: 9/2007 — 12/2009.
6. Somendra Chakraborty: 9/2007 — 5/2011.
7. Pablo Nigra: 2/2007 — 6/2008.
8. Jiankuai Diao: 9/2004 — 8/2005.
9. Rafael Salazar: 8/2003 — 8/2006.
10. Kamala Raghavan: 10/2003 — 9/2005.
11. Niny Z. Rao: 8/2002 - 7/2003.

Graduate students

1. Amir Nasrabadi: 2015-present; Ph.D. student.
2. Roger Larson: 2011-2013; MS student.
3. Yue Wang: 9/2010—1/2013; graduated with MS.
4. Brian Barnes: 8/2003—9/2010, Washington University. Ph.D.
5. Alicia Hopkins (FSU): Fall 2001 — 7/2002; could not move to St. Louis and left group.
6. Ryan Oyler (FSU): Fall 2001 — 7/2002 ; could not move to St. Louis and left group.
7. Heaya Summy (FSU): Fall 1999 — 7/2001; left program after two years.

Technicians

1. Brian Barnes: 10/2002-8/2003; joined graduate program as my student.
2. John Glennon: 10/2002-2/2003; joined graduate program in R. A. Loomis' group.

Undergraduates

1. Harrison Lee, Summer 2016 (REU student.)
2. Elaine Rosenthal, Summer 2016 (REU student.)
3. Anh Do, Summer 2015 (REU student.)
4. Layla Bakhtiari, Summer 2014 (REU student.)
5. Kate Nguyen, Summer 2013 (REU student.)
6. Sara Cheng, Summer 2012 (REU student.)
7. Amber Khan, Summer 2011 — 2012.
8. Brandyn Lee, Fall 2011.
9. Chidinma Chima-Okereke, Summer 2004 through Summer 2005, now at UCLA Medical School.
10. Ted Carnahan, Summer 2004 (WU).
11. R. Preston Clark, January-August 2003 (WU).
12. Deena Westbrook, Summer and Fall 2001 (FSU).
13. Over three years at Florida State University, I had eight freshman and sophomore undergraduates work for me in some capacity. Most of them came through the "honors general chemistry laboratory" sequence, where honors-track freshman would do an eight-week project in one of the research labs. I kept several of these on for an additional semester.

Professional societies

American Chemical Society
American Institute of Chemical Engineers

Other experience

Web design and publishing (1994—)
Developed WU *Center for Materials Innovation* website. Completely redesigned and rewrote the WU Chemistry Department web-site (2003–2009). Maintenance and additions to our group web-site.

Computer systems and administration (1990—)
Installation and administration experience with SGI, DEC Alpha (Digital Unix, Linux), PC (Windows, Linux), Apple, parallel clustering (ROCKS and OSCAR).

NSF Undergraduate Research Fellowship (1991)
Application of Path Integral Monte Carlo and PI Hybrid Monte Carlo techniques to dispersion oscillators, with Professor B. J. Berne at Columbia University. Continued this research in 1992.

Lab Assistant (1990)
Advanced Magnetics, Inc., Boston, MA. Lab techniques: organic synthesis techniques, column chromatography, use of magnetometry, flame ionization spectroscopy, and particle size counters.

Lab Assistant (1989)
Seragen Inc., Boston, MA. Lab techniques: quality control techniques in biotechnology; gel chromatography and BSA protein assay preparation.