

Publications of Gregory A. Voth

(As of 7/16/2014: Web of Science h-index = 72, total citations = 19,123; 16,283 w/o self citations;
Google Scholar h-index = 78, total citations = 22,366; 12,111 since 2009)

1. G. A. Voth, R. A. Marcus, and A. H. Zewail, "The Highly Excited C-H Stretching States of CHD₃, CHT₃, and CH₂D", *J. Chem. Phys.* **81**, 5494-5507 (1984).
2. G. A. Voth and R. A. Marcus, "Semiclassical Theory of Fermi Resonance Between Stretching and Bending Modes in Polyatomic Molecules", *J. Chem. Phys.* **82**, 4064-4072 (1985).
3. G. A. Voth and R. A. Marcus, "Semiclassical Dressed State Theory for the Vibrational Excitation of a Morse Oscillator by Radiation", *J. Phys. Chem.* **89**, 2208-2213 (1985).
4. S. M. Lederman, V. Lopez, G. A. Voth, and R. A. Marcus, "Quantum and Classical Energy Transfer Between Ligands of a Heavy Metal Atom", *Chem. Phys. Lett.* **124**, 93-98 (1986).
5. G. A. Voth and R. A. Marcus, "Adiabatically Reduced Coupled Equations for Intramolecular Dynamics Calculations", *J. Chem. Phys.* **84**, 2254-2261 (1986).
6. G. A. Voth, "On the Relationship of Classical Resonances to the Quantum Mechanics of Coupled Oscillator Systems", *J. Phys. Chem.* **90**, 3624-3629 (1986).
7. G. A. Voth, "Approximate Coupled Equations for Multiphoton Processes Induced by One or More Lasers", *Chem. Phys. Lett.* **129**, 315-320 (1986).
8. S. J. Klippenstein, G. A. Voth, and R. A. Marcus, "Iteratively Determined Effective Hamiltonians for the Adiabatically Reduced Coupled Equations Approach to Intramolecular Dynamics Calculations", *J. Chem. Phys.* **85**, 5019-5026 (1986).
9. G. A. Voth, "Quasidissipative Intramolecular Dynamics: An Adiabatically Reduced Coupled Equations Approach", *J. Chem. Phys.* **87**, 5272-5279 (1987).
10. G. A. Voth, "An Effective Golden Rule Decay Rate Expression for Quasidissipative IVR Processes", *J. Chem. Phys.* **88**, 5547-5552 (1988).
11. G. A. Voth, D. Chandler, and W. H. Miller, "Time Correlation Function and Path Integral Analysis of Quantum Rate Constants", *J. Phys. Chem.* **93**, 7009-7015 (1989).
12. S. M. Lederman, V. Lopez, V. Fairen, G. A. Voth, and R. A. Marcus, "Vibrational Energy Redistribution Across a Heavy Atom", *Chem. Phys.* **139**, 171-184 (1989).
13. G. A. Voth, D. Chandler, and W. H. Miller, "Rigorous Formulation of Quantum Transition State Theory and Its Dynamical Corrections", *J. Chem. Phys.* **91**, 7749-7760 (1989).
14. G. A. Voth, D. Chandler, and W. H. Miller, "A New Perspective on Quantum Mechanical Transition State Theory", in *Quantum Simulations of Condensed Matter Phenomena*, J. D. Doll and J. E. Gubernatis eds. (World Scientific, Singapore, 1990), pp. 391-400.
15. G. A. Voth, "Analytic Expression for the Transmission Coefficient in Quantum Mechanical Transition State Theory", *Chem. Phys. Lett.* **170**, 289-296 (1990).

16. B. G. Sumpter, G. A. Voth, D. W. Noid, and B. Wunderlich, "Infrared Laser Induced Chaos and Conformational Disorder in a Model Polymer Crystal: Melting Versus Ablation", *J. Chem. Phys.* **93**, 6081-6091 (1990).
17. G. A. Voth, "On the Use of Feynman-Hibbs Effective Potentials to Calculate Quantum Mechanical Free Energies of Activation", *J. Chem. Phys.* **94**, 4095-4098 (1991).
18. G. A. Voth, "A Feynman Path Integral Approach for Calculating Quantum Rate Constants in Complex Systems", *Ber. Bunsenges. Phys. Chem.* **95**, 393-399 (1991).
19. G. A. Voth and E. V. O'Gorman, "An Effective Barrier Model for Describing Quantum Mechanical Activated Rate Processes in Condensed Phases", *J. Chem. Phys.* **94**, 7342-7352 (1991).
20. D. H. Li and G. A. Voth, "A Feynman Path Integral Approach for Studying Intramolecular Effects in Proton Transfer Reactions", *J. Phys. Chem.* **95**, 10425-10431 (1991).
21. G. A. Voth, "Calculation of Equilibrium Averages with Feynman-Hibbs Effective Classical Potentials and Similar Variational Approximations", *Phys. Rev. A* **44**, 5302-5305 (1991).
22. H. Gai and G. A. Voth, "A Computer Simulation Method for Studying the Ablation of Polymer Surfaces by Ultraviolet Laser Radiation", *J. Appl. Phys.* **71**, 1415-1420 (1992).
23. J. B. Straus and G. A. Voth, "Studies on the Influence of Nonlinearity in Classical Activated Rate Processes", *J. Chem. Phys.* **96**, 5460-5470 (1992).
24. D. H. Li and G. A. Voth, "A Path Integral Einstein Model for Characterizing the Equilibrium States of Low Temperature Solids", *J. Chem. Phys.* **96**, 5340-5353 (1992).
25. G. R. Haynes and G. A. Voth, "Effect of Nonlinear Dissipation on Quantum Activated Rate Processes in Condensed Phases", *Phys. Rev. A* **15** *46*, 2143-2146 (1992).
26. J. Lobaugh and G. A. Voth, "A Partial Averaging Strategy for Low Temperature Fourier Path Integral Monte Carlo Calculations", *J. Chem. Phys.* **97**, 4205-4214 (1992).
27. R. P. McRae, G. K. Schenter, B. C. Garrett, G. R. Haynes, G. A. Voth, and G. C. Schatz, "Critical Comparison of Approximate and Accurate Quantum Mechanical Calculations of Reaction Rates for a Model Activated Reaction in Solution", *J. Chem. Phys.* **97**, 7392-7404 (1992).
28. A. L. R. Bug, A. Wilson, and G. A. Voth, "Nonlinear Vibrational Dynamics of a Neon Atom in C_{60} ", *J. Phys. Chem.* **96**, 7864-7869 (1992).
29. J. Lobaugh and G. A. Voth, "Calculation of Quantum Activation Free Energies for Proton Transfer Reactions in Polar Solvents", *Chem. Phys. Lett.* **198**, 311-315 (1992).
30. G. A. Voth, "A Theory for Treating Spatially-Dependent Friction in Classical Activated Rate Processes", *J. Chem. Phys.* **97**, 5908-5910 (1992).
31. J. B. Straus, J. M. Gomez-Llorente, and G. A. Voth, "Manifestations of Spatially-Dependent Friction in Classical Activated Rate Processes", *J. Chem. Phys.* **98**, 4082-4097 (1993).
32. D. H. Li and G. A. Voth, "A Variational Model for the Thermodynamical and Structural Properties of Impurities in Low Temperature Solids", *J. Chem. Phys.* **98**, 5734-5746 (1993).

