## Lawrence R. Pratt

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### EDUCATION

B.S., Michigan State University, 1972
M.S., University of Illinois, 1974
Ph.D., University of Illinois, 1977

### POST Ph.D PROFESSIONAL EXPERIENCE

Postdoctoral research fellow, Department of Chemistry, Harvard University, 1977-78.
Assistant Professor, Department of Chemistry, University of California, Berkeley, 1979-84.
Staff member, Los Alamos National Laboratory, 1984-2008.
Sabbatical leave (PR&TL) Stanford University/NASA Ames Research Center, January 1991 - June 1991.
Visiting Research Professor, Department of Chemical & Biomolecular Engineering, Johns Hopkins University, July 1998 - June 1999.
Professor, Herman and George R. Brown Chair, Department of Chemical & Biomolecular Engineering, Tulane University, January 2008-
Adjunct Professor of Physics, Tulane University, January 2008-
Interim Chairman of Tulane's Chemical & Biomolecular Engineering Department, 2010-2011

### RESEARCH INTERESTS

Statistical mechanics and thermodynamics, molecular theory of liquids, water and aqueous solutions relevant to molecular biophysics, molecular simulation and design of electrical energy storage materials.

### PROFESSIONAL ACTIVITIES

*Member:* American Chemical Society, American Institute of Chemical Engineers, American Physical Society

*Awards:*

2018 Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids, sponsored by ExxonMobil Research & Engineering

*Books:*

THE POTENTIAL DISTRIBUTION THEOREM AND MODELS OF MOLECULAR SOLUTIONS, T. L. Beck, M. E. Paulaitis, and L. R. Pratt (Cambridge University Press, 2006).

*Service:*

Organizer and chairman of Eighth West Coast Statistical Mechanics Conference, Department of Chemistry, University of California, Berkeley, June 1982.

Organizer: Symposium "Chemistry at Solution Interfaces" ACS Spring Meeting, Dallas, April 1989.

Nominating committee ACS Theoretical Chemistry Subdivision, 1989.

Award Committee for the Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids sponsored by E. I. du Pont de Nemours & Company and administered by the American Chemical Society. 1990-1992, 2008-2010, Chairman 2011.

Committee to review Molecular Sciences Research Center (Battelle Pacific Northwest Laboratory) program supported by the Division of Chemical Sciences in the U. S. Department of Energy's Office of Basic Energy Sciences. 1992

Committee to review NIH Center for Biomolecular Simulation at Columbia University, October 1995; December 2000.

Organizer: Workshop on Treatment of Electrostatic Interactions in Computer Simulation of Condensed Media, Santa Fe, June 1999, editor of conference volume *Simulation and Theory of Electrostatic Interactions in Solution. Computational Chemistry, Biophysics, and Aqueous Solutions*, AIP Conference Proceedings **492**, (1999).

Organizer: Special Session "Quantum Mechanics and Computational Modeling of Soft Matter," International Conference on Computational Nanoscience, March 2001.

Organizer: Symposium "Probing Molecular Aqueous Environments in Chemistry and Biology" ACS Spring Meeting, San Diego, April 2001.

Editorial Advisory Board for the *Journal of Chemical Theory and Computation* 2004-2010.

Interim Chair of Chemical & Biomolecular Engineering Department, 2010-2011.

Editorial Advisory Board for the *Journal of Statistical Physics* 2013-

Organizer, Telluride Workshop: "Ions in Aqueous Solutions and Molecular Biology: Theory, simulation, modeling," 2012, 2014, 2016.

External thesis examiner for Timothy Duignan, Department of Applied Mathematics, Research School of Physics and Engineering, Australian National University, 2015

**INVITED LECTURES**

1. Chemistry Department, University of Maine, November 1977.
2. Chemistry Department, Harvard University, December 1977.
3. CECAM Workshop on "Protein-Protein Interaction," Brussels, October 1979.
4. Chemistry Department, U. C., Davis, December 1979.
5. NRCC workshop on "The Problem of Long-ranged Forces in Computer Simulations of Condensed Matter," January 1980.
6. Gordon Research Conference on "Physics and Chemistry of Water and Aqueous Solutions," August 1980.
7. Gordon Research Conference on "Proteins," June 1981.
8. U. C., Davis, seminar series on computer simulation, 1981.
9. Planetary Biology Branch, NASA Ames Research Center, 1981.
10. Gordon Conference on "Chemistry at Interfaces," July 1982.
11. Gordon Research Conference on "Physics and Chemistry of Water and Aqueous Solutions," August 1982.
12. Chemistry Department, U.C., San Diego, October, 1982.
13. Faraday Symposium No. 17, "The Hydrophobic Interaction," December 1982.
14. 185th National Meeting of the ACS, Symposium on "Structure and Dynamics of Liquids," Seattle, March 1983.
15. Chemistry Department, UCLA, May 1983.
16. Los Alamos Chemistry Division, January 1984.
17. Los Alamos Center for Nonlinear Studies (exchange visitor), March 1984.
18. Chemistry Department, Brookhaven National Laboratory, April 1984.
19. Division of Computer Research and Technology, National Institutes of Health, April 1984.

20. 58th Colloid and Surface Science Symposium, Carnegie-Mellon University, June 1984.
21. Materials Science Theory Group, Argonne National Laboratory, June 1984.
22. Photophysics Section Eastman Kodak, Rochester, June 1984.
23. Chemical Engineering Department Princeton University, November 1984.
24. NSF Workshop on "Structures and Phase Behaviors of Simple Surfactant Solutions and Microemulsions," UCLA, January 1985.
25. Chemistry Department, U.C., San Diego, March 1985.
26. APS spring meeting, Baltimore, March 1985.
27. NSF workshop on "Future of Computer Simulation in Chemistry," Arden House, Harriman, NY, April 1985.
28. ACS spring meeting, Miami Beach, May 1985.
29. Gordon Research Conference on "Chemistry at Interfaces," July 1985.
30. CECAM discussion meeting on "Long Range Forces in Computer Simulation," August 1985.
31. Gordon Research Conference on "Physics and Chemistry of Liquids," August 1985.
32. Planetary Biology Branch, NASA Ames Research Center, December 1985.
33. 30th Annual Meeting of the Biophysical Society, San Francisco, February 1986.
34. ACS spring meeting, New York City, Hildebrand Award Symposium, April 1986.
35. Gordon Research Conference on "Biopolymers," Holderness School, June 1986.
36. Gordon Research Conference on "Physics and Chemistry of Water and Aqueous Solutions," Colby-Sawyer College, August 1986.
37. Electrochemical Society Meeting, Honolulu, October 1987.
38. Workshop on "The Role of Nonlinear Dynamics in Reaction Kinetics" sponsored by the California Coordinating Committee for Nonlinear Studies, Lake Arrowhead, California, March 1988.
39. 2nd NASP Workshop on hydrogen-materials interactions, Scottsdale, Arizona, June 1988.
40. Photographic Research Laboratory, Eastman Kodak, Rochester, July 1988.
41. Chemistry Department, Brown University, September 1988.
42. Chemistry Department, University of Michigan, January 1989.
43. Utah Workshop in Theoretical and Computational Chemistry, February 1989.
44. ACS Spring Meeting, Dallas, April 1989.
45. Theoretical Physics Institute, University of Minnesota, "Many-Body Encounter in Minnesota," May 1989.
46. Los Alamos Center for Nonlinear Studies Workshop "Quantum Simulation of Condensed Matter Phenomena," August 1989.
47. American Institute of Chemical Engineers 1989 Annual Meeting, San Francisco, November, 1989.
48. Department of Chemistry, Colorado State University, April 1990.
49. Theoretical Chemistry Research Group, University of Utah, April 1990.
50. Department of Chemistry, University of Utah, April 1990.
51. Department of Chemistry, Colorado University, April 1990.
52. Department of Chemistry, Ohio State University, April 1990.
53. Department of Chemistry, University of Cincinnati, April 1990.
54. Ohio Supercomputer Center Workshop on "Theory and Application of Density Functional Approaches to Chemistry," May 1990.
55. Department of Chemistry, University of Pittsburgh, May 1990.

