

Lev D. Gelb

Curriculum Vitae

Address

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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 Chemistry,
Washington University in St. Louis, 2006—present.
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

- First-principles molecular simulations
- New methods for free energy and phase equilibria calculations
- Potential model development
- Nanostructured and amorphous porous materials
- Capillary phenomena and confined phase equilibria
- High-performance computing
- Liquid structure theory
- Nucleation
- Multiscale modeling

Teaching experience

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.

“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, and kinetics. Washington University, Spring, 2003, Spring 2004, Spring 2008.

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. Florida State University, 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. Florida State University, Fall 1999, Fall 2000.

“Advanced Statistical Mechanics”, a graduate course in modern statistical mechanics with a focus on molecular simulation. Florida State University, 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

2009

42. “Thermodynamic and structural properties of finely-discretized on-lattice hard-sphere fluids: virial coefficients, free energies and direct correlation functions,” D. S. Siderius and L. D. Gelb, to appear in *J. Chem. Phys.*
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. “Phase change materials for data storage” \$25,000, Co-PI; with K. F. Kelton (WU Physics). 2008-2009.
2. “First-principles Monte Carlo simulations of fluid phase equilibria at extreme conditions”, National Science Foundation (#CHE-0718861), \$381,806, 2007-2009.
3. “DURIP: Acquisition of a computer system for first-principles simulations of molecular solids”, Army Research Office (# W911NF-07-1-0253), \$157,655, 2007.
4. “Collaborative Research: Cyberinfrastructure for Phase-Space Mapping – Free Energies, Phase Equilibria and Transition Paths”, National Science Foundation (#CHE-0626008), \$615,000. 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). 2006-2010.
5. “Three-dimensional reconstruction of mesoporous materials from gas adsorption and structure factor data”, ACS Petroleum Research Fund (#44674-AC10) \$80,000, 2006-2008.
6. “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.)

PENDING PROPOSALS

1. “CDI-Type I: Cyber-Enabled Chemical Imaging: From Terascale Data Colledge to Chemical Knowledge,” full proposal submitted 5/09 to NSF CDI program, PI: A. V. Walker (University of Texas at Dallas), Co-PI: L. D. Gelb. (\$131,669 subcontract.)
2. “Phase change materials for data storage” \$32,000, Co-PI; with K. F. Kelton (WU Physics), renewal proposal.
3. “High-Resolution Chemical Image Reconstruction Methods for Mass Spectrometry and Other Surface Analysis Techniques,” submitted 07/09 to NIST Recovery Act Measurement Science and Engineering Research Grants Program, PI: A. V. Walker (University of Texas at Dallas), Co-PI: L. D. Gelb. (\$661,437.)

EXPIRED AWARDS AND CONTRACTS

1. “Multi-Scale Modeling of Sol-Gel Materials”, National Science Foundation CAREER Award \$433,900, 2002-2006.
2. “Nucleation Control”, WU Center for Materials Innovation, \$15,000 collaborative project with K. F. Kelton (PI) and others, 2005. (Total award: \$60,000.)
3. “Materials for Hydrogen Storage”, WU Center for Materials Innovation, \$11,500, PI, collaborative project, 2005.
4. “Parallel molecular simulations of nano-scale bubble formation and collapse dynamics”, Research Corporation (Research Innovation Award) \$34,000, for 2001-2002.
5. “Computational Modeling of Nanoporous Silica Xerogels”, First-year Assistant Professor Award of \$10,000, from the FSU Council on Research and Creativity. 2000.
6. “Generation of computer graphics of silica aerogels,” Cabot Corporation, 2/2003, \$8,000.
7. “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).

OTHER AWARDS

The project “First-principles Monte Carlo simulations of fluid phase equilibria at extreme conditions” is supported by an MRAC allocation from the NSF TeraGrid, of approximately 950,000 processor core-hours in 2009. Since 2003 we have had continuous grants of computer resources via TeraGrid.

Conference Presentations and Seminars

2009

1. 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 Nanoporous 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

WASHINGTON UNIVERSITY

1. Condensed Matter Theory (Dept. of Physics) search committee, 2003-2004, 2006-2007 and 2008-2009 acad. years.
2. ACS national award committee member, 2007-present.
3. Inorganic Chemistry Faculty Search committee, 2007-2008 acad. year.
4. University Chancellor's Fellowship award committee, 2007-present.
5. Undergraduate curriculum committee, 2007-present.
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-present.
10. University mock-interviewer for Rhodes scholar candidates, 2003-present.
11. Chair, Departmental seminar committee, 2006-present.
12. Chair, Departmental web-site oversight committee, 2003-2009.
13. CSPC (Center for Scientific Parallel Computing) Oversight Committee, 2004-2008.
14. Graduate Admissions/Recruitment Committees, 2002-present.
15. Research Computing Committee, 2003-present. Currently Chair; also maintain Computational Chemistry facility (16-node system) obtained via CRIF grant, above.
16. Assisted with 2004 graduate brochure revision.
17. Redeveloped 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.
18. Developed and maintained the *Center for Materials Innovation* web-site, 2004-2009.
19. Dissertation committees: D. Zhou (as reader), C. Hogan (Chemical Engineering), A. Vitalis (Computational Biology), Brett Olsen (Computational Biology), Justin Xiang (Computational Biology), Jeff Anderson (Chemistry).
20. "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 (1999-2009)