33. Y.-C. Sun and G. A. Voth, "Path Integral Calculation of Hydrogen Diffusion Rates on Metal Surfaces", *J. Chem. Phys.* **98**, 7451-7458 (1993).
34. G. R. Haynes, G. A. Voth, and E. Pollak, "A Theory for the Thermally Activated Rate Constant in Systems with Spatially Dependent Friction", *Chem. Phys. Lett.* **207**, 309-316 (1993).
35. H. Gai and G. A. Voth, "Vibrational Energy Relaxation Dynamics of Si-H Stretching Modes on the H/Si(111)1'1 Surface", *J. Chem. Phys.* **99**, 740-743 (1993).
36. J. B. Straus and G. A. Voth, "A Computer Simulation Study of Free Energy Curves in Heterogeneous Electron Transfer", *J. Phys. Chem.* **97**, 7388-7391 (1993).
37. G. A. Voth, "Feynman Path Integral Formulation of Quantum Mechanical Transition State Theory", *J. Phys. Chem.* **97**, 8365-8377 (1993). (Invited Feature Article)
38. D. Scharf, G. J. Martyna, D. H. Li, G. A. Voth, and M. L. Klein, "Nature of Lithium Trapping Sites in the Quantum Solids *para*-Hydrogen and *ortho*-Deuterium", *J. Chem. Phys.* **99**, 9013-9020 (1993).
39. I. Bhattacharya-Kodali and G. A. Voth, "Integral Equation Calculation of Solvent Activation Free Energies for Electron and Proton Transfer Reactions", *J. Phys. Chem.* **97**, 11253-11257 (1993).
40. G. R. Haynes and G. A. Voth, "The Dependence of the Potential of Mean Force on the Solvent Friction: Consequences for Condensed Phase Activated Rate Theories", *J. Chem. Phys.* **99**, 8005-8008 (1993).
41. J. Cao and G. A. Voth, "A New Perspective on Quantum Time Correlation Functions", *J. Chem. Phys.* **99**, 10070-10073 (1993).
42. J. Lobaugh and G. A. Voth, "Quantum Mechanical Calculations of Tunneling Rates in Condensed Phases Systems", in *Reaction Dynamics in Clusters and Condensed Phases* (Kluwer Academic Publishers, The Netherlands, 1994), pp. 411-422.
43. D. H. Li and G. A. Voth, "Calculation of ESR Linewidths for Hydrogen Atom Impurities in Solid *para*-Hydrogen", *J. Chem. Phys.* **100**, 1785-1796 (1994).
44. Y.-C. Sun, H. Gai, and G. A. Voth, "Vibrational Energy Relaxation Dynamics of C-H Stretching Modes on the Hydrogen-Terminated H/C(111)1'1 Surface", *J. Chem. Phys.* **100**, 3247-3252 (1994).
45. J. Lobaugh and G. A. Voth, "A Path Integral Study of Electronic Polarization and Nonlinear Coupling Effects in Condensed Phase Proton Transfer Reactions", *J. Chem. Phys.* **100**, 3039-3047 (1994).
46. J. Cao and G. A. Voth, "The Formulation of Quantum Statistical Mechanics Based on the Feynman Path Centroid Density. I. Equilibrium Properties", *J. Chem. Phys.* **100**, 5093-5105 (1994).
47. J. Cao and G. A. Voth, "The Formulation of Quantum Statistical Mechanics Based on the Feynman Path Centroid Density. II. Dynamical Properties", *J. Chem. Phys.* **100**, 5106-5117 (1994).
48. D. E. Sagnella, J. Cao, and G. A. Voth, "A Semiclassical Reactive Flux Method for the Calculation of Condensed Phase Activated Rate Constants", *Chem. Phys.* **180**, 167-180 (1994).

49. H. Gai and G. A. Voth, "First-Principles Molecular Dynamics Study of Surface Vibrations and Vibrational Mode Coupling on the H/Si(111)1x1 Surface", *J. Chem. Phys.* **101**, 1734-1737 (1994).
50. J. Cao and G. A. Voth, "The Formulation of Quantum Statistical Mechanics Based on the Feynman Path Centroid Density. III. Phase Space Formalism and Analysis of Centroid Molecular Dynamics", *J. Chem. Phys.* **101**, 6157-6167 (1994).
51. J. Cao and G. A. Voth, "The Formulation of Quantum Statistical Mechanics Based on the Feynman Path Centroid Density. IV. Algorithms for Centroid Molecular Dynamics", *J. Chem. Phys.* **101**, 6168-6183 (1994).
52. J. Cao and G. A. Voth, "The Formulation of Quantum Statistical Mechanics Based on the Feynman Path Centroid Density. V. Quantum Instantaneous Normal Mode Theory of Liquids", *J. Chem. Phys.* **101**, 6184-6192 (1994).
53. G. R. Haynes, G. A. Voth, and E. Pollak, "A Theory for the Activated Barrier Crossing Rate Constant in Systems Influenced by Space and Time Dependent Friction", *J. Chem. Phys.* **101**, 7811-7822 (1994).
54. J. B. Straus, A. Calhoun, and G. A. Voth, "Calculation of Solvent Free Energies for Heterogeneous Electron Transfer at the Water–Metal Interface: Classical versus Quantum Behavior", *J. Chem. Phys.* **102**, 529-539 (1995).
55. J. Cao and G. A. Voth, "Modeling Physical Systems by Effective Harmonic Oscillators: The Optimized Quadratic Approximation", *J. Chem. Phys.* **102**, 3337-3348 (1995).
56. J. Cao, C. Minichino, and G. A. Voth, "The Computation of Electron Transfer Rates: The Nonadiabatic Instanton Solution", *J. Chem. Phys.* **103**, 1391-1399 (1995).
57. G. A. Voth, "A Feynman Path Integral Formulation of Quantum Mechanical Transition State Theory", in *New Trends in Kramers' Reaction Rate Theory*, P. Talkner and P. Hänggi, eds. (Kluwer Academic Publishers, The Netherlands, 1995). (Invited)
58. J. Cao and G. A. Voth, "A Theory for Time Correlation Functions in Liquids", *J. Chem. Phys.* **103**, 4211-4220 (1995).
59. R. Hernandez, J. Cao, and G. A. Voth, "On the Feynman Path Centroid Density as a Phase Space Distribution in Quantum Statistical Mechanics", *J. Chem. Phys.* **103**, 5018-5026 (1995).
60. C. P. Ursenbach and G. A. Voth, "Effect of Solvent on Semiconductor Surface Electronic States: A First-Principles Study", *J. Chem. Phys.* **103**, 7569-7575 (1995).
61. Y.-C. Sun, H. Gai, and G. A. Voth, "Vibrational Energy Relaxation Dynamics of Si–H Stretching Modes on Stepped H/Si(111)1x1 Surfaces", *Chem. Phys.* **200**, 357-368 (1995).
62. G. R. Haynes and G. A. Voth, "Reaction Coordinate Dependent Friction in Classical Activated Barrier Crossing Dynamics: When It Matters and When It Doesn't", *J. Chem. Phys.* **103**, 10176-10182 (1995).
63. J. Cao and G. A. Voth, "Semiclassical Approximations to Quantum Dynamical Time Correlation Functions" *J. Chem. Phys.* **104**, 273-285 (1996).