56. 200th ACS National Meeting, August 1990.
57. NIH, DCRT/PSL, August 1990.
58. Pacific Northwest Lab (Battelle), Richland, Washington, September 1990.
59. Department of Chemical Engineering, North Carolina State University, December 1990.
60. Department of Chemistry, University of North Carolina, December 1990.
61. Department of Chemistry, Clemson University, December 1990.
62. Department of Chemistry, University of California, Santa Cruz, January 1991.
63. Symposium on Interfacial Chemistry, American Physical Society Meeting, March 1991.
64. Department of Pharmaceutical Chemistry, University of California, San Fransicso, April 1991.
65. Condensed Matter Physics Seminar, Michigan State University, April 1991.
66. Department of Chemistry, Wayne State University, April 1991.
67. First Canadian Symposium on Computational Chemistry, Sherbrooke, Quebec, May 1991.
68. BIOSYM Technologies, July 1991.
69. LANL Structural Biology Colloquium, July 1991.
70. Department of Chemistry, Washington State University, August 1991.
71. Department of Chemistry, University of New Mexico, November 1991.
72. Workshop on "Structure and Function of Protobiological Membranes," NASA Ames Research Center, December 1991.
73. Department of Chemistry, University of Texas (Arlington), February 1991.
74. Workshop on the Environmental Chemistry of Ground Water, sponsored by Battelle PNL, Seattle, May 1992.
75. Department of Chemistry, Brown University, May 1992.
76. Workshop on Water-Biomolecule Interactions, sponsored by the European Biophysical Societies Association, Palermo, June 1992.
77. Division of Computer Research and Technology, NIH, May 1993.
78. Department of Chemical Engineering, University of Delaware, May 1993.
79. 1994 ACS Spring Meeting, Symposium "Structure and Reactivity in Aqueous Solution," San Diego, March 1994.
80. 1994 Gordon Research Conference on "Water and Aqueous Solutions," Holderness, August 1994.
81. Chemistry Department, Rutgers University, September 1994.
82. Chemistry Department, Columbia University, September 1994.
83. Department of Chemical Engineering, University of Delaware, September 1994.
84. Biophysical Society Meeting, San Francisco, February 1995.
85. Harvard University Martin Karplus 65th Birthday Symposium, March 1995.
86. Department of Chemistry, Brown University, March 1995.
87. Department of Chemistry, Florida International University, September 1995.
88. Structural Biology Program, NCI-Frederick Cancer Research and Development Center, Frederick MD, October 1995.
89. Pacific Symposium on Biocomputing '96, Hawaii, January 1996.
90. International Congress on Theoretical Chemical Physics, New Orleans, April 1996.
91. ACS Central Regional Meeting, Dayton, June 1996.
92. American Conference on Theoretical Chemistry, Park City, July 1996.

93. Workshop on "Implicit Solvent Models in Biomolecular Simulation," Biophysical Society Meeting, New Orleans, March 1997.
94. Electrochemical Society Meeting, Montreal, May 1997.
95. American Physical Society Meeting, Los Angeles, March 1998.
96. CECAM Workshop "Implicit solvent models for biomolecular simulations," Lyon, France, May 1998.
97. NATO Advanced Study Institute "Liquid State Theory" Patti Marina, Sicily, July 1998.
98. Telluride Workshop on Condensed Phase Dynamics, Telluride, July 1998.
99. Idaho National Engineering and Environmental Laboratory, Idaho Falls, July 1998.
100. Electrochemical Society Meeting, Boston, November 1998.
101. Johns Hopkins University, "Biophysical Evening Series," December 1998.
102. Department of Chemical Engineering, Johns Hopkins University, Short Course on "Hydration Models for Biophysics and Molecular Theory of Aqueous Solutions ," December 1998.
103. Sanibel Symposium, St. Augustine, FL, March 1999.
104. ACS Spring Meeting 1999, Anaheim, CA, March 1999.
105. Workshop on Emerging Methods in Computational Chemistry and Materials Science, Aberdeen, MD, April 1999.
106. Rutgers University Chemistry Department, October 1999.
107. Purdue University Chemistry Department, March 2000.
108. Joint Northwest Rocky Mountain Regional ACS Meeting, Idaho Falls, June 2000.
109. Sandia National Laboratory (ABQ), Biomolecular Materials and Interfaces Group, September 2000.
110. International Symposium on Structure, Dynamics, and Folding of Proteins as Viewed from the Pressure Axis, Otsu, Japan, January 2001.
111. Chemical Engineering Department, Johns Hopkins University, Short Course on "Modeling Life's Matrix: Theory and Modeling of Aqueous Solutions," April 2001.
112. Chemistry Department, Vassar College, April 2001.
113. Chemical Engineering Department, Rennselaer Polytechnic Institute, April 2001.
114. CECAM Meeting "Electrostatics for complex molecular systems: Continuum models and beyond." Ecole Normale Superiore, Lyon, France. June 2001.
115. Snowbird Workshop on Polarizability for Biomolecular Simulation, December 2001.
116. ICAM (Institute for Complex Adaptive Materials) Workshop on "Self-organizing biomolecules: the evolving picture," Santa Fe, January 2002.
117. ICCN (International Conference on Computational Nanotechnology), Puerto Rico, April 2002.
118. MRS meeting San Francisco, April 2002.
119. Department of Chemistry, University of Houston, July 2002.
120. Idaho National Engineering & Environmental Laboratory, Idaho Falls, July 2002.
121. ACS National Meeting, Boston, September 2002.
122. Department of Chemistry, University of Wisconsin, October 2002.
123. Southwest Theoretical Chemistry Conference, University of Houston, November 2002.
124. Department of Chemistry, University of New Orleans, January 2003.
125. Department of Chemistry, University of Pittsburgh, June 2003.
126. Bunsen International Discussion Meeting, Schloss Velen, September 2003.
127. Department of Chemistry, Iowa State University, November 2003.