Papers: 84, 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. |
| Conference proceedings volumes. | | |

Proposals: 29, for NSF, DOE, CRDF, ACS (PRF), Research Corp, LA Board of Regents, NSERC (Canada), NASA/EPSCoR.

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

Books: 1, for *Springer*.

CONFERENCE SESSIONS CHAIRED/ORGANIZED

1. First-Principles Simulations (Chair, Sessions I and II), AIChE Annual Meeting, Philadelphia, PA.
2. First-Principles Simulations of Condensed Phases (chair), AIChE Annual Meeting, Salt Lake City, UT 2007.
3. Keith Gubbins 70th Birthday Celebration II (chair), AIChE Annual Meeting, Salt Lake City, UT 2007.
4. Hydrogen storage, (vice-chair), AIChE Annual Meeting, San Francisco, CA 2006.
5. Best practices in Electronic Structure Calculations (vice-chair), AIChE Annual Meeting, San Francisco, CA 2006.
6. Frontiers in Nanoscience and Technology (chair), AIChE Annual Meeting, Austin, TX. 2004.
7. Recent Advances in Molecular Simulation: Monte Carlo Methods (co-chair), AIChE Annual Meeting, Austin, TX. 2004.
8. Frontiers in Nanoscience and Technology (co-chair), AIChE Annual Meeting, San Francisco, CA. 2003.
9. Molecular Modeling and Design of Nanostructured Adsorbents (chair), AIChE Annual Meeting, Indianapolis, IN. 2002.
10. Poster Session - Fundamentals of Adsorption and Ion Exchange (co-chair), AIChE Annual Meeting, Reno, NV. 2001.
11. Physical Chemistry Session (chair), Florida ACS Annual Meeting, Orlando, FL. 2001.
12. Physical Chemistry Session (chair), Florida ACS Annual Meeting, Orlando, FL. 2000.

Research Associates and Students Supervised

POSTDOCTORAL ASSOCIATES

1. Subhashis Biswas: 2/2009 — present.
2. Daniel Siderius: 9/2007 — present.
3. Somendra Chakraborty: 9/2007 — present.
4. Pablo Nigra: 2/2007 — 6/2008.
5. Jiankuai Diao: 9/2004 — 8/2005.
6. Rafael Salazar: 8/2003 — 8/2006.
7. Kamala Raghavan: 10/2003 — 9/2005.
8. Niny Z. Rao: 8/2002 - 7/2003.

GRADUATE STUDENTS

1. Brian Barnes: 8/2003—present, Washington University. Ph.D. candidate.
2. Alicia Hopkins (FSU): Fall 2001 — 7/2002; could not move to St. Louis and left group.
3. Ryan Oyler (FSU): Fall 2001 — 7/2002 ; could not move to St. Louis and left group.
4. 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, now in R. A. Loomis' group.

UNDERGRADUATES

1. Chidinma Chima-Okereke - Summer 2004 through Summer 2005, now at UCLA Medical School.
2. Ted Carnahan - Summer 2004 (WU).
3. R. Preston Clark - January-August 2003 (WU).
4. Deena Westbrook - Summer and Fall 2001 (FSU).
5. 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

Skills

COMPUTATIONAL METHODS (1991—)

Molecular dynamics and Monte Carlo codes, quantum chemistry, 3D visualization techniques, computer animation techniques, digital video production, reaction kinetics modeling, numerical mathematics techniques, curve fitting, programming of vector processing machines, SIMD and MIMD parallel codes, Fortran, some C, some C++, MPI, Java, Python.

COMPUTER SYSTEMS AND ADMINISTRATION (1990—)

Used in research: IBM SP2, IBM SP3, SGI CRAY T3D and T3E, DEC Alpha (Digital Unix, Linux), CONVEX C2, AMT (DAP-500), Sun, Unix, PC (Windows, Linux), Macintosh.

Administration experience with: SGI, DEC Alpha (Digital Unix, Linux), PC (Windows, Linux), Macintosh, parallel clustering.

OTHER EXPERIENCE

Web design and publishing

Developed WU *Center for Materials Innovation* website, www.cmi.wustl.edu. Completely redesigned and rewrote the WU Chemistry Department web-site www.chemistry.wustl.edu (2003); maintenance and additions to our group web-site (1999-current).

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.