64. J. Lobaugh and G. A. Voth, "The Quantum Dynamics of an Excess Proton in Water", *J. Chem. Phys.* **104**, 2056-2069 (1996).
65. J. Cao, L. Ungar, and G. A. Voth, "A Novel Method for Simulating Quantum Dissipative Systems", *J. Chem. Phys.* **104**, 4189-4197 (1996).
66. G. A. Voth, "Path Integral Centroid Methods in Quantum Statistical Mechanics and Dynamics", *Adv. Chem. Phys.* **93**, 135-218 (1996). (Invited)
67. M. Pavese and G. A. Voth, "Pseudopotentials for Centroid Molecular Dynamics: Application to Self-Diffusion in Liquid *para*-Hydrogen", *Chem. Phys. Lett.* **249**, 231-236 (1996).
68. Y. Boroda and G. A. Voth, "A Theory for Adiabatic Electron Transfer Processes Across the Semiconductor/Electrolyte Interface", *J. Chem. Phys.* **104**, 6168-6183 (1996).
69. D. E. Sagnella and G. A. Voth, "The Structure and Dynamics of Hydronium in the Gramicidin Ion Channel", *Biophys. J.* **70**, 2043-2051 (1996).
70. G. A. Voth and R. M. Hochstrasser, "Transition State Dynamics and Relaxation Processes in Solution: A Frontier of Physical Chemistry", *J. Phys. Chem.* **100**, 13034-13049 (1996) (Centennial Issue).
71. A. Calhoun and G. A. Voth, "Electron Transfer Across the Electrode/Electrolyte Interface: Influence of Redox Ion Mobility and Counterions", *J. Phys. Chem.* **100**, 10746-10753 (1996).
72. J. Cao and G. A. Voth, "A Theory for the Quantum Activated Rate Constant in Dissipative Systems", *Chem. Phys. Lett.* **261**, 111-116 (1996).
73. A. Calhoun, M. Pavese, and G. A. Voth, "Hyper-Parallel Algorithms for Centroid Molecular Dynamics: Application to Liquid *para*-Hydrogen", *Chem. Phys. Lett.* **262**, 415-420 (1996).
74. J. Cao and G. A. Voth, "A Unified Framework for Quantum Activated Rate Processes: I. General Theory", *J. Chem. Phys.* **105**, 6856-6870 (1996).
75. L. W. Ungar, N. F. Scherer, and G. A. Voth, "Classical Molecular Dynamics Simulation of the Photoinduced Electron Transfer Dynamics of Plastocyanin", *Biophys. J.* **72**, 5-17 (1997).
76. J. Lobaugh and G. A. Voth, "A Quantum Model for Water: Equilibrium and Dynamical Properties", *J. Chem. Phys.* **106**, 2400-2410 (1997).
77. M. J. Murphy, G. A. Voth, and A. L. R. Bug, "Classical and Quantum Transition State Theory for the Diffusion of Helium in Silica Sodalite", *J. Phys. Chem.* **101**, 491-503 (1997).
78. J. Cao and G. A. Voth, "A Unified Framework for Quantum Activated Rate Processes: II. The Nonadiabatic Limit", *J. Chem. Phys.* **106**, 1769-1779 (1997).
79. C. P. Ursenbach, A. Calhoun, and G. A. Voth, "A First-Principles Simulation of the Water/Semiconductor Interface", *J. Chem. Phys.* **106**, 2811-2818 (1997).
80. C. Minichino and G. A. Voth, "Potential Energy Surfaces for Chemical Reactions: An Analytical Representation from Coarse Grained Data with an Application to Proton Transfer in Water", *J. Phys. Chem.* **101**, 4544-4552 (1997).

81. M. Pavese, S. Chawla, D. Lu, J. Lobaugh, and G. A. Voth, "Quantum Effects and the Excess Proton in Water," *J. Chem. Phys.* **107**, 7428-7432 (1997).
82. S. Jang and G. A. Voth, "Simple Reversible Molecular Dynamics Algorithms for Nosé-Hoover Chain Dynamics," *J. Chem. Phys.* **107**, 9514-9526 (1997).
83. Y. Boroda, A. Calhoun, and G. A. Voth, "A Theory for Electron Transfer across the Electrode/Electrolyte Interface Involving Multiple Redox Ions," *J. Chem. Phys.* **107**, 8940-8954 (1997).
84. C. D. Schwieters and G. A. Voth, "A Semiclassical Method for the Calculation of Nonadiabatic Tunneling Rates," *J. Chem. Phys.* **108**, 1055-1062 (1998).
85. Y. Boroda and G. A. Voth, "A Theory for Electron Transfer between an Electrode and a Multilevel Acceptor/Donor Species in an Electrolyte Solution," *J. Electroanal. Chem.* **450**, 95-107 (1998).
86. A. Calhoun and G. A. Voth, "The Computer Simulation of Electron Transfer Processes Across the Electrode/Electrolyte Interface: A Treatment of Solvent and Electrode Polarizability," *J. Electroanal. Chem.* **450**, 253-264 (1998).
87. S. Jang and G. A. Voth, "Lithium Impurity Recombination in Solid *para*-Hydrogen: A Path Integral Quantum Transition State Theory Study," *J. Chem. Phys.* **108**, 4098-4106 (1998).
88. M. T. M. Koper and G. A. Voth, "A Theory for Adiabatic Bond Breaking Electron Transfer Reactions at Metal Electrodes," *Chem. Phys. Lett.* **282**, 100-106 (1998).
89. R. Hernandez and G. A. Voth, "Quantum Time Correlation Functions and Classical Coherence," *Chem. Phys.* **233**, 243-256 (1998).
90. S. Chawla and G. A. Voth, "Exact Exchange in *Ab Initio* Molecular Dynamics Simulations: An Efficient Plane-Wave based Algorithm," *J. Chem. Phys.* **108**, 4697-4700 (1998).
91. M. Pavese and G. A. Voth, "Quantum and Classical Simulations of an Excess Proton in Water", *Ber. Bunsenges. Phys. Chem.* **102**, 527-532 (1998).
92. D. Lu and G. A. Voth, "Proton Transfer in the Enzyme Carbonic Anhydrase: An *Ab Initio* Study," *J. Am. Chem. Soc.* **120**, 4006-4014 (1998).
93. D. Lu and G. A. Voth, "Molecular Dynamics Simulations of Human Carbonic Anhydrase II: Insights into Experimental Results and the Role of Solvation," *Proteins* **33**, 119-134 (1998).
94. M. T. M. Koper and G. A. Voth, "A Three-Dimensional Potential Energy for Dissociative Adsorption and Associative Desorption at Metal Electrodes," *J. Chem. Phys.* **109**, 1991-2001 (1998).
95. U. W. Schmitt and G. A. Voth, "A Multi-State Empirical Valence Bond Model for Proton Transport in Water," *J. Phys. Chem. B* **102**, 5547-5551 (1998).
96. A. Calhoun and G. A. Voth, "The Computer Simulation of Correlated Electron Transfer Across the Electrode/Electrolyte Interface Involving Multiple Redox Species," *J. Chem. Phys.* **109**, 4569-4575 (1998).
97. A. Calhoun and G. A. Voth, "Isotope Effects in Electron Transfer Across the Electrode/Electrolyte Interface: A Measure of Solvent Mode Quantization," *J. Phys. Chem. B* **102**, 8563-8568 (1998).

