Shekhar Garde

Dean of Engineering
Elaine S. and Jack S. Parker Endowed Professor
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RESEARCH

- Fundamental understanding of the role of water in biological self-assembly and interactions at the molecular level using state-of-the-art statistical mechanical theory, modeling, and simulations.
- Hydrophobic hydration and interactions; solvation of ions, osmolytes, and complex bio and nano interfaces; water-mediated interactions and assembly in bulk and interfacial environments; proteins under pressure; development of molecular theory, simulation tools, and coarse-graining methods.

EDUCATION

1988 – 1992	B. Chem. Eng., Chemical Engineering, University of Bombay, 1992
1992 – 1997	Ph. D., Chemical Engineering, University of Delaware, 1997

EXPERIENCE/APPOINTMENTS

2014 – present	Dean, School of Engineering, Rensselaer Polytechnic Institute
2007 – 2014	Head of the Department of Chemical and Biological Engineering (reappointed for a second term in 2012)
2006 –	Full Professor and Elaine and Jack S. Parker Chair in Engineering Chemical and Biological Eng., Rensselaer Polytechnic Institute, Troy, NY
2004 – 2006	Associate Professor Chemical and Biological Eng., Rensselaer Polytechnic Institute, Troy, NY
1999 – 2004	Assistant Professor Chemical Engineering, Rensselaer Polytechnic Institute, Troy, NY.
1997 – 1999	Directors Postdoctoral Fellow T-10 Theoretical Biology and Biophysics Group, Los Alamos Natl. Lab., NM.

HONORS & AWARDS

- More than 130 invited lectures at Universities, Industry, and National/International Conferences, including several Keynote Lectures.
- 2014 *Guest Editor*, Special Issue of the Materials Research Society Bulletin on Water at functional interfaces (with Mark Schlossman).
- 2014 Elected *fellow of American Institute of Medical and Biological Engineering* (AIMBE).
- 2013 *Best of Web Award* by Center for Digital Education to the Nanospace Project (Garde = co-PI)
- 2011 *Robert W. Vaughan Lecturer*, Chemical Engineering, California Institute of Technology.
- 2011 *V. V. Mariwala Award Lecturer*, Institute of Chemical Technology, Mumbai, India.
- 2011 Alkyl Amines Padmabhushan B. D. Tilak *Chemcon Distinguished Speaker Award*, Indian Institute of Chemical Engineers.
- 2011 *Explore~Imagine~Discover Award* by the Children's Museum of Science and Technology, in the Capital District, NY.
- 2009-present, Member of the Advisory Council, Chemical Engineering at US Military Academy, West Point, NY; 2009-present.
- 2007 *Outstanding Team Award*, for the Molecularium PI team given by the School of Engineering, Rensselaer Polytechnic Institute.

- Co-executive Producer and the Director of Simulations for the Molecularium^{TM} project (see www.molecularium.com). The first Molecularium movie *Riding Snowflakes* received the Domefest-2005 award in July 2005. A 2D and 3D IMAX film, *Molecules to the Max* was released nationwide in 2010. The next platform, Nanospace, a web-based gaming portal was released in late 2012.
- 2004 *Rensselaer Early Career Award*, Rensselaer Polytechnic Institute, for outstanding achievements (by junior faculty) in research and education.
- 2003 *School of Engineering Excellence in Research Award*, Rensselaer Polytechnic Institute.
- 2001 *CAREER, National Science Foundation*'s Faculty Early Career Award.
- 2001 Inducted into Sigma-Xi @Rensselaer.
- 1997-99 *Director's Postdoctoral Fellowship* by the Los Alamos National Laboratory.

PUBLICATIONS [total = 85, citations ~5800, h-index = 39 (per Google Scholar)]

86. S. Parimal, S. M. Cramer, and S. Garde, "Application of a spherical harmonics expansion approach for calculating ligand density distributions around proteins", Phys. Chem. B (Accepted, to be **Featured on the Cover**) (2014)
85. V. Venkateshwaran, S. Vembanur, and S. Garde, "On the enhancement of water-mediated ion-ion interactions at the water vapor-liquid interface", Proc. Natl. Acad. Sci. USA, 111 (24), 8729-8734 (2014).
84. S. Vembanur, V. Venkateshwaran, and S. Garde, "Structure and dynamics of single hydrophobic/ionic heteropolymers at the vapor-liquid interface of water", Langmuir, 30 (16), 4654–4661 (2014).
83. A. J. Patel and S. Garde, "An Efficient Method to Characterize the Context-Dependent Hydrophobicity of Proteins", J. Phys. Chem. B, 118 (6), 1564-1573 (2014). **Featured on the Cover.**
82. S. Vembanur, A. J. Patel, S. Sarupria, and S. Garde, "On the thermodynamics and kinetics of hydrophobic interactions at interfaces", J. Phys. Chem. B, 117 (35), 10261–10270 (2013).
81. A. Fiore, V. Venkateshwaran, and S. Garde, "Trimethylamine N-Oxide (TMAO) and tert-Butyl Alcohol (TBA) at Hydrophobic Interfaces: Insights from Molecular Dynamics Simulations", Langmuir, 29(25), 8017-8024 (2013).
80. A. J. Patel, P. Varilly, S. N. Jamadagni, D. Chandler, and S. Garde, "Sitting on the edge: How biomolecules use hydrophobicity to tune their interactions and function", J. Phys. Chem. B., 116, 2498-2503 (2012).
79. H. Acharya, N. J. Mozdzierz, P. Keblinski, and S. Garde, "How chemistry, nanoscale roughness, and the direction of heat flow affect thermal conductance of solid-water interfaces", Ind. & Eng. Chem. Res., 51, 1767-1773 (2012).
78. S. Garde and A. J. Patel, "Unraveling the hydrophobic effect, one molecule at a time", Proc. Natl. Acad. Sci. USA, 108, 16491-16492 (2011).
77. A. Freed, S. Garde, and S. M. Cramer, "Molecular simulations of multimodal ligand-protein binding: elucidation of binding sites and correlation with experiments", J. Phys. Chem. B, **115,** 13320-13327 (2011) [**on the Cover of Nov 17rd issue].**
76. A. J. Patel, P. Varilly, S. N. Jamadagni, H. Acharya, S. Garde, and D. Chandler, "Extended surfaces modulate hydrophobic interactions of neighboring solutes", Proc. Natl. Acad. Sci., 108, 17678-17683 (2011).
75. A. J. Patel, P. Varilly, D. Chandler, and S. Garde, "Quantifying density fluctuations in volumes of all shapes and sizes using indirect umbrella sampling", J. Stat. Phys., **145**(2), 265-275 (2011).
74. S. N. Jamadagni, R. Godawat, and S. Garde, "Hydrophobicity of proteins and interfaces: Insights from density fluctuations", Annual Reviews of Chemical and Biomolecular Engineering, 2, 147-171 (2011).
73. *Non-peer-reviewed* Editorial: S. Garde, A. Nigam, and K.D.P. Nigam, "Homage/Dedication of the issue to Prof. E. Bruce Nauman (1937-2009)", Chemical Engineering and Processing, 49, 633-334 (2010).