128. Department of Chemistry, University of Cincinnati, March 2004.
129. Workshop of the Institute for Complex Adaptive Materials "Dynamic Energy Landscapes and Functional Systems," Santa Fe, April 2004.
130. CECAM Workshop "Continuing challenges in free energy calculations: Theory and applications in chemistry and biology." Ecole Normale Superiore, Lyon, France. May 2004.
131. Department of Chemistry, University of California at Berkeley, June 2004.
132. Gordon Research Conference on "Water and Aqueous Solutions," August 2004.
133. Institute for Mechanics and Computation, Stanford University, November 2004.
134. 2005 Berkeley Mini Statistical Mechanics Meeting, UC Berkeley, January 2005.
135. Mesilla "Tex-Mex" Theoretical Chemistry Conference, April 2005.
136. Varenna "Water of Life" workshop, April 2005.
137. Symposium "Ions in Complex Systems," national ACS meeting, Washington DC, September 2005.
138. Department of Chemistry, University of Alabama (Tuscaloosa), October 2005.
139. Department of Chemistry, University of Alabama (Huntsville), October 2005.
140. PACIFICHEM, Honolulu, December 16, 2005.
141. PACIFICHEM, Honolulu, December 19, 2005.
142. Workshop on *Quantitative Quantum Chemistry* in honour of Thom Dunning, Santa Fe, March 2006.
143. DOE Workshop "Grotthus 2006," Washington DC, June 2006. see http://www.cbms.utah.edu/~ derry/doe_proton_workshop/index.html
144. Southwest Regional Meeting of the ACS, Houston, October 2006.
145. Retreat for DOE Institute for Multi-scale Modeling of Biological Interactions, Johns Hopkins, November 2006.
146. AIChE National Meeting, San Fransico, November 2006.
147. Greater Boston (Harvard/MIT/BU/BC) Theoretical Chemistry Lectures, December 2006.
148. Rice Theoretical and Computational Biology Conference, December 2006.
149. Army Alkaline Membrane Workshop, December 2006.
150. Center for Non-linear Studies (LANL) Colloquium, January 2007: *Theory of Liquids and Landau's "neither convincing nor useful" Epithet.*
151. $47^{\underline{\text{th}}}$ Sanibel Symposium, St. Simons Island, GA, February 2007.
152. ACS meeting Boston, August 2007.
153. Department of Chemical & Biomolecular Engineering, Tulane University, September 2007.
154. Astrobiology Science Conference 2008, Santa Clara, April 2008.
155. Southeastern Theoretical Chemistry Association 2008 Meeting, University of Alabama.
156. Workshop on "Aqueous Solutions and Their Interfaces," Crete 2008.
157. ACS meeting Philadelpia, August 2008.
158. APS meeting Pittsburg, March 2009.
159. University of Maryland Statistical Physics Group, April 2009.
160. 1st University of Maryland Symposium on Theoretical Chemistry "Water from the molecule to the macroscopic," April 2009.
161. Department of Chemistry, University of New Orleans, October 2009.
162. American Institute of Chemical Engineers, Nashville, November 2009.

163. American Chemical Society Spring National Meeting, San Francisco, March 2010.
164. 217th Electrochemical Society Meeting, Vancouver, April 2010.
165. Argonne National Laboratory, "Symposium on Research Opportunities on Electrochemical Energy Storage, Beyond Lithium Ion: Computational Perspectives," May 2010.
166. Goldsmidt Conference 2010, Knoxville, June 2010.
167. Telluride Research Conference on "Ions in solution," July 2010.
168. American Chemical Society Fall National Meeting, Boston 2010.
169. University of Tennessee, College of Engineering Distinguished Lecture Series, November 2010.
170. University of Tennessee, Department of Chemical & Biomolecular Engineering, statistical mechanics class "quasi-chemical theory," November 2010.
171. American Chemical Society SE/SW regional meeting, New Orleans, Decemeber 2010.
172. 104th Statistical Mechanics Conference (Lebowitz/Rutgers conference), December 2010.
173. American Chemical Society Fall National Meeting, Denver 2011.
174. Studium Conference 'Water in biological systems,' Orléans, France, December 2011.
175. American Chemical Society National Meeting, San Diego, March 2012.
176. CECAM Workshop "Free energy calculations: From theory to applications," Ecole des Ponts, Champs-sur-Marne, France, June 2012.
177. ACS SW Regional Meeting Baton Rouge, January 2013.
178. LONI Institute HPC Symposium Baton Rouge, June 2013.
179. "Aquo Incognita, Galileo 400 years on, the Florentine Debates." Florence, July 2013. [http : //apple.csgi.unifi.it/ fondazione/aquaincognita.html]
180. Telluride Scientific Research Workshop "Hydrophobic effects," June 2014.
181. American Chemical Society Fall National Meeting, San Francisco 2014.
182. Department of Chemistry, Notre Dame University, November 2014.
183. 227th Annual Meeting of the Electrochemical Society, Chicago, May 24-28, 2015
184. NSF workshop "Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions," Washington DC, May 31- June 4, 2015
185. Department of Chemical & Biomolecular Engineering, Rice University, October 15, 2015.
186. 115th Statistical Mechanics Meeting, Rutgers University, May 8, 2016.
187. Los Alamos National Laboratory P&T Colloquium, November 3, 2016
188. Conference on Polymers for Fuel Cells, Energy Storage, and Conversion, Asilomar February 2017
189. ACS Symposium "Liquid Theory: in Honor of Ben Widom's Upcoming 90th Birthday," ACS National Meeting, Washington DC August, 2017

**PUBLICATIONS, Hirsch index: $h = 57$ (Google Scholar)**

1. D. Chandler and L. R. Pratt, *J. Chem. Phys.* **65**, 2925(1976): "Statistical Mechanics of Chemical Equilibrium and Intramolecular Structures of Nonrigid Molecules in Condensed Phases."
2. L. R. Pratt and D. Chandler, *J. Chem. Phys.* **66**, 148(1977): "Interaction Site Cluster Series for the Helmholtz Free Energy and Variational Principle for Chemical Equilibria and Intramolecular Structures."
3. L. R. Pratt and D. Chandler, *J. Chem. Phys.* **67**, 3683(1977): "Theory of the Hydrophobic Effect."
4. L. R. Pratt, C. S. Hsu, and D. Chandler, *J. Chem. Phys.* **68**, 4202(1978): "Statistical Mechanics of Small Chain Molecules. I. Effects of Liquid Packing on Conformational Structures."
5. C. S. Hsu, L. R. Pratt, and D. Chandler, *J. Chem. Phys.* **68**, 4213(1978): "Statistical Mechanics of Small Chain Molecules. II. Intermolecular Pair Correlations in n-Butane."
6. E. L. Pollock, B. J. Alder, and L. R. Pratt, *Proc. Natl. Acad. Sci. USA* **77**, 49(1980): "Relation Between the Local Field at Large Distance for a Charge or Dipole and the Dielectric Constant."
7. L. R. Pratt and D. Chandler, *J. Soln. Chem.* **9**, 1(1980): "Hydrophobic Interactions and Osmotic Second Virial Coefficients for Methanol in Water."
8. L. R. Pratt, *Molec. Phys.* **40**, 347): "Effective Field a Dipole in Non-Polar Polarizable Fluids."
9. L. R. Pratt and D. Chandler, *J. Chem. Phys.* **72**, 4045(1980): "Effective Intramolecular Potentials for Molecular Bromine in Argon. Comparison of Theory with Simulation."
10. L. R. Pratt, R. O. Rosenberg, B. J. Berne, and D. Chandler, *J. Chem. Phys.* **73**, 1002(1980): "Comment on the Structure of a Simple Liquid Solvent Near a n-Butane Solute Molecule."
11. L. R. Pratt and D. Chandler, *J. Chem. Phys.* **73**, 3430(1980): "Hydrophobic Solvation of Nonspherical Solutes."
12. L. R. Pratt and D. Chandler, *J. Chem. Phys.* **73**, 3434(1980): "Effects of Solute-Solvent Attractive Forces on Hydrophobic Correlations."
13. L. R. Pratt and S. W. Haan, *J. Chem. Phys.* **74**, 1864(1981). "Effects of Periodic Boundary Conditions on Equilibrium Properties of Computer Simulated Fluids. I. Theory."
14. L. R. Pratt and S. W. Haan, *J. Chem. Phys.* **74**, 1873(1981). "Effects of Periodic Boundary Conditions on Equilibrium Properties of Computer Simulated Fluids. II. Applications to Simple Liquids."
15. L. R. Pratt, *Molec. Phys.* **43**, 1163(1981): "Connection Between Central Force Model Treatment of Polyatomic Liquids and the Interaction Site Cluster Expansion."
16. L. R. Pratt, D. L. Ermak, and B. J. Alder, *J. Phys. Chem.* **85**, 3221(1981): "Hard Sphere Solids with One Fluid Component."
17. S. W. Haan and L. R. Pratt, *Chem. Phys. Lett.* **79**, 436(1981): "Monte Carlo Study of a Simple Model for Micelle Structure." [Erratum, *Chem. Phys. Lett.* **81**, 386(1981)].
18. Book Review: "The Hydrophobic Effect: Formation of Micelles and Biological Membranes" *J. Am. Chem. Soc.* **103**, 7697(1981).
19. A. L. Nichols III and L. R. Pratt, *J. Chem. Phys.* **76**, 3782 (1982): "Theory of Surface Structure of Dilute Electrolyte Solutions."
20. A. L. Nichols III and L. R. Pratt, *J. Chem. Phys.* **77**, 1070(1982): "Slow Decay of Ion Correlations Parallel to an Electrolyte Solution Surface."
21. L. R. Pratt, *J. Chem. Phys.* **77**, 979 (1982): "A New Monte Carlo Method for Direct Estimation of Cluster Partition Functions. Application to Micellar Aggregates."
22. M. A. Wilson, A. L. Nichols III, and L. R. Pratt, *J. Chem. Phys.* **78**, 5129(1983): "Theory of Electrolyte Solution Interfaces at Finite Dilution."