98. M. Pavese, D. R. Berard, and G. A. Voth, "Ab initio Centroid Molecular Dynamics: A Fully Quantum Method for Condensed Phase Dynamics Simulations," *Chem. Phys. Lett.* **300**, 93-98 (1999).
99. P.-N. Roy and G. A. Voth, "On the Feynman Path Centroid Density for Bose-Einstein and Fermi-Dirac Statistics," *J. Chem. Phys.* **110**, 3647-3652 (1999).
100. Y. Pak and G. A. Voth, "Reactive Flux Calculations of Methyl Vinyl Ketone Reacting with Cyclopentadiene in Water," *J. Phys. Chem.* **103**, 925-931 (1999).
101. A. Calhoun, M. T. M. Koper, and G. A. Voth, "Largescale Computer Simulation of an Electrochemical Bond Breaking Reaction," *Chem. Phys. Lett.* **305**, 94-100 (1999).
102. A. Calhoun, M. T. M. Koper, and G. A. Voth, "Electrochemical Bond Breaking Reactions: A Comparison of Largescale Simulation Results with Analytical Theory" *J. Phys. Chem. B* **103**, 3442-3448 (1999).
103. C. D. Schweiters and G. A. Voth, "An Extension of Path Integral Quantum Transition State Theory to the Case of Nonadiabatic Activated Dynamics," *J. Chem. Phys.* **111**, 2869-2877 (1999).
104. S. Jang and G. A. Voth, "Path Integral Centroid Variables and the Formulation of Their Exact Real Time Dynamics," *J. Chem. Phys.* **111**, 2357-2370 (1999).
105. S. Jang and G. A. Voth, "A Derivation of Centroid Molecular Dynamics and Other Approximate Time Evolution Methods for Path Integral Centroid Variables," *J. Chem. Phys.* **111**, 2371-2384 (1999).
106. P. Vath, M. B. Zimmt, D. V. Matyushov, and G. A. Voth, "Temperature Dependence of the Solvent Reorganization Energy of Electron Transfer in Highly Polar Solvents," *J. Phys. Chem. B* **103**, 9130-9140 (1999).
107. D. V. Matyushov and G. A. Voth, "A Perturbation Theory for Solvation Thermodynamics: Dipolar-Quadrupolar Liquids," *J. Chem. Phys.* **111**, 3630-3638 (1999).
108. H. S. Randa, L. R. Forrest, G. A. Voth, and M. S. P. Sansom, "Molecular Dynamics of Synthetic Leucine-Serine Ion Channels in a Phospholipid Membrane," *Biophys. J.* **77**, 2400-2410 (1999).
109. L. W. Ungar, M. D. Newton, and G. A. Voth, "Classical and Quantum Simulation of Electron Transfer Through a Polypeptide," *J. Phys. Chem. B* **34**, 7367-7382 (1999).
110. P.-N. Roy, S. Jang, and G. A. Voth, "Feynman Path Centroid Dynamics for Fermi-Dirac Statistics," *J. Chem. Phys.* **111**, 5303-5305 (1999).
111. U. W. Schmitt and G. A. Voth, "Quantum Properties of the Excess Proton in Liquid Water," *Israel J. Chem.* **39**, 483-492 (1999).
112. U. W. Schmitt and G. A. Voth, "The Computer Simulation of Proton Transport in Water," *J. Chem. Phys.* **111**, 9361-9381 (1999).
113. S. Jang, C. D. Schweiters, and G. A. Voth, "A Modification of Path Integral Quantum Transition State Theory for Asymmetric and Metastable Potentials," *J. Phys. Chem. A* **103**, 9527-9538 (1999).

114. S. Jang, S. Jang, and G. A. Voth, "Quantum Molecular Dynamics Simulations of Low Temperature High Energy Density Matter: Solid *p*-H₂/Li and *p*-H₂/B," *J. Phys. Chem. A* **103**, 9512-9520 (1999).
115. S. Jang, Y. Pak, and G. A. Voth, "Quantum Dynamical Simulation of the Energy Relaxation Rate of the CN⁻ Ion in Water," *J. Phys. Chem. A* **103**, 10289-10293 (1999).
116. D. V. Matyushov and G. A. Voth, "A Theory of Electron Transfer and Steady-State Optical Spectra with Varying Electronic Polarizability," *J. Phys. Chem. A* **103**, 10981-10992 (1999).
117. J. P. Lewis, T. D. Sewell, R. B. Evans, and G. A. Voth, "Electronic Structure Calculation of the Structures and Energies of the Three Pure Polymorphic Forms of Crystalline HMX," *J. Phys. Chem. B* **104**, 1009-1013 (2000).
118. D. R. Reichman and G. A. Voth, "Self-Consistent Harmonic Theory of Solvation in Glassy Systems: Classical Solvation," *J. Chem. Phys.* **112**, 3267-3279 (2000).
119. D. R. Reichman and G. A. Voth, "Self-Consistent Harmonic Theory of Solvation in Glassy Systems: Quantum Solvation," *J. Chem. Phys.* **112**, 3280-3284 (2000).
120. T. C. Henderson, P. A. McMurtry, P. J. Smith, G. A. Voth, C. A. Wight, and D. W. Pershing, "Simulating Accidental Fires and Explosions," *Computing in Science and Engineering*, **2**, 64-76 (2000).
121. S. Jang and G. A. Voth, "A Relationship Between Centroid Dynamics and Path Integral Quantum Transition State Theory" *J. Chem. Phys.* **112**, 8747-8757 (2000).
122. M. Pavese, S. Jang, and G. A. Voth, "Centroid Molecular Dynamics: A Quantum Dynamics Method Suitable for the Parallel Computer," *Parallel Computing* **26**, 1025-1041 (2000). (Special Issue on Computational Chemistry).
123. M. Cuma, U. W. Schmitt, and G. A. Voth, "A Multi-State Empirical Valence Bond Model for Acid-Base Chemistry in Aqueous Solution," *Chem. Phys.* **258**, 187 (2000).
124. D. V. Matyushov and G. A. Voth, "Reorganization Parameters of Electronic Transitions in Electronically Delocalized Systems: I. Electron Transfer Reactions," *J. Phys. Chem. A* **104**, 6470-6484 (2000).
125. D. V. Matyushov and G. A. Voth, "Reorganization Parameters of Electronic Transitions in Electronically Delocalized Systems: II. Optical Spectra," *J. Phys. Chem. A* **104**, 6485-6494 (2000).
126. D. R. Reichman, P.-N. Roy, S. Jang, and G. A. Voth, "A Feynman Path Centroid Dynamics Approach for the Computation of Time Correlation Functions Involving Non-Linear Operators," *J. Chem. Phys.* **113**, 919-929 (2000).
127. G. K. Schenter, B. C. Garrett, and G. A. Voth, "The Quantum Vibrational Dynamics of Cl⁻(H₂O)_n Clusters," *J. Chem. Phys.* **113**, 5171 (2000).
128. J. R. Krumrine, S. Jang, M. H. Alexander, and G. A. Voth, "Quantum Molecular Dynamics and Spectral Simulation of a Boron Impurity in Solid *para*-Hydrogen," *J. Chem. Phys.* **113**, 9079-9089 (2000).