72. S. N. Jamadagni, C. Bosoy, and S. Garde, “Designing heteropolymer to fold into unique structures *via* water-mediated interactions”, J. Phys. Chem. B., 114, 13282-13288 (2010).
71. ON THE COVER**:** A. Kalra, S. Garde, and G. Hummer, “Lubrication by molecularly thin water films confined between nanostructured membranes”, European Physical Journal – Special Topics, in press, 189, 147-154 (2010).
70. G. Anand, S. N. Jamadagni, S. Garde, and G. Belfort, "Self assembly of TMAO at hydrophobic interfaces and its effect on protein adsorption: Insights from experiments and simulations", Langmuir, 26, 9695-9702 (2010).
69. H. Acharya, S. Vembanur, S. N. Jamadagni and S. Garde, "Mapping hydrophobicity at the nanoscale: Applications to heterogeneous surfaces and proteins", Faraday Disc., 146, 353-365 (2010).
68. S. Sarupria, T. Ghosh, A. E. Garcia, and S. Garde, "Studying Pressure Denaturation of a Protein by Molecular Dynamics Simulations", Proteins: Struct Funct Bioinform, 78, 1641-1651 (2010).
67. R. Godawat, S. N. Jamadagni, and S. Garde, "Unfolding of hydrophobic polymers in guanidinium chloride solutions", J. Phys. Chem. B, 114, 2246-2254 (2010).
66. R. H. Coridan, N. W. Schmidt, G. H. Lai, R. Godawat, M. Krisch, S. Garde, P. Abbamonte, and G. C. L. Wong, "Hydration dynamics at femtosecond timescales and Angstrom lengthscales from inelastic x-ray scattering", Phys. Rev. Lett., 103, 237402 (2009).
65. C. H. Chen, S. Malkova, F. Long, S. Garde, W. Cho, and M. L. Schlossman, "Configuration of PKCα-C2 Domains Bound to SOPC:SOPS Lipid Monolayers", Biophys. J., 97, 2794-2802 (2009).
64. M. V. Athawale, S. N. Jamadagni, and S. Garde, "How hydrophobic hydration responds to solute size and attractions: Theory and simulations", J. Chem. Phys., 131, 115102 (2009).
63. C. J. Fennell, A. Bizjak, V. Vlachy, K. Dill, S. Sarupria, S. Rajamani, and S. Garde, "Ion pairing in molecular simulations of aqueous alkali halide solutions (vol 113, pg 6782, 2009)", J. Phys. Chem. B., 113, 14837-14838 (2009).
62. R. Godawat, S. N. Jamadagni, and S. Garde, "Characterizing hydrophobicity of interfaces using cavity formation, solute binding, and water correlations", Proc. Natl. Acad. Sci. USA, part of the special issue on liquids and structural glasses, 106 (36) 15119 - 15124 (2009).
61. S. Sarupria, and S. Garde, "Quantifying water density fluctuations and compressibility of hydration shells of hydrophobic solutes and proteins", Phys. Rev. Lett., 103, 037803 (2009).
60. ON THE COVER: S. N. Jamadagni, R. Godawat, and S. Garde, "How Surface Wettability Affects Binding, Folding, and Dynamics of Hydrophobic Polymers at Interfaces, Langmuir, 25, 13092-13099 (2009).
59. N. Shenogina, R. Godawat, P. Keblinski, and S. Garde, "How Wetting and Adhesion Affect Thermal Conductance of a Range of Hydrophobic to Hydrophilic Aqueous Interfaces", Phys. Rev. Lett., 102, 156101 (2009).
58. ON THE COVER: S. N. Jamadagni, R. Godawat, J. S. Dordick, and S. Garde, "How Interfaces Affect Hydrophobically Driven Polymer Folding", Part of the special section "Aqueous Solutions and Their Interfaces", J. Phys. Chem. B, 113(13), 4093-4101 (2009).
57. FEATURED ARTICLE: C. J. Morrison, R. Godawat, S. A. McCallum, S. Garde, and S. M. Cramer, "Mechanistic studies of displacer-protein binding in chemically selective displacement systems using NMR and MD simulations", Biotechnology and Bioengineering, 102(5), 1428-1437 (2009).
56. N. Shenogina, P. Keblinski, and S. Garde, “Strong frequency dependence of dynamical coupling between protein and water”, J. Chem. Phys., 129, 155105 (2008).
55. G. Goel, M. V. Athawale, S. Garde, and T. M. Truskett, “Attractions, water structure, and thermodynamics of hydrophobic collapse”, 112, 13193-13196 (2008).
54. R. Godawat, S. Jamadagni, J. R. Errington, and S. Garde, “Structure, stability, and rupture of free and supported liquid films and assemblies in molecular simulations”, Ind. Eng. Chem. Res., 47, 3582-3590 (2008).
53. M. V. Athavale, S. Sarupria, and S. Garde, “Enthalpy-entropy contributions to salt and osmolyte effects on hydrophobic hydration and interactions”, 112, 5661-5670 (2008).