23. A. L. Nichols III and L. R. Pratt, *J. Chem. Soc. Faraday Symp.* **17**, 129(1982): "Disentanglement of Hydrophobic and Electrostatic Contributions to the Film Pressures of Ionic Surfactants."
24. R. A. LaViolette and L. R. Pratt, *Phys. Rev. A* **28**, 2482(1983): "Free Energy of Nucleating Droplets via Cluster-Integral Series."
25. B. Owenson and L. R. Pratt, *J. Phys. Chem.* **88**, 2905(1984): "Molecular Statistical Thermodynamics of Model Micellar Aggregates."
26. A. Pohorille, L. R. Pratt, S. K. Burt, and R. D. MacElroy, *J. Biomolec. Struct. Dyn.* **1**, 1257(1984): "Solution Influence on Biomolecular Equilibria: Nucleic Acid Base Associations."
27. A. L. Nichols III and L. R. Pratt, *J. Chem. Phys.* **80**, 6225(1984): "Salt Effects on the Surface Tensions of Dilute Electrolyte Solutions: Influence of Nonzero Relative Solubility of the Salt between the Coexisting Phases."
28. M. A. Wilson, A. L. Nichols III, and L. R. Pratt, *J. Chem. Phys.* **81**, 579(1984): "Hydrophobic Interaction of Amphiphilic Ions with Water-Hydrocarbon Liquid Interfaces."
29. P. Phillips, R. A. LaViolette, and L. R. Pratt, *J. Chem. Phys.* **80**, 1605(1984): "Multiple Nucleation Pathways Near Triple Points of Ar-Kr Mixtures."
30. B. Owenson and L. R. Pratt, *J. Phys. Chem.* **89**, 6048(1984): "Monte Carlo Calculation of the Molecular Structure of Surfactant Bilayers."
31. R. A. Harris and L. R. Pratt, *J. Chem. Phys.* **82**, 856(1985): "Discretized Propagators, Hartree and Hartree-Fock Approximations, and the Hohenberg-Kohn Theorem."
32. R. A. Harris and L. R. Pratt, *J. Chem. Phys.* **82**, 5084(1985): "Discretized Propagators in Hartree and Hartree-Fock Theory. II. Responses to Static Electric and Magnetic Fields."
33. R. A. Harris and L. R. Pratt, *J. Chem. Phys.* **83**, 4024(1985): "A Method for Systematic Inclusion of Electron Correlation in Density Functionals."
34. L. R. Pratt, *Ann. Rev. Phys. Chem.* **36**, 433(1985): "Theory of Hydrophobic Effects."
35. L. R. Pratt and D. Chandler, *Methods in Enzymology* **127**, 48(1985): "Theoretical and Computational Studies of Hydrophobic Interactions."
36. A. Pohorille and L. R. Pratt, *Methods in Enzymology* **127**, 64(1985): "Theoretical Methods for Obtaining Free Energies of Biomolecular Equilibria in Aqueous Solution."
37. M. A. Wilson, A. Pohorille, and L. R. Pratt, *J. Chem. Phys.* **83**, 5832(1985): "Molecular Dynamics Test of the Brownian Description of $Na^+$ Motion in Water."
38. L. R. Pratt, B. Owenson, and Zhewei Sun, *Advances in Colloid and Interface Science* **26**, 69(1986): "Molecular Theory of Micelle Formation in Aqueous Solution."
39. L. R. Pratt, *J. Chem. Phys.* **85**, 5045(1986): "A Statistical Method for Identifying Transition States in High Dimensional Problems."
40. J. Geldard and L. R. Pratt, *J. Chem. Ed.* **64**, 425 (1987): "Statistical Determination of Normal Modes."
41. L. R. Pratt, *J. Chem. Phys.* **87**, 1245 (1987): "Fluctuation Method for the Calculation of Elastic Constants of Solids."
42. M. A. Wilson, A. Pohorille, and L. R. Pratt, *J. Phys. Chem.* **91**, 4873(1987): "Molecular Dynamics of the Water Liquid-Vapor Interface."
43. A. Pohorille, L. R. Pratt, R. A. LaViolette, M. A. Wilson, and R. D. MacElroy, *J. Chem. Phys.* **87**, 6070 (1987): "Comparison of the Structure of Harmonic Aqueous Glasses and Liquid Water."
44. L. R. Pratt, G. G. Hoffman, and R. A. Harris, *J. Chem. Phys.* **88**, 1818 (1988): "Statistical Theory of Electron Densities."
45. M. A. Wilson, A. Pohorille, and L. R. Pratt, *J. Chem. Phys.* **88**, 3281(1988): "Surface Potential of the Water Liquid-Vapor Interface."