129. D. Matyushov and G. A. Voth, "Modeling the Free Energy Surfaces of Electron Transfer in Condensed Phases," *J. Chem. Phys.* **113**, 5413-5424 (2000).
130. U. W. Schmitt and G. A. Voth, "The Isotope Substitution Effect on the Hydrated Proton," *Chem. Phys. Lett.* **329**, 36-41 (2000).
131. J. P. Lewis, K. R. Glaesemann, R. B. Evans, K. VanOpdorp, and G. A. Voth, "Ab Initio Calculations of Reactive Pathways for Gas-Phase a-Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (a-HMX)" *J. Phys. Chem. A* **104**, 11384-11389 (2000).
132. T. J. F. Day, U. W. Schmitt, and G. A. Voth, "The Mechanism of Hydrated Proton Transport in Water," *J. Am. Chem. Soc.* **122**, 12027-12028 (2000).
133. G. A. Voth, "Feynman Path Centroid Dynamics," in *Progress in Theoretical Chemistry and Physics, Vol. 5*, S. D. Schwartz, Ed. (Kluwer, Dordrecht, 2000), Chap. 2, pp. 47-68.
134. M. T. M. Koper and G. A. Voth, "Molecular Dynamics of Bond-Breaking Electron-Transfer Reactions at Metal-Liquid Interfaces," *CATTECH* **4**, 51-55 (2000). (Highlight Article)
135. M. L. Brewer, U. Schmitt, and G. A. Voth, "The Formation and Dynamics of Proton Wires in Channel Environments," *Biophys. J.* **80**, 1691-1702 (2001).
136. S. Izvekov, A. Mazzolo, K. VanOpdorp, and G. A. Voth, "Ab initio Molecular Dynamics Simulation of the Cu(110)-Water Interface," *J. Chem. Phys.* **114**, 3248 (2001).
137. M. Ovchinnikov, V. A. Apkarian, and G. A. Voth, "Semiclassical Molecular Dynamics Computation of Spontaneous Light Emission in the Condensed Phase: Resonance Raman Spectra," *J. Chem. Phys.* **114**, 7130-7143 (2001).
138. G. Ayton, S. Bardenhagen, P. McMurtry, D. Sulsky, and G. A. Voth, "Interfacing Molecular Dynamics with Continuum Dynamics in Computer Simulation: Toward an Application to Biological Membranes," *IBM J. Res. Dev.* **45**, 417-426 (2001).
139. M. Cuma, U. W. Schmitt, and G. A. Voth, "A Multi-State Empirical Valence Bond Model for Weak Acid Dissociation in Aqueous Solution," *J. Phys. Chem. A* **105**, 2814-2823 (2001).
140. G. Ayton, S. Bardenhagen, P. McMurtry, D. Sulsky, and G. A. Voth, "Interfacing Continuum and Molecular Dynamics: An Application to Lipid Bilayers," *J. Chem. Phys.* **114**, 6913-6924 (2001).
141. J. P. Lewis, K. R. Glaesemann, G. A. Voth, J. Fritsch, A. A. Demkov, J. Ortega, and O. F. Sankey, "Further Developments in the Local-Orbital Density-Functional-Theory Tight-Binding Method," *Phys. Rev. B* **64**, 195103-1:10 (2001).
142. H. B. Schlegel, J. M. Millam, S. S. Iyengar, G. A. Voth, A. D. Daniels, G. E. Scuseria, and M. J. Frisch, "Ab Initio Molecular Dynamics: Propagating the Density Matrix with Gaussian Orbitals," *J. Chem. Phys.* **114**, 9758-9763 (2001).
143. A. E. Lefohn, M. V. Ovchinnikov, and G. A. Voth, "A Multi-State Empirical Valence Bond Approach to a Polarizable and Flexible Water Model," *J. Phys. Chem. B* **105**, 6628-6637 (2001).
144. N. V. Blinov, P.-N. Roy, and G. A. Voth, "Path Integral Formulation of Centroid Dynamics for Systems Obeying Bose-Einstein Statistics," *J. Chem. Phys.* **115**, 4484 (2001).