52. J.C. Rasaiah, S. Garde, and G. Hummer, “Water in Nonpolar Confinement: From Nanotubes to Proteins and Beyond”, Annual Reviews in Physical Chemistry, 59, 713-740 (2008).
51. L. Yang and S. Garde, “Modeling the selective partitioning of cations into negatively charged nanopores”, J. Chem. Phys., 126, 084706 (2007).
50. M. V. Athawale, G. Goel, T. M. Truskett, and S. Garde, “Effects of Lengthscales and attractive interactions on the collapse of hydrophobic polymers in water”, Proc. Natl. Acad. Sci., 104, 733-738 (2007).
49. P. Shemella, B. Pereira, P. Van-Roey, G. Belfort, S. Garde, and S. Nayak, "Mechanism for intein C-terminal cleavage: A proposal from quantum mechanical calculations", Biophys J., 92, 847-853 (2007).
48. B. Pereira, S. Jain, S, Sarupria, and S. Garde, "Pressure dependence of compressibility of a micelle and a protein: Insights from cavity formation analysis", Molecular Physics, 105, 189-199 (2007).
47. A.M. Tikhonov, H. Patel, S. Garde, and M. L. Schlossman, “Tail ordering due to head group hydrogen bonding interactions in surfactant monolayers at water-oil interface”, J. Phys. Chem. B, 110, 19093-19096 (2006).
46. S. Jain, S. Garde, and S. K. Kumar, “Do inverse Monte Carlo algorithms yield thermodynamically consistent interaction potentials”, Ind. & Eng. Chem. Res., 45, 5614-5618 (2006).
45. B. Pereira, S. Jain, and S. Garde, "Quantifying the protein core flexibility through analysis of cavity formation", J. Chem. Phys., 124, 074704 (2006).
44. H. Patel, S. Garde, and E. B. Nauman, “Detailed molecular simulations to investigate multicomponent diffusion models”, AIChE Journal, 52, 1304-1307 (2006).
43. H. Liu, S. Garde, and S. K. Kumar, “Direct determination of phase behavior of square-well fluids”, J. Chem. Phys., 123, 174505 (2005).
42. H. Patel, S. Garde, and P. Keblinski, “Thermal resistence of nanoscopic liquid-liquid interfaces: Dependence on chemistry and molecular architecture”, Nanoletters, 5, 2225-2231 (2005).
41. S. Rajamani, T. M. Truskett, and S. Garde, “Hydrophobic hydration from small to large lengthscales: Understanding and manipulating the crossover”, Proc. Natl. Acad. Sci. USA, 102, 9475-9480 (2005).
40. S. Garde, L. S. Schadler, and R. W. Siegel, "Molecularium explores the world of materials", Materials Research Society Bulletin, 30, 132-133 (2005) (Not peer reviewed).
39. M. V. Athawale, J. S. Dordick, and S. Garde, "Osmolyte trimethylamine-N-oxide (TMAO) does not affect the strength of hydrophobic interactions: Origin of osmolyte compatibility", Biophysical Journal, 89, 858-866 (2005).
38. H. Ashbaugh, H. Patel, S. K. Kumar, and S. Garde, “Mesoscale model of polymer melt structure: Self-consistent mapping of molecular correlations to coarse-grained potentials”, Journal of Chemical Physics, 112, 104908-1-5 (2005).
37. T. Ghosh, A. Kalra, and S. Garde, "On the salt-induced stabilization of pair and many-body hydrophobic interactions", Journal of Physical Chemistry B, 109, 642-651 (2005).
36. S. Rajamani, T. Ghosh, and S. Garde, “Size dependent ion hydration, its asymmetry, and convergence to macroscopic behavior”, Journal of Chemical Physics, 120, 4457-4466 (2004).
35. F. Xia, D. Nagrath, S. Garde, and S. M. Cramer, "Evaluation of selectivity changes in HIC systems using a preferential interaction based analysis", J. Chromatography, 87 (3), 354-363 (2004).
34. A. Kalra, G. Hummer, and S. Garde, “Selective partitioning and transport of methanes in hydrated carbon nanotubes”, Journal of Physical Chemistry B, 108, 544-549 (2004).
33. L. Yang, J. S. Dordick, and S. Garde, “Hydration of enzyme is consistent with its activity in non-aqueous solutions”, Biophysical Journal, 87, 812-821 (2004).
32. H. Patel, E. B. Nauman, and S. Garde, “Molecular structure and hydrophobic solvation thermodynamics at an octane-water interface”, Journal of Chemical Physics, 119, 9199-9206 (2003).
31. T. Ghosh, S. Garde, and A. E. Garcia, “Role of backbone hydration and salt bridge formation in stability of alpha-helix in solution”, Biophysical Journal, 85, 3187-3193 (2003).