46. G. G. Hoffman, L. R. Pratt, and R. A. Harris, *Chem. Phys. Letts.* **148**, 313 (1988): "Monte Carlo Integration of Density Functional Theory: Fermions in a Harmonic Well."
47. M. A. Wilson, A. Pohorille, and L. R. Pratt, *Chem. Phys.* **129**, 209(1989): "Interaction of a Sodium Ion with the Water Liquid-Vapor Interface."
48. M. A. Wilson, A. Pohorille, and L. R. Pratt, *J. Chem. Phys.* **90**, 5211(1989): "Comment on 'Study on the Liquid-Vapor Interface of Water...'." See also B. Yang, D. E. Sullivan, B. Tjipto-Margo, and C. G. Gray, *J. Phys. Condens. Matter* **3**, F109(1991): "Molecular Orientational Structure of the Water Liquid/Vapour Interface."
49. L. R. Pratt and J. Eckert, *Phys. Rev. B* **39**, 13 170(1989): "Molecular Dynamics of a Dilute Solution of Hydrogen in Palladium."
50. L. R. Pratt, *Phys. Rev. A* **40**, 6077 (1989): "Lower Bound on the Ground State Energies of Atoms and Molecules by Variational Quantum Monte Carlo."
51. L. R. Pratt, G. G. Hoffman, and R. A. Harris, *J. Chem. Phys.* **92**, 6687 (1990): "Ground State Densities from Electron Propagators: Optimized Thomas-Fermi Approximation for Short Wavelength Modes."
52. G. G. Hoffman and L. R. Pratt, *Proceedings of the International Workshop on Quantum Simulation of Condensed Matter Phenomena*, edited by J. D. Doll and J. E. Gubernatis (World Scientific Publishing Co. Pte. Ltd., Teaneck NJ, 1990), pages 105-115: "Optimized Thomas-Fermi potential for discrete propagator electron density functional calculations."
53. A. Pohorille and L. R. Pratt, *J. Am. Chem. Soc.* **112**, 5066(1990): "Cavities in Molecular Liquids and the Theory of Hydrophobic Solubilities." See also "Simulated Liquids Point to New Solutions," *Science News*, 7 July 1990, page 5.
54. G. G. Hoffman and L. R. Pratt, *Proc. Roy. Soc. A* **435**, 245(1991). "Statistical Theories of Electron Densities: Multiple Scattering Perturbation Theory."
55. L. R. Pratt, *J. Phys. Chem.* **96**, 25(1991): "Contact Potentials of Solution Interfaces: Phase Equilibrium and Interfacial Electric Fields."
56. L. R. Pratt, *CLS Division 1991 Annual Review*: "Oil and Water Don't Mix." LA-UR-91-1783. National Technical Information Service, U. S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161.
57. G. G. Hoffman, R. A. Harris, and L. R. Pratt, *Can. J. Chem.* **70**, 478(1992): "Statistical Theory of Electron Densities at Nonzero Temperatures."
58. L. R. Pratt and A. Pohorille, *Proc. Nat. Acad. Sci. USA* **89**, 2995(1992): "Theory of Hydrophobicity: Transient Cavities in Molecular Liquids."
59. D. L. Lynch, J. D. Doll, S. W. Rick, M. A. Gomez, and B. W. Spath, L. R. Pratt, *J. Chem. Phys.* **97**, 5177(1992): "Spectroscopic Studies of Surface and Subsurface Hydrogen/Metal Systems."
60. R. A. Harris and L. R. Pratt, *Chem. Phys. Letts.* **203**, 399(1993): "Simple Effective Hamiltonian for Low-Frequency Responses."
61. L. R. Pratt and A. Pohorille, *Proceedings of the EBSA 1992 International Workshop on Water-Biomolecule Interactions*, edited by M. U. Palma, M. B. Palma-Vittorelli, and F. Parak (Societá Italiana de Fisica, Bologna, 1993), pp. 261-268: "Hydrophobic Effects from Cavity Statistics."
62. L. R. Pratt and R. A. Keller, *J. Phys. Chem.* **97**, 10254 (1993): "Estimate of the Probability of Diffusional Misordering in High-Speed DNA Sequencing."
63. G. G. Hoffman and L. R. Pratt, *Molec. Phys.* **82**, 245(1994): "Comparison of Electron Density Functional Models."
64. L. R. Pratt, G. Hummer, and A. E. García, *Biophys. Chem.* **51**, 147(1994): "Ion Pair Potentials-of-Mean-Force In Water."
65. G. J. Tawa and L. R. Pratt in *Structure and reactivity in aqueous solution: Characterization of chemical and biological systems,* ACS Symposium Series 568, edited by C. J. Cramer and D. G. Truhlar (American Chemical Society, Washington DC, 1994), pp. 60-70: "Tests of Dielectric Model Descriptions of Chemical Charge Displacements in Water."

66. G. J. Tawa and L. R. Pratt, *J. Am. Chem. Soc.* **117**, 1625(1995): "Theoretical Calculation of the Water Ion Product $K_W$."

67. G. Hummer, L. R. Pratt, and A. E. García, *J. Phys. Chem.* **99**, 14188(1995): "The Hydration Free Energy of Water."

68. G. Hummer, L. R. Pratt, and A. E. García, *J. Phys. Chem.* **100**, 1206(1996): "Free Energy of Ionic Hydration." See also F. Figueirido, G. S. Del Buono, R. M. Levy, *J. Phys. Chem. B* **101**, 5622 (1997).

69. S. A. Corcelli, J. D. Kress, L. R. Pratt, and G. J. Tawa, *Pacific Symposium on Biocomputing '96*, edited by L. Hunter and T. E. Klein (World Scientific, Singapore, 1995), pp. 142–159. "Mixed-direct-iterative Methods for Boundary Integral Formulations of Continuum Dielectric Solvation Models."

70. G. J. Tawa, R. L. Martin, L. R. Pratt, and R. V. Russo, *J. Phys. Chem.* **100**, 1515 (1996): "Solvation Free Energy Calculations Using a Continuum Dielectric Model for the Solvent and Gradient Corrected Density Functional Theory for the Solute."

71. S. Garde, G. Hummer, A. E. García, L. R. Pratt, and M. E. Paulaitis, *Phys. Rev. E* **53**, R4310 (1996): "Hydrophobic Hydration: Inhomogeneous Water Structure Near Nonpolar Molecular Solutes."

72. G. Hummer, S. Garde, A. E. García, A. Pohorille, and L. R. Pratt, *Proc. Natl. Acad. USA***93**, 8951 (1996): "An Information Theory Model of Hydrophobic Interactions." See also the commentary B. J. Berne, *Proc. Natl. Acad. USA* **93**, 8800 (1996): "Inferring the hydrophobic interaction from the properties of neat water."

73. S. Garde, G. Hummer, A. E. García, M. E. Paulaitis, and L. R. Pratt, *Phys. Rev. Letts.* **77** , 4966 (1996): "Origin of Entropy Convergence in Hydrophobic Hydration and Protein Folding." See also comments by S. Marcelja, *Biophys. J.* **78**, 593–594 (1999).

74. L. R. Pratt, G. J. Tawa, G. Hummer, A. E. García, and S. A. Corcelli, *Int. J. Quant. Chem.* **64**, 121(1997): "Boundary Integral Methods for the Poisson Equation of Continuum Dielectric Solvation Models."

75. G. J. Tawa, R. L. Martin, and L. R. Pratt, *Int. J. Quant. Chem.* **64**, 143 (1997): "Reaction Field Spectral Shifts with Semi-Empirical Molecular Orbital Theory."

76. G. Hummer, L. R. Pratt, A. E. García, B. J. Berne, and S. W. Rick, *J. Phys. Chem. B* **101**, 3017(1997): "Electrostatic Potentials and Free Energies of Solvation of Polar and Charged Molecules."

77. G. Hummer, L. R. Pratt, and A. E. García, *J. Am. Chem. Soc.* **119**, 8523 (1997): "Multistate Gaussian Model for Polar and Ionic Hydration."

78. G. Hummer, L. R. Pratt, and A. E. García, *J. Chem. Phys.* **107**, 9275 (1997): "Ion Sizes and Finite-Size Corrections for Ionic-Solvation Free Energies."

79. G. Hummer, S. Garde, A. E. García, M. E. Paulaitis, and L. R. Pratt, *Proc. Natl. Acad. USA* **95**, 1552 (1998): "The Pressure Dependence of Hydrophobic Interactions Is Consistent with the Pressure Denaturation of Proteins."

80. L. R. Pratt, *Hydrophobic Effects,* in *the Encyclopedia of Computational Chemistry,* Schleyer, P. v. R.; Allinger, N. L.; Clark, T.; Gasteiger, J.; Kollman, P. A.; Schaefer III, H. F.: Schreiner, P. R., Eds.; John Wiley & Sons, Chichester, 1998.

81. R. L. Martin, P. J. Hay, and L. R. Pratt, *J. Phys. Chem. A* **102**, 3565-3573 (1998): "Hydrolysis of Ferric Ion in Water and Conformational Equilibrium."

82. L. R. Pratt and R. A. LaViolette, *Molec. Phys.* **94**, 909(1998): "Quasi-chemical Theories of Associated Liquids."

83. S. J. Paddison, L. R. Pratt, T. Zawodzinski, D. W. Reagor, *Fluid Phase Equilibria* **150**, 235(1998): "Molecular Modeling of Trifluoromethanesulfonic Acid for Solvation Theory."

84. G. Hummer, L. R. Pratt, and A. E. García, *J. Phys. Chem. A* **102**, 7885(1998): "Molecular Theories and Simulation of Ions and Polar Molecules in Water."