145. S. Izvekov and G. A. Voth, "Ab initio Molecular Dynamics Simulation of the Ag(111)–Water Interface," *J. Chem. Phys.* **115**, 7196-7206 (2001).
146. S. Jang, S. Jang, and G. A. Voth, "Applications Of Higher Order Composite Factorization Schemes In Imaginary Time Path Integral Simulations," *J. Chem. Phys.* **115**, 7832-7842 (2001).
147. E. Geva, Q. Shi, and G. A. Voth, "Quantum Mechanical Reaction Rate Constants from Centroid Molecular Dynamics Simulations," *J. Chem. Phys.* **115**, 9209-9222 (2001).
148. S. S. Iyengar, H. B. Schlegel, J. M. Millam, G. A. Voth, G. E. Scuseria, and M. J. Frisch, "Ab Initio Molecular Dynamics: Propagating the Density Matrix with Gaussian Orbitals. II. Generalization based on Mass-weighting, Idempotency, Energy Conservation, and Choice of Initial Conditions," *J. Chem. Phys.* **115**, 10291-10302 (2001).
149. J. Kim, U. W. Schmitt, J. A. Gruetzmacher, G. A. Voth, and N. F. Scherer, "The Vibrational Spectrum of the Hydrated Proton: Comparison of Experiment, Simulation, and Normal Mode Analysis," *J. Chem. Phys.* **116**, 737-746 (2002).
150. G. Ayton, A. M. Smondyrev, S. G. Bardenhagen, P. McMurtry, and G. A. Voth, "Calculating the Bulk Modulus for a Lipid Bilayer with Non-Equilibrium Molecular Dynamics Simulation," *Biophys. J.* **82**, 1226-1238 (2002).
151. A. M. Smondyrev and G. A. Voth, "Molecular Dynamics Simulation of Proton Transport Near the Surface of a Phospholipid Membrane," *Biophys. J.* **82**, 1460-1468 (2002).
152. S. Izvekov and G. A. Voth, "Car-Parrinello Molecular Dynamics Simulation of Liquid Water: New Results," *J. Chem. Phys.* **116**, 10372-10376 (2002).
153. J.-L. Liao and G. A. Voth, "Numerical Approaches for Computing Nonadiabatic Electron Transfer Rate Constants," *J. Chem. Phys.* **116**, 9174-9187 (2002).
154. G. Narayanan, S. Izvekov, and G. A. Voth, "Ab initio Molecular Dynamics Simulation of the H/InP(100)–Water Interface," *J. Chem. Phys.* **117**, 872-884 (2002).
155. G. Ayton, A. M. Smondyrev, S. G. Bardenhagen, P. McMurtry, and G. A. Voth, "Interfacing Molecular Dynamics and Macro-scale Simulations for Lipid Bilayer Vesicles," *Biophys. J.* **83**, 1026-1038 (2002).
156. A. M. Smondyrev and G. A. Voth, "Molecular Dynamics Simulation of Proton Transport Through the Influenza A Virus M2 Channel," *Biophys. J.* **83**, 1987-1996 (2002).
157. T. J. F. Day, A. V. Soudackov, M. Cuma, U. W. Schmitt, and G. A. Voth, "A Second Generation Multi-State Empirical Valence Bond Model for Proton Transport in Aqueous Systems," *J. Chem. Phys.* **117**, 5839-5849 (2002).
158. J.-L. Liao and G. A. Voth, "A Centroid Molecular Dynamics Approach for Nonadiabatic Dynamical Processes in Condensed Phases: The Spin-Boson Case," *J. Phys. Chem. B* **106**, 8449-8455 (2002).
159. H. B. Schlegel, S. S. Iyengar, X. Li, J. M. Millam, G. A. Voth, G. E. Scuseria, and M. J. Frisch, "Ab Initio Molecular Dynamics: Propagating the Density Matrix with Gaussian Orbitals. III. Comparison with Born-Oppenheimer Dynamics," *J. Chem. Phys.* **117**, 8694-8704 (2002).

160. G. Ayton and G. A. Voth, "Bridging Microscopic and Mesoscopic Simulations of Lipid Bilayers," *Biophys. J.* **83**, 3357-3370 (2002).
161. D. T. Mirjianian, M. H. Alexander, and G. A. Voth, "Path Integral Molecular Dynamics Simulation of Solid *Para*-Hydrogen with an Aluminum Impurity," *Chem. Phys. Lett.* **365**, 487-493 (2002).
162. D. V. Matyushov and G. A. Voth, "New Developments in the Theoretical Description of Charge-Transfer Reactions in Condensed Phases," *Reviews in Computational Chemistry*, Volume 18, K. B. Lipkowitz and D. B. Boyd, Editors (John Wiley and Sons, New York, 2002), pp. 147-210.
163. S. S. Iyengar, H. B. Schlegel, G. A. Voth, J. M. Millam, G. E. Scuseria, and M. J. Frisch, "*Ab Initio* Molecular Dynamics: Propagating the Density Matrix with Gaussian Orbitals. IV. Formal Analysis of the Deviations from Born-Oppenheimer Dynamics," *Israel. J. Chem.* **42**, 191-202 (2003).
164. J. Jeon, A. E. Lefohn, and G. A. Voth, "An Improved Polarflex Water Model," *J. Chem. Phys.* **118**, 7504-7518 (2003).
165. S. D. Shellman, J. P. Lewis, K. R. Glaesemann, K. Sikorski, and G. A. Voth, "Massively Parallel Linear-Scaling Algorithm in the *Ab Initio* Tight-Binding FIREBALL Method," *J. Comp. Phys.* **188**, 1-15 (2003).
166. D. W. Small, D. M. Matyushov, and G. A. Voth, "The Theory of Electron Transfer Reactions: What May Be Missing?" *J. Am. Chem. Soc.* **125**, 7470-7478 (2003).
167. S. S. Iyengar, C. J. Burnham, M. K. Petersen, and G. A. Voth "Modeling Condensed Phase Chemistry Through Molecular Dynamics Simulation," *Computers in Science and Engineering* **5**, 22-31 (2003). (Invited)
168. Y. Wu and G. A. Voth, "Computational Studies of Proton Transport through the M2 Channel", *FEBS Letters* **552**, 23-27 (2003).
169. Y. Wu and G. A. Voth, "A Computer Simulation Study of the Hydrated Proton in a Synthetic Proton Channel," *Biophys. J.* **85**, 864-875 (2003).
170. G. A. Voth, "The Computer Simulation of Proton Transport in Biomolecular Systems," *Frontiers in Bioscience* **8**, 1384-1397 (2003).
171. S. S. Iyengar, H. B. Schlegel, and G. A. Voth, "Atom-centered Density Matrix Propagation (ADMP): Generalizations using Bohmian Mechanics," *J. Phys. Chem.* **107**, 7269-7277 (2003).
172. M. G. Del Popolo and G. A. Voth, "On the Structure and Dynamics of Ionic Liquids," *J. Phys. Chem. B* **108**, 1744-1752 (2004).
173. G. Ayton, H. L. Tepper, D. T. Mirjianian, and G. A. Voth, "A New Perspective on the Coarse-grained Dynamics of Fluids," *J. Chem. Phys.* **120**, 4074-4088 (2004).
174. Y. Wu and G. A. Voth, "Computer Simulations of Proton Transport Through the M2 Channel of the Influenza A Virus" in *Viral Membrane Proteins: Structure, Function and Drug Design*, edited by W. Fischer (Kluwer Academic/Plenum Publishers, New York, 2004), Chap. 10.
175. N. Rega, S. S. Iyengar, G. A. Voth, H. B. Schlegel, T. Vreven, and M. J. Frisch, "Hybrid *Ab Initio* Empirical Molecular Dynamics: Combining the ONIOM Scheme with the Atom-centered Density Matrix Propagation (ADMP) Approach," *J. Phys. Chem. B* **108**, 4210 - 4220 (2004).