30. A. Kalra, S. Garde, and G. Hummer, "Osmotic water transport through carbon nanotube membranes", Proc. Natl. Acad. Sci. USA, 100, 10175-10180 (2003). (An invited commentary on this article was also published in the same issue of PNAS)
29. C. Bystroff and S. Garde, "Helix Propensities of Short Peptides: Molecular dynamics versus bioinformatics", Proteins: Structure, Function, and Genetics, 50, 552-562 (2003).
28. T. Ghosh, A. E. Garcia, and S. Garde, "Water-mediated three-Particle interactions between hydrophobic solutes: size, salt, and pressure dependences", Journal of Physical Chemistry B., 107, 612-617 (2003).
27. T. Ghosh, A. E. Garcia, and S. Garde, "Enthalpy and entropy contributions to the pressure dependence of hydrophobic interactions", Journal of Chemical Physics, 116, 2480-2486 (2002).
26. S. Garde, L. Yang, J. S. Dordick, and M. E. Paulaitis, "Molecular dynamics simulations of C_8E_5 micelles in explicit water: structure and hydrophobic solvation thermodynamics", Molecular Physics, 100, 2299-2306 (2002).
25. S. Garde, G. Hummer, and R. Khare, "Effect of chain length on microscopic density fluctuations and solvation in polymeric fluids", ACS Symposium on Polymeric Materials: Science and Engineering, 85, 449 (2001).
24. T. Ghosh, A. E. Garcia, and S. Garde, "Molecular dynamics simulations of pressure effects on hydrophobic interactions", Journal of American Chemical Society, 123, 10997-11003 (2001).
23. A. Kalra, N. Tugcu, S. Cramer, and S. Garde, "Salting-in and salting-out of hydrophobic solutes in aqueous salt solutions", Journal of Physical Chemistry B., 105, 6380-6386 (2001).
22. S. Garde and H. S. Ashbaugh, "Temperature dependence of hydrophobic hydration and entropy convergence in an isotropic model of water", Journal of Chemical Physics, 115, 977-982 (2001).
21. G. Hummer, A. E. Garcia, and S. Garde, "Helix nucleation kinetics using molecular simulations in explicit solvent", Proteins: Structure Function & Genetics, 42, 77-84 (2001).
20. G. Hummer, A. E. Garcia, and S. Garde, "Conformational diffusion and helix formation kinetics", Physical Review Letters, 85, 2637-2640 (2000).
19. G. Hummer, S. Garde, A. E. Garcia, and L. R. Pratt, "New perspectives on hydrophobic effects", Chemical Physics, 258, 349-370 (2000).
18. S. Garde, R. Khare, and G. Hummer, "Free energy of cavity formation in polymers", Journal of Chemical Physics, 112, 1574-1578 (2000).
17. S. Garde, G. Hummer, and M. E. Paulaitis, "Hydration of tetramethylammonium ion: from water structure to the free energy of hydration", Proceedings of AIP Conference: Simulation and Theory of Electrostatic Interactions in Solution, L. R. Pratt and G. Hummer (eds.), Santa Fe, New Mexico, 202-224 (1999).
16. S. Garde, A. E. Garcia, L. R. Pratt, and G. Hummer, "Temperature dependence of the solubility of nonpolar gases in water", Biophysical Chemistry, 78, 21-32 (1999).
15. L. R. Pratt, S. Garde, and G. Hummer, "Theories of hydrophobic effects and the description of free volume in complex liquids", Proceedings of the NATO Advanced Study Institute: New approaches to and new problems in liquid state theory, C. Caccamo et al. (eds.), Kluwer Academic Publishers, the Netherlands (1999).
14. M. A. Gomez, L. R. Pratt, G. Hummer, and S. Garde, "Molecular realism in default models for information theories of hydrophobic effects", Journal of Physical Chemistry B, 103, 3520 (1999).
13. H. S. Ashbaugh, S. Garde, G. Hummer, E. W. Kaler, and M. E. Paulaitis, "Conformational equilibria of hydrophobic solutes in aqueous solution: relationship to inhomogeneous water structure", Biophysical Journal, 77, 645-654 (1999).
12. S. Garde, G. Hummer, and M. E. Paulaitis, "Free energy of hydration of a molecular ionic solute: tetramethylammonium ion", Journal of Chemical Physics, 108, 1552-1561 (1998). (citations **34**)
11. G. Hummer and S. Garde, "Cavity expulsion and weak dewetting of hydrophobic solutes in water" Physical Review Letters, 80, 4193-4196 (1998).
10. G. Hummer, S. Garde, A. E. Garcia, M. E. Paulaitis, and L. R. Pratt, "Hydrophobic effects on a molecular scale", Journal of Physical Chemistry B, Feature article, 102,10469-10482, (1998).

9. G. Hummer, S. Garde, A. E. Garcia, M. E. Paulaitis, and L.R. Pratt, "The pressure dependence of hydrophobic interactions is consistent with the observed pressure denaturation of proteins", Proc. Natl. Acad. Sci. USA. 95, 1552-1555 (1998).
8. G. Hummer, L. R. Pratt, A. E. Garcia, S. Garde, B. J. Berne, and S. W. Rick, "Reply to comment on `Electrostatic potentials and free energies of solvation of polar and charged molecules", Journal of Physical Chemistry B, 102, 3841-3843 (1998).
7. S. Garde, G. Hummer, M. E. Paulaitis, and A. E. Garcia, "Hydration of biological macromolecules: From small solutes to proteins and nucleic acids", in Proceedings of the 1996 MRS Fall Meeting Symposium on Statistical Mechanics in Physics and Biology, edited by D. Wirtz, T. C. Halsey, 463, 21 (1997).
6. S. Garde, G. Hummer, A. E. Garcia, M. E. Paulaitis, and L. R. Pratt, "Origin of the entropy convergence in hydrophobic hydration and protein folding", Physical Review Letters, 77, 4966-4968 (1996).
5. S. Garde, G. Hummer, A. E. Garcia, L. R. Pratt, and M. E. Paulaitis, "Hydrophobic hydration: inhomogeneous water structure near nonpolar molecular solutes", Physical Review E, 53, R4310-4313 (1996).
4. S. Garde, G. Hummer, and M. E. Paulaitis, "Hydrophobic interactions: conformational equilibria and the association of nonpolar molecules in water", Faraday Discussions, 103, 125 (1996).
3. G. Hummer, S. Garde, A. E. Garcia, A. Pohorille, and L. R. Pratt, "An information theory model of hydrophobic interactions", Proc. Natl. Acad. Sci. USA. 93, 8951-8955 (1996). (An invited commentary on this article was also published in the same issue of PNAS).
2. M. E. Paulaitis, S. Garde, and H. S. Ashbaugh, "The hydrophobic effect", Current Opinion in Colloids and Interfaces, 1, 376-383 (1996).
1. M. E. Paulaitis, H. S. Ashbaugh, and S. Garde, "The entropy of hydration of simple hydrophobic solutes", Biophysical Chemistry, 51, 349 (1994).