85. M. A. Gomez and L. R. Pratt, *J. Chem. Phys.* **109**, 8783(1998): "Construction of Simulation Wavefunctions for Aqueous Species: $D_3O^+$."

86. L. R. Pratt, S. Garde, and G. Hummer, in NEW APPROACHES TO PROBLEMS IN LIQUID STATE THEORY, NATO Science Series **529**, edited C. Caccamo, J.-P. Hansen, and G. Stell (Kluwer, Netherlands, 1999), 407–420: "Theories of Hydrophobic Effects and the Description of Free Volume in Complex Liquids."

87. G. Hummer, S. Garde, A. E. García, M. E. Paulaitis, and L. R. Pratt, *J. Phys. Chem. B* **102**, 10469(1998): "Hydrophobic Effects on a Molecular Scale."

88. S. Garde, A. E. García, L. R. Pratt, and G. Hummer, *Biophys. Chem.* **78**, 21–32, (1999): "Temperature Dependence of the Solubility of Nonpolar Gases in Water."

89. S. J. Paddison, L. R. Pratt, and T. A. Zawodzinski, Jr., in *Proton Conducting Membrane Fuel Cells II,* S. Gottesfeld and T. F. Fuller, Editors, PV 98-27, the Electrochemical Society Proceedings Series, Pennington, NJ (1999), pp 99–105: "Theoretical Structure of Triflic Acid-Water Clusters and the Molecular Mechanism of Proton Dissociation."

90. M. A. Gomez, L. R. Pratt, G. Hummer, and S. Garde, *J. Phys. Chem. B* **103**, 3520–3523, (1999): "Molecular Realism in Default Models for Information Theories of Hydrophobic Effects."

91. S. J. Paddison, L. R. Pratt, and T. A. Zawodzinski, Jr., *J. New Mat. Electrochem. Sys.* **2**, 183–188(1999): "Conformations of Perfluoroether Sulfonic Acid Side Chains for the Modeling of Nafion."

92. B. S. Jorgensen, R. C. Dye, M. A. Gomez, L. R. Pratt, and J. E. Meadows, *Fusion Technology* **37**, 124-130(2000): "Concentrating Low Level Tritiated Water Through Isotope Exchange."

93. L. R. Pratt and S. B. Rempe, *Simulation and Theory of Electrostatic Interactions in Solution*, AIP Conference Proceedings **492**, (1999), eds. L. R. Pratt and G. Hummer, pp. 172–201: "Quasi-chemical Theory and Implicit Solvent Models for Simulations."

94. G. Hummer, L. R. Pratt, A. E. García, and M. Neumann, *Simulation and Theory of Electrostatic Interactions in Solution*, AIP Conference Proceedings **492**, (1999), eds. L. R. Pratt and G. Hummer, pp. 84–103: "Treatment of Electrostatic Interactions In Computer Simulations and Calculations of Thermodynamic Properties Such As Free Energies and Pressures."

95. S. B. Rempe, L. R. Pratt, Gerhard Hummer, J. D. Kress, Richard L. Martin, and Antonio Redondo, *J. Am. Chem. Soc.* **122**, 966–967 (2000): "The Hydration Number of $Li^+$ in Liquid Water."

96. G. Hummer, S. Garde, A. E. García, L. R. Pratt, *Chem. Phys.* **258**, 349-370(2000): "New Perspectives on Hydrophobic Effects."

97. S. B. Rempe and L. R. Pratt, *Fluid Phase Equilibria*, **183-184**, 121(2001): "The Hydration Number of $Na^+$ in Liquid Water."

98. S. J. Paddison, L. R. Pratt, and T. A. Zawodzinski, Jr., *J. Phys. Chem. A* **105**, 6266–6268(2001): "Variation of the Dissociation Constant of Triflic Acid with Hydration."

99. L. R. Pratt, R. A. LaViolette, M. A. Gomez, and M. E. Gentile, *J. Phys. Chem. B* **105**, 11662–11668 (2001): "Quasi-Chemical Theory for the Statistical Thermodynamics of the Hard Sphere Fluid."

100. L. R. Pratt, *Annu. Rev. Phys. Chem.* **53**, 409–436 (2002): "Molecular Theory of Hydrophobic Effects: 'She is too mean to have her name repeated.'"

101. L. R. Pratt, *Chem. Rev.* **102**, 2625(2002): "Introduction: Water."

102. L. R. Pratt and A. Pohorille, *Chem. Rev.,* **102**, 2671–2691(2002): "Hydrophobic Effects and Modeling of Biophysical Aqueous Solution Interfaces."

103. P. Grabowski, D. Riccardi, M. A. Gomez, D. Asthagiri, and L. R. Pratt, *J. Phys. Chem. A* **106**, 9145 (2002): "Quasi-chemical Theory and the Standard Free Energy of $H^+$(aq)."

104. M. E. Paulaitis and L. R. Pratt, *Adv. Prot. Chem.* **62**, 283-310(2002): "Hydration Theory for Molecular Biophysics."

105. M. Eikerling, S. J. Paddison, L. R. Pratt, and T. A. Zawodzinski, Jr., *Chem. Phys. Letts.* **368**, 108–114 (2003): "Defect Structure for Proton Transport in Triflic Acid Monohydrate Solid."

106. D. Asthagiri and L. R. Pratt *Chem. Phys. Letts.* **371**, 613–619 (2003): "Quasi-Chemical Studies of $Be^{2+}$ Speciation in Water."

107. H. S. Ashbaugh, D. Asthagiri, L. R. Pratt, and S. B. Rempe, *Biophys. Chem.* **105**, 321–336(2003): "Hydration of Krypton and Consideration of Clathrate Models of Hydrophobic Effects from the Perspective of Quasi-Chemical Theory."

108. L. R. Pratt, in THEORY IN ACTION: HIGHLIGHTS IN THE THEORETICAL DIVISION AT LOS ALAMOS 1943-2003, LA-14000-H (history report unclassified): "Modeling and Molecular Theory of Liquids."

109. D. Asthagiri, L. R. Pratt, H. S. Ashbaugh *J. Chem. Phys.* **119**, 2702 –2708 (2003): "Absolute Hydration Free Energies of Ions, Ion-Water Clusters, and Quasi-chemical Theory."

110. L. R. Pratt and H. S. Ashbaugh, *Phys. Rev. E* **68**, 021505 (2003): "Self Consistent Molecular Field Theory for Packing in Classical Liquids."

111. D. Asthagiri, L. R. Pratt, J. D. Kress, and M. A. Gomez, *Chem. Phys. Letts.* **380**, 530-535 (2003): "The hydration state of $HO^-$(aq)."

112. D. Asthagiri, L. R. Pratt, J. D. Kress *Phys. Rev. E* **68**, 041505 (2003): "Free Energy of Liquid Water on the Basis of Quasi-Chemical Theory and *Ab Initio* Molecular Dynamics."

113. R. A. LaViolette, K. L. Copeland, and L. R. Pratt, *J. Phys. Chem. A* **107**, 11267 (2003): "Cages of Water Coordinating Kr in Aqueous Solution."

114. D. Asthagiri, L. R. Pratt, M. E. Paulaitis, and S. B. Rempe, *J. Am. Chem. Soc.* **126**, 1285-1289(2003): "Hydration Structure and Free Energy of Biomolecularly Specific Aqueous Dications, including $Zn^{2+}$ and First-Transition-Row Metals."

115. S. B. Rempe, D. Asthagiri, L. R. Pratt, *PCCP* **6**, 1966-1969 (2004): "Inner Shell Definition and Absolute Hydration Free Energy of $K^+$(aq) on the Basis of Quasi-chemical Theory and *Ab Initio* Molecular Dynamics."