176. B. Ilan, E. Tajkhorshid, K. Schulten, and G. A. Voth, "The Mechanism of Proton Exclusion in Aquaporin Channels," *Proteins: Structure, Function, and Bioinformatics* **55**, 223-228 (2004).
177. G. S. Ayton and G. A. Voth, "The Simulation of Biomolecular Systems at Multiple Length and Time Scales," *Int. J. for Multiscale Comp. Eng. (IJMCE)* (Special Issue: Invited Article) **2**, 291-311 (2004).
178. B. J. Ka and G. A. Voth, "Combining the Semiclassical Initial Value Representation with Centroid Dynamics," *J. Phys. Chem. B* **108**, 6883-6892 (2004).
179. S. Izvekov, M. Parrinello, C. J. Burnham, and G. A. Voth, "Effective Force Fields for Condensed Phase Systems from *Ab Initio* Molecular Dynamics: A New Method for Force-Matching," *J. Chem. Phys.* **120**, 10896-10913 (2004).
180. A. Violi, A. F. Sarofim, and G. A. Voth, "Kinetic Monte Carlo-Molecular Dynamics Approach To Model Soot Inception," *Combust. Sci. and Tech.* **176**, 991-1005 (2004).
181. T. D. Hone and G. A. Voth, "A Centroid Molecular Dynamics Study of Liquid *para*-Hydrogen and *ortho*-Deuterium," *J. Chem. Phys.* **121**, 6412-6422 (2004).
182. T. Yan, C. J. Burnham, M. G. Del Popolo, and G. A. Voth, "Molecular Dynamics Simulation of Ionic Liquids: The Effect of Electronic Polarizability," *J. Phys. Chem. B* **108**, 11877-11881 (2004).
183. M. K. Petersen, S. S. Iyengar, T. J. F. Day, and G. A. Voth, "The Hydrated Proton at the Water Liquid/Vapor Interface," *J. Phys. Chem. B* **108**, 14804-14806 (2004).
184. J. L. McWhirter, G. S. Ayton, and G. A. Voth, "Coupling Field Theory with Mesoscopic Dynamical Simulations of Multi-Component Lipid Bilayers," *Biophys. J.* **87**, 3242-3263 (2004).
185. G. S. Ayton and G. A. Voth, "Mesoscopic Lateral Diffusion in Lipid Bilayers," *Biophys. J.* **87**, 3299-3311 (2004).
186. H. Lapid, N. Agmon, M. K. Petersen, and G. A. Voth, "A Bond-order Analysis of the Mechanism for Hydrated Proton Mobility in Liquid Water," *J. Chem. Phys.* **122**, 014506(1-11) (2005).
187. A. Venkatnathan and G. A. Voth, "Superposition State Molecular Dynamics," *J. Chem. Theory Comp.* **1**, 36-40 (2005).
188. T. D. Hone, S. Izvekov, and G. A. Voth, "Fast Centroid Molecular Dynamics: A Force-Matching Approach for the Predetermination of the Effective Centroid Forces," *J. Chem. Phys.* **122**, 054105(1-7) (2005).
189. J. Jeon and G. A. Voth, "The Dynamic Stress Responses to Area Change in Planar Lipid Bilayer Membranes," *Biophys. J.* **88**, 1104-1119 (2005).
190. S. Izvekov and G. A. Voth, "A Multiscale Coarse-Graining Method for Biomolecular Systems," *J. Phys. Chem. B* **109**, 2469-2473 (2005).
191. M. K. Petersen, F. Wang, N. P. Blake, H. Metiu, and G. A. Voth, "Excess Proton Solvation and Delocalization in a Hydrophilic Pocket of the Proton Conducting Polymer Membrane NafionTM," *J. Phys. Chem. B* **109**, 3727-3730 (2005).

192. S. S. Iyengar, T. J. F. Day, and G. A. Voth, "On the Amphiphilic Behavior of the Hydrated Proton: An *Ab Initio* Molecular Dynamics Study," *Int. J. Mass. Spec.* **241**, 197-204 (2005).
193. S. Izvekov and G. A. Voth, "Effective Force Field for Liquid Hydrogen Fluoride from *Ab Initio* Molecular Dynamics Simulation Using the Force-Matching Method," *J. Phys. Chem. B* **109**, 6573-6586 (2005).
194. E. Geva, S. Jang, and G. A. Voth, "Quantum Rate Theory: A Path Integral Centroid Perspective," in Encyclopedia of Materials Modeling: Vol. I, Fundamental Models and Methods, S. Yip, Editor (2005).
195. H. L. Tepper and G. A. Voth, "Protons May Leak Through Pure Lipid Bilayers via a Concerted Mechanism," *Biophys. J.* **88**, 3095-3108 (2005).
196. F. Wang and G. A. Voth, "A Linear-Scaling Self-Consistent Generalization of the Multi-State Empirical Valence Bond Model for Multiple Excess Protons in Aqueous Systems", *J. Chem. Phys.* **122**, 144105(1-9) (2005).
197. H. L. Tepper and G. A. Voth, "A Coarse-Grained Model for Double-Helix Molecules in Solution: Spontaneous Helix Formation and Equilibrium Properties," *J. Chem. Phys.* **122**, 124906(1-11) (2005).
198. J. Xu and G. A. Voth, "Computer Simulation of Explicit Proton Translocation in Cytochrome c Oxidase: The D-Pathway," *Proc. Nat. Acad. Sci. USA* **102**, 6795-6800 (2005).
199. G. S. Ayton, J. L. McWhirter, P. McMurtry, and G. A. Voth, "Coupling Field Theory with Continuum Mechanics: A Simulation of Domain Formation in Giant Unilamellar Vesicles," *Biophys. J.* **88**, 3855-3869 (2005).
200. R. Chang, G. S. Ayton, and G. A. Voth, "Multi-Scale Coupling of Mesoscopic and Atomistic-Level Lipid Bilayer Simulations," *J. Chem. Phys.* **122**, 244716(1-12) (2005).
201. S. Izvekov and G. A. Voth, "*Ab Initio* Molecular Dynamics Simulation of Aqueous Proton Solvation and Transport Revisited," *J. Chem. Phys.* **123**, 044505(1-9) (2005).
202. S. S. Iyengar, M. K. Petersen, T. J. F. Day, C. J. Burnham, V. E. Tiege, and G. A. Voth, "The Properties of Ion-Water Clusters. I. The Protonated 21-Water Cluster," *J. Chem. Phys.* **123**, 084309(1-9) (2005).
203. Y. Wang and G. A. Voth, "Unique Spatial Heterogeneity in Ionic Liquids," *J. Am. Chem. Soc.* **127**, 12192-12193 (2005).
204. J.-W. Chu and G. A. Voth, "Allostery of Actin Filaments: Molecular Dynamics Simulations and Coarse-Grained Analyses," *Proc. Natl. Acad. Sci. USA* **102**, 13111-13116 (2005).
205. S. Izvekov, A. Violi, and G. A. Voth, "Systematic Coarse-Graining of Nanoparticle Interactions in Molecular Dynamics Simulation," *J. Phys. Chem. B* **109**, 17019-17024 (2005).
206. Y. Wu and G. A. Voth, "A Computational Study of the Open and Closed States of the Influenza A M2 Proton Channel," *Biophys. J.* **89**, 2402-2411 (2005).
207. Q. Shi and G. A. Voth, "Multiscale Modeling of Phase Separation in Mixed Lipid Bilayers," *Biophys. J.* **89**, 2385-2394 (2005).