INVITED PRESENTATIONS (total > 135)

1. Centennial seminar speaker, University of Delaware, 2014.
2. Gordon Research Conference on Water and Aqueous Solutions (Discussion Leader), Holderness, NH, August, 2014.
3. Gordon Conference on Polymer Physics, Mount Holyoke College, July 2014.
4. Telluride Science Research Center Workshop of Hydrophobicity, June, 2014.
5. ACS Symposium on Hydrophobicity, ACS National Meeting, Dallas, TX, March 2014.
6. University at Albany, Department of Chemistry, Albany, NY, March 11, 2014.
7. Laufer Center for Physical and Quantitative Biology, Stony Brook, October 29, 2013.
8. Northwestern University, Department of Chemical Engineering, September 26, 2013.
9. Enrico Fermi School on Water, **Varenna Lectures**, Varenna, Italy, July 7-12, 2013.
10. University of Pennsylvania, Department of Chemical & Biomolecular Engineering, April 24, 2013.
11. Northeastern University, Department of Chemical Engineering, April 17, 2013.
12. Johns Hopkins University, Department of Chemical & Biomolecular Engineering, April 4, 2013.
13. University of Maryland College Park, Department of Chemical & Biomolecular Engineering, April 2, 2013.
14. Department of Physics and Astronomy, RPI, March 27, 2013.
15. **Keynote Speaker,** 8th HIC/RPC meeting Advancements, Applications and Theory in Downstream Processing, Savannah, Georgia, March 3-7, 2013.
16. University of Wisconsin, Madison, Department of Chemical Engineering, Nov 13, 2012.
17. University of Colorado, Department of Chemical Engineering, Oct 9th, 2012.
18. New England Complex Fluids Workshop, Brandeis University, Sept 21, 2012.
19. Purdue University Department of Chemical Engineering, Sept 18th, 2012
20. Gordon Research Conference on Water and Aqueous Solutions, Holderness School, NH, August, 2012.

21. Pennsylvania State University Department of Chemical Engineering, Nov. 3rd, 2011.
22. **Keynote Speech**, High Performance Computing Conference, Rensselaer Polytechnic Institute, Oct 27th, 2011.
23. **Keynote Speaker**, Area 1a American Institute of Chemical Engineering Annual Conference, Minneapolis, October 2011.
24. **Highlight talk,** Thermophysical Properties of Biological Systems – II, American Institute of Chemical Engineers, Annual Conference, Minneapolis, October, 2011.
25. ACS Colloids Division Symposium in honor of Prof. Eli Ruckenstein, Denver, Colorado, August 28, 2011.
26. American Conference on Theoretical Chemistry, Telluride, Colorado, August 18-22, 2011.
27. University of Akron, Polymers and Advanced Materials Lecture Series, Akron, OH, April 29th, 2011.
28. Brandeis University, Department of Physics Seminar, April 26, 2011.
29. University of California at Santa Barbara, April 15, 2011.
30. **Robert W. Vaughan Lecture**, Chemical Engineering, Cal Tech, April, 14, 2011.
31. **Keynote Speaker**, Chemical Biophysics Symposium, University of Toronto, April, 2011.
32. ACS Symposium on Hydrophobic Surfaces, Anaheim, CA, March, 2011.
33. Texas Tech University, Departmental Seminar, Feb 4, 2011.
34. University at Albany, Chemistry Department Seminar, Jan 28, 2011.
35. **Keynote Speaker**, Golden Jubilee Celebration, Tavanappa Patne High School, Kolhapur, India, January 3, 2011.
36. Alkyl Amines Padmabhushan B. D. Tilak Chemcon **Distinguished Speaker Award**, Indian Institute of Chemical Engineers, Dec 28, 2010.
37. Dr. V. V. Mariwala **Award Lecture**, Institute of Chemical Technology, University of Mumbai, Matunga, Mumbai, India, December 26, 2010.
38. Department of Chemical Engineering, University of Massachusetts, Amherst, Nov 16, 2010
39. Cornell University, Biophysics Seminar Series, Ithaca, NY, November 2010.
40. A symposium in honor of Richard W. Siegel, Center for Biotechnology and Interdisciplinary Disciplinary Studies, Rensselaer Polytechnic Institute, Troy NY, October 11, 2010.
41. Department of Chemical Engineering, Virginia Tech, Blacksburgh, October 6, 2010.
42. Special ACS Symposium in Honor of Bruce J. Berne, Boston, MA, August 21, 2010.
43. 17th Canadian Symposium on Theoretical Chemistry, Edmonton, Alberta, Canada, July 25-30, 2010.
44. Telluride Science Research Center Meeting on *Ions in Aqueous Solutions and Molecular Biology: Theory, Simulation, Modelling*, June 21-25, 2010.
45. Telluride Science Research Center Meeting on *Thermal Transport at the Nanoscale*, July 12-16, 2010.
46. Yeshiva University, Department of Physics Seminar, May 4th, 2010.
47. Faraday Discussions of the Royal Society of Chemistry (London), Richmond, VA, April 14, 2010.
48. Department of Chemistry Seminar, University of Delaware, April 5, 2010.
49. Genentech Research and Development, San Francisco, March 24, 2010.
50. New York University Chemistry Department Seminar, March 12, 2010.
51. Departmental Seminar, Chemical and Biological Engineering, Georgia Institute of Technology, Atlanta, GA, Feb 10, 2010.
52. NYTaC3, New York Theoretical and Computational Chemistry Conference, New York City, Jan 11, 2010.
53. Berkeley Mini Statistical Mechanics Meeting, University of California, Berkeley, CA, Jan 8-10, 2010.
54. "Multiscale Modeling and Simulations of Hard and Soft Materials" workshop and conference, Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore, Dec 17-20, 2009. Presented 3 workshop talks, led 1 interactive discussion, 1 conference talk, and 1 talk on the Molecularium Project.