116. D. Asthagiri, L. R. Pratt, J. D. Kress, M. A. Gomez *Proc. Natl. Acad. Sci USA* **101**, 7229–7233(2004): "Hydration and Mobility of $HO^-$(aq)."

117. H. S. Ashbaugh, L. R. Pratt, M. E. Paulaitis, J. Clohecy, and T. L. Beck, *J. Am. Chem. Soc.* **127**, 2808 – 2809 (2005): "Deblurred observation of the molecular structure of an oil-water interface."

118. D. Asthagiri, L. R. Pratt, and J. D. Kress, *Proc. Natl. Acad. Sci USA* **102**, 6704–6708(2005): "*Ab initio* molecular dynamics and quasichemical study of $H^+$(aq)."

119. H. S. Ashbaugh and L. R. Pratt, *Rev. Mod. Phys.* **78**, 159-178(2006): "Scaled-particle theory and the length scales of hydrophobicity." See also: February 1, 2006 issue of *Virtual Journal of Biological Physics Research,* and February 13, 2006 issue of *Virtual Journal of Nanoscale Science & Technology.*

120. A. Paliwal, D. Asthagiri, L. R. Pratt, H. S. Ashbaugh, M. E. Paulaitis, *J. Chem. Phys.* **124**, 224502(2006): "An analysis of molecular packing and chemical association in liquid water using quasi-chemical theory."

121. D. Asthagiri, L. R. Pratt, and M. E. Paulaitis, *J. Chem. Phys.* **125**, 124701(2006): "Role of fluctuations in a snug-fit mechanism of KcsA channel selectivity." See also July 15, 2006 issue of *Virtual Journal of Biological Physics Research.*

122. T. L. Beck, M. E. Paulaitis, and L. R. Pratt *Cambridge University Press* (2006): THE POTENTIAL DISTRIBUTION THEOREM AND MODELS OF MOLECULAR SOLUTIONS.

123. L. R. Pratt and D. Asthagiri, in FREE ENERGY CALCULATIONS. THEORY AND APPLICATIONS IN CHEMISTRY AND BIOLOGY, Springer Series in Chemical Physics, Vol. 86 (2007), Chipot, C.; Pohorille, Andrew (Eds.):"Potential distribution methods and free energy models of molecular solutions."

124. M. A. Gomez, L. R. Pratt, J. D. Kress, and D. Asthagiri, *Surf. Sci.* **601**, 1608-1614(2007): "Water adsorption and dissociation on BeO (001) and (100) surfaces."

125. H. S. Ashbaugh and L. R. Pratt, *J. Phys. Chem. B* **111**, 9330 - 9336(2007): "Contrasting non-aqueous against aqueous solvation on the basis of scaled-particle theory."

126. T. M. McCleskey, D. S. Ehler, T. S. Keizer, D. N. Asthagiri, L. R. Pratt, R. Michalczyk, and B. L. Scott, *Angew. Chemie - Int. Ed.* **46**, 2669 – 2671, (2007): "Beryllium displacement of $H^+$ from strong hydrogen bonds."

127. D. Asthagiri, H. S. Ashbaugh, A. Piryatinski, M. E. Paulaitis, and L. R. Pratt, *J. Am. Chem. Soc.* **129**, 10133 - 10140 (2007): "*Non-van der Waals* treatment of the hydrophobic solubility of $CF_4$."

128. J. K. Shah, D. Asthagiri, L. R. Pratt, and M. E. Paulaitis, *J. Chem. Phys.* **127**, 144508 (2007): "Balancing local order and long-ranged interactions in the molecular theory of liquid water."

129. S. Chempath, B. R. Einsla, L. R. Pratt, C. S. Boncella, J. M. Macomber, J. A. Rau, and B. S. Pivovar, *J. Phys. Chem. C* **112**, 3179 – 3182 (2008): "Mechanism of tetraalkylammonium headgroup degradation in alkaline fuel cell membranes."

130. D. Asthagiri, S. Merchant, L. R. Pratt, *J. Chem. Phys.* **128**, 244512 (2008): "Role of attractive methane-water interactions in the potential of mean force between methane molecules in water." Selected for the July 1, 2008 issue of *Virtual Journal of Biological Physics Research.*

131. S. Chempath and L. R. Pratt, *J. Phys. Chem. B* **113**, 4147-4151(2009): "Distribution of binding energies of a water molecule in the water liquid-vapor interface."

132. S. Chempath, L. R. Pratt, and M. E. Paulaitis, *J. Chem. Phys.* **130**, 054113 (2009): "Quasi-chemical theory with a soft cutoff."

133. L. Yang, B. H. Fishbine, A. Migliori, and L. R. Pratt, *J. Am. Chem. Soc.* **131**, 12373-12376 (2009): "Molecular simulation of electric double-layer capacitors based on carbon nanotube forests."

134. P. Zhu, T. Harris, M. Driver, C. Campbell, L. R. Pratt, K. Papadopoulos, *J. Phys. Chem. C*, **113**, 16458-16463 (2009): 'Dissolution Kinetics of [Hmim][$BF_4$] Ionic Liquid Droplets in 1-Pentanol."

135. D. Asthagiri, P. D. Dixit, S. Merchant, M. E. Paulaitis, L. R. Pratt, S. B. Rempe, and S. Varma, *Chem. Phys. Letts. (Frontier Article with cover graphics)* **485**, 1-7 (2010): "Ion selectivity from local configurations of ligands."

136. L. Yang, B. H. Fishbine, A. Migliori, L. R. Pratt, *J. Chem. Phys.* **132**, 044701(2010): "Dielectric saturation of liquid propylene carbonate in electrical energy storage applications." See also: February 1, 2010 issue of *Virtual Journal of Nanoscale Science & Technology.*

137. S. Chempath, L. R. Pratt and M. E. Paulaitis, *Chem. Phys. Letts.*, **487**, 24–27(2010): "Distributions of extreme contributions to binding energies of molecules in liquids."

138. A. C. Beveridge, J. H. Jett, R. A. Keller, L. R. Pratt, and T. M. Yoshida, *Analyst*, **135**, 1333-1338(2010): "Reduction in Diffusion Broadening in Flow Experiments by Analysis of Time-Gated Single-Molecule Data."

139. S. Chempath, J. M. Boncella, L. R. Pratt, N. Henson, B. S. Pivovar, *J. Phys. Chem. C*, **114**, 11977-11983(2010): "Density functional theory study of degradation of tetraalkylammonium hydroxides."

140. M. I. Chaudhari, L. R. Pratt, and M. E. Paulaitis, *J. Chem. Phys.,* **133** 231102(2010): "Direct observation of a hydrophobic bond in loop-closure of a capped $(\text{-}OCH_2CH_2\text{-})_n$ oligomer in water."

141. P. Zhu, X. You, L. R. Pratt, and K. D. Papadopoulos, *J. Chem. Phys.,* **134** 054502(2011): "Generalizations of the Fuoss Approximation for Ion Pairing."

142. L. J. Thibodeaux, K. T. Valsaraj, V. T. John, K. D. Papadopoulos, L. R. Pratt, and N. S. Pesika, *Environmental Engineering Science*, **28** 87-93(2011): "Marine Oil Fate: Knowledge Gaps, Basic Research, and Development Needs; A Perspective Based on the Deepwater Horizon Spill."

143. S. Varma, D. M. Rogers, L. R. Pratt, and S. B. Rempe, *J. Gen. Physiol.* **137**, 479-488 (2011): "Design principles for $K^+$ selectivity in membrane transport."