55. Department of Chemical and Biomolecular Engineering Seminar, University of Houston, Nov 20, 2009.
56. Gordon Research Conference on "Biological Molecules in the Gas Phase", in the session on Hydration, Jul 5-10, 2009.
57. "Proteins and Water", A special invitation only workshop, Arizona State University, May 12, 2009.
58. Department of Chemical Engineering, Clarkson University, Apr 21, 2009.
59. Department of Chemistry, Purdue University, Mar 25, 2009.
60. Department of Chemical and Environmental Engineering, University of California at Riverside, Feb 6, 2009.
61. National Chemical Laboratory, Pune, India, Jan 7, 2009.
62. Presentation on the Molecularium Project at the Opening celebration of Experimental Media and Performing Arts Center (EMPAC), research symposium titled “Insight/Outlook”, Oct 5, 2008.
63. Departmental Seminar, Department of Chemical and Biomolecular Engineering, U. Connecticut, Oct 14, 2008
64. Departmental Seminar, Department of Chemical and Biomolecular Engineering, U. Oklahoma, Sept 25, 2008
65. ACS Symposium, ACS National Meeting, Philadelphia, PA, August 2008.
66. A special conference on Water at Interfaces, in Crete, Greece, June 2008.
67. American Institute of Chemical Engineers and ACS joint conference symposium, April 2008.
68. American Physical Society, March, 2008
69. Department of Chemistry, University of Utah, Nov. 2007
70. Department of Chemical Engineering, Lehigh University, Bethelehem, PA, Sept 26, 2007.
71. Department of Biomedical Engineering, Washington University, St. Louis, Sept 21, 2007.
72. Gordon Research Conference on *Physics and Chemistry of Liquids*, NH, July 29, 2007.
73. National Institutes of Health, Laboratory of Chemical Physics, NIDDK, Bethesda, MD, June 8th, 2007.
74. ACS symposium 2007 on “Structure, Dynamics, and Solvation at Liquid-Liquid Interfaces”, March 25th, 2007.
75. ICampus, symposium on “Learning without barriers/Technology without borders” celebrating MIT-Microsoft Icampus alliance, Dec 1-2, 2006.
76. Department of Chemical Engineering, Northwestern University, Evanston, IL, Nov 2, 2006.
77. “Bio and Nanotechnology – a modelers view”, Bethlehem Highschool, Delmar, NY, October, 2006.
78. “From Modeling to Moviemaking”, Undergraduate Lecture Series, Nanotechnology Center, RPI, June 2006.
79. “Modeling of Bio and Nano Systems: How and Why?”, Chautauqua Lectures, Nanotechnology Center, RPI, June 2006.
80. “Molecular Modeling of Bio and Nanosystems”, Key Executives Conference, Rensselaer Polytechnic Institute, Troy, NY, April 6, 2006.
81. “Simulations in Colloidal and Complex Fluids”, American Chemical Society Symposium, March 2006.
82. Center for Medical Science, Wadsworth Center, Albany, NY, March 2006.
83. *FOMMS* (Foundations of Molecular Modeling and Simulation) “Tools for Innovation” meeting, Semiahmoo, Blaine, WA, USA, 2006.
84. *ICFAI* and Shivaji University Special Seminar Series, Kolhapur, India, Dec. 2005.
85. CHEMCON – *Annual Congress of Indian Institute of Chemical Engineers*, Delhi, India, December 2005.
86. Department of Chemical Engineering, Princeton University, Dec 7, 2005.
87. Department of Chemical Engineering, University of Florida, November 14, 2005.
88. Department of Chemical and Biomolecular Engineering, Rice University, October 27, 2005.
89. Department of Chemistry, Virginia Commonwealth University, October 20, 2005.
90. Department of Chemical Engineering, University of California at Santa Barbara, October 13, 2005.

91. Department of Chemical and Biomolecular Engineering, Ohio State University, Sept. 22, 2005.
92. Nanotechnology workshop, The Model Institutions for Excellence (MIE) a National Science Foundation sponsored program at Universidad Metropolitana in San Juan, Puerto Rico, September 16-17, 2005.
93. Department of Chemical Engineering, University of Pittsburgh, September 9, 2005.
94. Gordon Research Conference on "Cellular Osmoregulation: Sensors, Transducers, and Regulators", Salve Regina University, August 2005.
95. Domefest 2005, Domie Award and lecture on Molecularium (with Owen Bush and Kurt Przybilla), Albuquerque, NM, July 2005.
96. Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, May 2, 2005.
97. Department of Chemical and Biological Engineering, *Columbia University*, April 19, 2005.
98. Department of Chemistry, *Mount Holyoke College*, MA, April 20, 2005.
99. *Materials Research Society* Spring Meeting, San Francisco, CA, March 29, 2005.
100. *ACS Symposium* on "Water: Structure, Dynamics, and Reactions Across the Phase Diagram", American Chemical Society Spring National Meeting, San Diego, CA, March 14, 2005.
101. Center for Molecular and Engineering Thermodynamics, *University of Delaware*, February 2005.
102. *University of Delaware Engineering Banquet Keynote speaker*, "Molecularium: A magical musical adventure into the world of molecules", February 25, 2005.
103. *US-Korea Nanotechnology Forum*, "Molecularium: A new way to approach science education of children", Los Angeles, CA, February 17-18, 2005.
104. Biotechnology Symposium, *Rensselaer Polytechnic Institute*, September 2004.
105. *Jawaharlal Nehru Center for Advanced Research*, Bangalore, India, August 2004.
106. *Indo-US Nanotechnology Workshop* sponsored by the US National Science Foundation, Bangalore, India, August 2004.
107. Department of Physics – Condensed Matter Seminar, *University of Illinois at Chicago*, March 4, 2004.
108. Medical Textiles Conference, Clemson University, March (2004).
109. Department of Chemical Engineering Seminar, SUNY Buffalo, February 4, 2004.
110. Department of Chemical Engineering Seminar, Massachusetts Institute of Technology, October 31, 2003.
111. Department of Chemical Engineering Seminar, Carnegie Mellon University, October 21, 2003.
112. Department of Chemical Engineering Seminar, University of Notre Dame, September 23, 2003.
113. Department of Chemical Engineering and Physical Chemistry Seminar, University of Texas - Austin, September 18, 2003.
114. Fifth Canadian Computational Chemistry Conference, University of Toronto, Canada, July 27, 2003.
115. Mid West Statistical Mechanics Meeting, Ohio State University, May 2003.
116. Department of Chemical Engineering, Washington University, St. Louis, November 11, 2002.
117. Department of Chemical Engineering, University of Virginia, October 24, 2002.
118. Department of Chemical Engineering, *University of Delaware*, October 18, 2002.
119. Lindsay Lecturer, Department of Chemical Engineering, *Texas A & M University*, Sept 17, 2002.
120. "Nanobiotechnology: what is it really?" Diversity day workshop at *Rensselaer Polytechnic*, February 9, 2002.
121. Department of Chemistry, *Rensselaer Polytechnic*, Troy, NY, November 15, 2001.
122. Condensed Matter and Optics Seminar, Department of Physics, *Rensselaer Polytechnic Institute*, Troy, NY, October 1, 2001.
123. *Unilever Research Labs*., Edgewater, NJ, September 25, 2001.
124. *Biotechnology in the Capital Region* Conference on Imaging and Bioengineering, Rensselaerville, NY, September 14, 2001.
125. *ACS Polymer Symposium, Chicago*, August 2001.

126. New York State Capital Region MENSA, May 2001.
127. Department of Chemistry, *State University of New York, Binghamton*, September 2000.
128. Department of Chemistry, *University of Maine*, May 2000.
129. Department of Chemical Engineering, *Rensselaer Polytechnic Institute*, February 1999.
130. Department of Chemical Engineering, *Pennsylvania State University*, February 1999.
131. Department of Chemical Engineering, *University of Illinois at Urbana Champaign*, February 1999.
132. Department of Chemical Engineering, *University of Pennsylvania, Philadelphia*, February 1999.
133. Department of Chemical Engineering, *University of Iowa*, Iowa City, February 1999.
134. Department of Chemical Engineering, *Washington University*, St. Louis, November 1998.
135. Theory Division, *Los Alamos National Laboratory*, Los Alamos, NM 1995.
136. Thermodynamics Group Meeting, *Massachusetts Institute of Technology*, Department of Chemical Engineering, Summer, 1996.

GARDE GROUP STUDENT MENTORING

Postdoctoral students:

Alums:

Amish Patel (PhD Berkeley, Previous post-doc in David Chandler Group, Berkeley Chemistry). Currently, Assistant Professor, University of Pennsylvania, Chemical Engineering.

Parbati Biswas (currently faculty at Delhi University, India)

Ph. D. (Graduated, total 15**)**

15. V. Vasudevan (co-advised with Joel Plawsky), Title: Ions, Osmolytes, and polymers at aqueous interfaces: Insights from molecular theory and simulations, 2014.

14. Siddharth Parimal (co-advised with Steve Cramer) Title: Molecular Investigations of Multimodal Ligand-Protein Interactions, 2014; to join Biogen-Idec.

13. Srivathsan Vembanur, Title: "Molecular-level studies of water and water-mediated interactions at aqueous interfaces", currently a postdoc at SUNY's RNA Institute, Albany, NY.

12. Hari Acharya, Title: "Influence of interfaces on hydrophobicity, and on heat and momentum transport", currently at Bayer in San Francisco, CA.

11. Natalia Shenogina, Title: "Thermal coupling at aqueous and biomolecular interfaces", May 2010.
Cuttently at a national lab in Ohio.

10. Sumanth Jamadagni, Title: "How interfaces affect the behavior of water and water-mediated interactions: Molecular Theory and Simulations", May 2010.
Currently at Procter and Gamble Research, Cincinnati, OH.

9. Sapna Sarupria, Title:Understanding pressure effects on biological self-assembly: Role of hydration and water-mediated interactions", July 2009.
Currently a post-doc at Princeton University.

8. Rahul Godawat, Title: Hydration and assembly in interfacial environments: Thermodynamic, Structural, and Kinetic Studies", April, 2009.
Currently at Genzyme Corporation, MA.

7. Brian Pereira, Title "Mechanistic studies of Intein Splicing by Molecular Modeling, Simulation, and Molecular Biology Experiments", May 2008.
Currently a post-doc at MIT.

6. Manoj Athawale, Title: "Hydrophobicity in the multidimensional space of lengthscales, attractions, and thermodynamic conditions", June 2007.
Currently at Intel Corporation, Portland, Oregon.

5. Sowmi Rajamani, Title: "Molecular simulation studies of hydration phenomena relevant to biological systems", May 2006.
Currently at Intel Corporation, Portland, Oregon.

4. Harshit Patel, Title: "Molecular Dynamics Studies of Alkane Polymers: In Melts and at Interfaces", May 2005. (coadvised by E. B.Nauman)
Currently an independent entrepreneur in Mumbai, India.
3. Lu Yang , Title: "Understanding Hydration in Biological and Colloidal Systems", December, 2004. (coadvised by J. D. Dordick)
Currently at Applied Materials, CA.
2. Tuhin Ghosh Title: "Hydration in Biological Systems", March 2004.
Currently at Ronin Financial, San Francisco, CA.
1. Amrit Kalra, Title: "Exploring Carbon Nanotubes and Their Assemblies as Molecular Channels", August 2003.
Currently at Shell Oil Company, Houston, Texas.