144. M. Hamsa Priya, L. R. Pratt, and M. E. Paulaitis, *Langmuir* **27**, 13713-13718 (2011): "Effect of PEG End-Group Hydrophobicity on Lysozyme Interactions in Solution Characterized by Light Scattering."

145. J. D. Weeks and L. R. Pratt, *J. Stat. Phys.* **145**, 207-208(2011): "Introduction to Special Issue on Water and Associated Liquids."

146. D. M. Rogers, D. Jiao, L. R. Pratt, and S. B. Rempe, *Ann. Rep. Comp. Chem.* **8**, 71-128 (2012): "Structural Models and Molecular Thermodynamics of Hydration of Ions and Small Molecules."

147. A. Pohorille and L. R. Pratt, *Origin of Life and Evolution of Biospheres* **42**, (2012): "Is Water the Universal Solvent for Life?" [See also: L. R. Pratt, A. Pohorille, and D. Asthagiri, http://arxiv.org/abs/physics/0701282: "What is special about water as a matrix of life?"]

148. P. Zhu, L. R. Pratt, and K. D. Papadopoulos, *J. Chem. Phys.* **137**, 174501(2012): "Pairing of 1-hexyl-3-methylimidazolium and tetrafluoroborate ions in *n*-pentanol."

149. X. You, M. I. Chaudhari, L. R. Pratt, N. Pesika, K. M. Aritakula, and S. W. Rick, *J. Chem. Phys.* **138**, 114708 (2013): "Interfaces of Propylene Carbonate."

150. D. Sabo, D. Jiao, S. Varma, L. R. Pratt, and S. B. Rempe, *Annu. Rep. Prog. Chem. Soc. C* (2013): "Case study of $Rb^+$(aq), quasi-chemical theory of ion hydration, and the *no split occupancies* rule." DOI: 10.1039/C3PC90011H [See also: http://arxiv.org/abs/1303.3210 .]

151. M. I. Chaudhari, S. Holleran, H. S. Ashbaugh, and L. R. Pratt, *Proc. Natl. Acad. Sci. USA* **110**, 20557-20562 (2013): "Molecular-scale Hydrophobic Interactions between Hard-sphere Reference Solutes are Attractive and Endothermic." (See also: http://arxiv.org/abs/1303.6597v1.)

152. W. Zhang, X. You, and L. R. Pratt, *J. Phys. Chem. B* **118**, 7730-7738 (2013): "Multi-scale theory in the molecular simulation of electrolyte solutions."

153. X. You, M. I. Chaudhari, and L. R. Pratt, AQUA INCOGNITA, pp. 434-442, editors B. W. Ninham and P. Lo Nostro (Connor Court Publishing Pty Ltd., 2014): "Comparison of Mechanical and Thermodynamical Evaluations of Electrostatic Potential Differences between Electrolyte Solutions."

154. M. I. Chaudhari and L. R. Pratt, OIL SPILL REMEDIATION: COLLOID CHEMISTRY-BASED PRINCIPLES AND SOLUTIONS, pp. 247-257, editors P. Somasundaran, R. S. Farinato, P. Patra, and K. Papadopoulos (John Wiley & Sons, Hoboken New Jersey, 2014): "Microstructures of capped ethylene oxide oligomers in water and n-hexane."
[See: http://arxiv.org/abs/1303.6597 and https://dx.doi.org/10.6084/m9.figshare.3123898.v1. ]

155. M. I. Chaudhari, L. R. Pratt, and M. E. Paulaitis, *J. Phys. Chem. B* (2014): "Loop-Closure and Gaussian Models of Collective Structural Characteristics of Capped PEO Oligomers in Water." DOI: 10.1021/jp504244x

156. M. I. Chaudhari, D. Sabo, L. R. Pratt, and S. B. Rempe, *J. Phys. Chem. B* (2014): "Hydration of Kr(aq) in dilute and concentrated solutions." DOI: 10.1021/jp508866h

157. M. I. Chaudhari, L. R. Pratt, and M. E. Paulaitis, *J. Chem. Phys.* **141**, 244908 (2014): "Concentration dependence of the Flory-Huggins interaction parameter in aqueous solutions of capped PEO chains." http://dx.doi.org/10.1063/1.4904386

158. L. R. Pratt *Encyclopedia of Astrobiology,* Springer-Verlag, Berlin (2014): "Hydrophobic Effect," DOI 10.1007/978-3-642-27833-4_704-3

159. X. You, L. R. Pratt, and S. W. Rick: "The role of attractive interactions in the dynamics of molecules in liquids," arXiv:1411.1773 [physics.chem-ph] (2014)

160. W. Zhang and L. R. Pratt, *ECS Transactions* **66**, 1-5 (2015): "AIMD Results for a Concentrated Solution of Tetra-ethylammonium Tetra-fluoroborate in Propylene Carbonate."

161. X. You, M. I. Chaudhari, S. B. Rempe, and L. R. Pratt, *ECS Transactions*, **69**, 107-111 (2015): "Dielectric Properties of Ethylene Carbonate and Propylene Carbonate using Molecular Dynamics Simulations."

162. X. You, M. I. Chaudhari, S. B. Rempe, and L. R. Pratt, *J. Phys. Chem. B* (2015): "Dielectric Relaxation of Ethylene Carbonate and Propylene Carbonate from Molecular Dynamics Simulations." (DOI: 10.1021/acs.jpcb.5b09561)

163. M. I. Chaudhari, S. B. Rempe, D. Asthagiri, and L. Tan, L. R. Pratt, *J. Phys. Chem. B* (2015): "Molecular Theory and the Effects of Solute Attractive Forces on Hydrophobic Interactions." (DOI: 10.1021/acs.jpcb.5b09552)

164. L. R. Pratt, M. I. Chaudhari, and S. B. Rempe, *J. Phys. Chem. B* (2016): "Statistical Analyses of Hydrophobic Interactions: A Mini-Review." (DOI: 10.1021/acs.jpcb.6b04082)

165. M. I. Chaudhari, J. Nair, L. R. Pratt, F. Soto, P. Balbuena, S. B. Rempe, *J. Chem. Theory & Comp.* (2016): "Scaling Atomic Partial Charges of Carbonate Solvents for Lithium Ion Solvation and Diffusion." (DOI: 10.1021/acs.jctc.6b00824)

166. M. Oguntoye, M. Johnson, L. R. Pratt, N. S. Pesika, *ACS Applied Materials & Interfaces* **8**, 27454-27457 (2016): "Triboelectricity Generation from Vertically Aligned Carbon Nanotube Arrays."

167. M. I. Chaudhari, L. R. Pratt, and S. B. Rempe, *Molecular Simulation* (2017): "Utility of Chemical Computations in Predicting Solution Free Energies of Metal Ions." (DOI: 10.1080/08927022.2017.1342127)

168. A. Muralidharan, M. I. Chaudhari, S. B. Rempe, and L. R. Pratt *Electrochem. Soc. Trans.* **77**, 1155–1162 (2017): "Molecular Dynamics Simulations of Lithium Ion Transport through a Model Solid Electrolyte Interphase (SEI) Layer."

169. M. I. Chaudhari, S. B. Rempe, and L. R. Pratt, *J. Chem. Phys.* (in press 2017): "Quasi-chemical Theory of $F^-$(aq): The *'no split occupancies rule'* revisited."

170. L. Tan, L. R. Pratt and M. I. Chaudhari: "Molecular-scale Description of SPAN80 Desorption from the Squalane-Water Interface." (arXiv:1603.04033v1, [physics.chem-ph, see also DOI: 10.6084/m9.figshare.3114928]

171. L. R. Pratt, D. Asthagiri, and S. B. Rempe, LA-UR-05-5986: "Momentum truncation errors and inferences of $Li^+$ hydration number on the basis of neutron diffraction from aqueous solutions."