M. S. (Graduated: total 4**)**

4. Ishita Manjrekar, Title: "Hydration in Biological Systems", 2007
   Currently a technology consultant to a Hedge Fund in San Francisco, CA.
3. Hongjun Liu, Title: "Phase behavior of square well fluids", 2006
   Currently a Ph.D. student at Columbia University
2. Sandeep Jain, Title: "Multiscale coarse-graining of polymeric melt systems", 2005
   Currently at Lehman Brothers, NY City.
1. Erik Storm, Title: "Molecular Modeling of Intein Structure", August, 2003.
   Currently at Bristol-Myers-Squibb Company, Syracuse, NY.

Current Postdocs:

Ketan Khare (co-advised with Pankaj Karande)

Current PhD students:

Eugene Wu	
Lijuan Li	
Cecily Wilbanks	(chemistry student, co-advised with Linda B. McGown)
John Kwak	(co-advised with Pankaj Karande)
Suvrajit Banerjee	(co-advised with Steven Cramer)

Undergraduate Students:

Robert Gottlieb (2012)	Christine Artim (2014)
Nick Mozdzierz (2011, 2012)	Andrew Fiore (2012, 2013)
Zach Whiteman (2008)	Cuyler Bates (2010)
Nai'l Mitchell (2007)	Steve Roy (2007)
Galina Gartsman (2007)	Christian Bosoy (2007, 2008, 2009, 2010)
Joseph Reynolds (2005)	Nathan Marsan (2005, high school student)
Caitlin Scott (2005, 2006, 2007)	Ashish Adhikari (2004)
Jake Cohen (2004)	Saryu Jindal (2004)
Monica Berrondo (2003)	Archana Fotedar (2003)
Seema Jaisinghani (2003)	Anya Esonis (2003)
Hsiao Nancy Lin (2002)	Shifalika Kanwar (2002)
Rebecca Rosenberg Beran (2002)	Jerome Covey (2002)
Pamela Sarro (2001)	Brian Golenberg (2001)

Visiting researchers:

Avni Jain, From UT Austin – Truskett group (2010)
Gaurav Goel, From UT Austin – Truskett group (2005)
Hank Ashbaugh, Tulane University (2006)
Prof. Kelvin Chu, University of Vermont (2003).

MEMBER

American Association for Advancement of Science
American Institute of Chemical Engineers
Biophysical Society
American Chemical Society
American Physical Society
Materials Research Society
American Society for Engineering Education
Sigma Chi Scientic Research Society

REVIEWER

Journals:

American Institute of Physics, Proceedings
Australian Journal of Chemistry
Biophysical Journal
Biochemistry
Chemical Reviews
Fluid Phase Equilibria
Journal of Chemical Physics
Journal of Physical Chemistry, B
Journal of the American Chemical Society
Journal of Chemical Theory and Computation
Langmuir
Macromolecules
Molecular Physics
Nature
Nature Communications
Physica A –statistical mechanics and its applications
Physical Chemistry Chemical Physics
Physical Review (B)
Physical Chemistry Chemical Physics
Physical Review Letters
Polymer Journal
Proceedings of the National Academy of Sciences, USA
Proteins: Structure Function and Genetics
Science

Funding agencies (acted as a reviewer for):

American Chemical Society Petroleum Research Fund
Bank of America (Virginia Trust)
Department of Energy
National Science Foundation (reviewer and **panelist**: NSF-CAREER, MRSEC, unsolicited proposals, NER; site visitor: STC)
NATO Postdoctoral fellowships
Air-force office of research (AFOSR)

PROFESSIONAL ACTIVITIES

1. Session Chair, "Sampling Non-equilibrium and biological systems", David Chandler's 70th Birthday Symposium, MIT, Boston, MA, Oct 18, 2014.

2. Discussion leader, Gordon Research Conference on Water and Aqueous Solutions, Holderness, NH, August 2014.
3. Guest Editor of a special issue of the Materials Research Society Bulletin on Water at Functional Interfaces, 2014 (with Mark Schlossman).
4. Co-organizer, ACS Symposium on "Single Molecules at Interfaces" with Dan Schwartz, Dallas, Texas, March 2014.
5. Co-organizer, Telluride Science Research Center Workshop (with Ruhong Zhou) on "Hydrophobicuty: from theory and simulations to experiments" 2012, 2014.
6. Organizing Committee, FOMMS (Foundations of Molecular Modeling and Simulations) conference, 2012.
7. Chair for "Thermophysical properties of biological systems I and II", AIChE Conference, 2007.
8. Chair/co-chair for "Thermophysical properties of biological systems I, II, and III", AIChE Conference, 2006.
9. Programming chair of Area 1a for AIChE 2005 Fall Meeting, Cincinnati, Ohio, 2005.
10. Session co-chair at the Annual AIChE conference for session "Molecular simulations, Recent Advances", 2003.
11. Session co-chair at the annual AIChE conference for "Computing and Simulations at Work in Molecular Science and Life Sciences"**,** San Franscisco, 2003.
12. Session co-chair at the annual AIChE conference for "Water in Inhomogeneous Environments" session, San Francisco, 2003.
13. Chair (organizer) of the American Chemical Society multi-day symposium on "Water in Novel Environments and Biological Systems" Boston, 2002.
14. Session chair at the annual AIChE conference for "Water in Inhomogeneous Environments" session, Indianapolis, 2002.
15. Session chair at the annual AIChE conference for "Thermodynamics of Aqueous and Ionic Solutions" session, Indianapolis, 2001.