208. P. D. Blood, G. S. Ayton, and G. A. Voth, "Probing the Molecular-Scale Lipid Bilayer Response to Shear Flow using Nonequilibrium Molecular Dynamics" *J. Phys. Chem. B* **109**, 18673-18679 (2005).
209. S. Izvekov and G. A. Voth, "Multiscale Coarse-Graining of Liquid State Systems," *J. Chem. Phys.* **123**, 134105(1-13) (2005).
210. B. J. Ka and G. A. Voth, "An Efficient and Accurate Implementation of Centroid Molecular Dynamics Using a Gaussian Approximation," *J. Phys. Chem. A* **109**, 11609-11617 (2005).
211. N. P. Blake, M. K. Petersen, G. A. Voth, and H. Metiu, "The Structure of Hydrated Na^+ -NafionTM Polymer Membranes," *J. Phys. Chem. B* **109**, 24244-24253 (2005).
212. S. Paramore, G. S. Ayton, D. T. Mirijanian, and G. A. Voth, "Extending a Spectrin Repeat Unit I. Linear Force-Extension Response," *Biophys. J.* **90**, 92-100 (2006).
213. S. Paramore, G. S. Ayton, and G. A. Voth, "Extending a Spectrin Repeat Unit II. Rupture Behavior," *Biophys. J.* **90**, 101-111 (2006).
214. Y. Wu, H. L. Tepper, and G. A. Voth, "A Flexible Simple Point Charge Water Model with Improved Liquid State Properties," *J. Chem. Phys.* **124**, 024503(1-12) (2006).
215. C. M. Maupin, K. F. Wong, A. V. Soudakov, S. Kim, and G. A. Voth, "A Multi-State Empirical Valence Bond Description of Protonatable Amino Acids," *J. Phys. Chem. A* **110** 631-639 (2006).
216. T. Yan, S. Li, W. Jiang, X. Gao, B. Xiang, and G. A. Voth, "Structure of the Liquid/Vacuum Interface of Room Temperature Ionic Liquids: A Molecular Dynamics Study," *J. Phys. Chem. B* **110**, 1800-1806 (2006).
217. Y. Wang, S. Izvekov, T. Yan, and G. A. Voth, "Multiscale Coarse-Graining of Ionic Liquids," *J. Phys. Chem. B* **110**, 3564-3575 (2006).
218. J.-W. Chu and G. A. Voth, "Coarse-Grained Modeling of the Actin Filament Derived from Atomistic-Scale Simulations," *Biophys. J.* **90**, 1572-1582 (2006).
219. G. S. Ayton, J. L. McWhirter, and G. A. Voth, "A Second Generation Lipid Bilayer Model: Connections to Field Theory Descriptions of Membranes and Nonlocal Hydrodynamics," *J. Chem. Phys.* **124**, 064906(1-12) (2006).
220. C. J. Burnham, M. K. Petersen, T. J. F. Day, S. S. Iyengar, and G. A. Voth, "The Properties of Ion-Water Clusters. II. Solvation Structures of Na^+ , Cl^- , And H^+ Clusters as a Function of Temperature," *J. Chem. Phys.* **124**, 024327(1-9) (2006).
221. S. Izvekov and G. A. Voth, "Multiscale Coarse-graining of Mixed Phospholipid/Cholesterol Bilayer," *J. Chem. Theory Comp.* **2**, 637-648 (2006).
222. T. D. Hone, P. J. Rossky, and G. A. Voth, "A Comparative Study of Imaginary Time Path Integral based Methods for Quantum Dynamics," *J. Chem. Phys.* **124**, 154103(1-9) (2006).
223. G. A. Voth, "Computer Simulation of Proton Solvation and Transport in Aqueous and Biomolecular Systems," *Acc. Chem. Res.* **39**, 143-150 (2006).

224. M. K. Petersen and G. A. Voth, "The Amphiphilic Character of the Hydrated Proton in Methanol-Water Solutions," *J. Phys. Chem. B* **110**, 7085-7089 (2006).
225. H. Chen, Y. Wu, and G. A. Voth, "Origins of Proton Transport Behavior from Selectivity Domain Mutations of the Aquaporin-1 Channel," *Biophys. J.* **90**, L73-L75 (2006).
226. J.-W. Chu, S. Izvekov, and G. A. Voth, "The Multiscale Challenge for Biomolecular Systems: Coarse-grained Modeling," *Mol. Sim.* **32**, 211-218 (2006).
227. V. Krishna and G. A. Voth, "Evaluation of Nonlinear Quantum Time Correlation Functions within the Centroid Dynamics Formulation," *J. Phys. Chem. B* **110**, 18953-18957 (2006).
228. J. Xu and G. A. Voth, "Free Energy Profiles for H⁺ Conduction in the D-Pathway of Cytochrome c Oxidase: A Study of the Wild Type and N98D Mutant Enzymes," *Biochim. et Biophys. Acta-Bioenergetics* **1757**, 852-859 (2006).
229. Q. Shi, S. Izvekov, and G. A. Voth, "Mixed Atomistic and Coarse-grained Molecular Dynamics: Simulation of a Membrane Bound Ion Channel," *J. Phys. Chem. B* **110**, 15045-15048 (2006).
230. M. K. Petersen and G. A. Voth, "Characterization of the Solvation and Transport of the Hydrated Proton in the Perfluorosulfonic Acid Membrane Nafion™," *J. Phys. Chem. B* **110**, 18594-18600 (2006).
231. Y. Wang and G. A. Voth, "Tail Aggregation and Domain Diffusion in Ionic Liquids," *J. Phys. Chem. B* **110**, 18601-18608 (2006).
232. P. D. Blood and G. A. Voth, "Observation of Bin/amphiphysin/Rvs (BAR) Domain-Induced Membrane Curvature by Means of Molecular Dynamics Simulation," *Proc. Natl. Acad. Sci. USA* **103**, 15068-15072 (2006).
233. S. Paramore and G. A. Voth, "Examining the Influence of Linkers and Tertiary Structure in the Forced Unfolding of Multiple-Repeat Spectrin Molecules," *Biophys. J.* **91**, 3436-3445 (2006).
234. S. Izvekov and G. A. Voth, "Modeling Real Dynamics in the Coarse-grained Representation of Condensed Phase Systems," *J. Chem. Phys.* **125**, 151101(1-4) (2006).
235. Harald L. Tepper and Gregory A. Voth, "Mechanisms of Passive Ion Permeation through Lipid Bilayers: New Insights from Simulations," *J. Phys. Chem. B* **110**, 21327-21337 (2006).
236. Y. Gebremichael, G. S. Ayton, and G. A. Voth, "Mesoscopic Modeling of Bacterial Flagellar Microhydrodynamics" *Biophys. J.* **91**, 3640-3652 (2006).
237. F. Paesani, W. Zhang, D. Case, T. L. Cheatham, III, and G. A. Voth, "An Accurate and Simple Quantum Model for Liquid Water," *J. Chem. Phys.* **125**, 184507(1-11) (2006).
238. D. T. Mirijanian, J.-W. Chu, G. S. Ayton, and G. A. Voth, "Atomistic and Coarse-grained Analysis of Double Spectrin Repeat Units: The Molecular Origins of Flexibility," *J. Mol. Biol.* **365**, 523-534 (2007).
239. H. Chen, B. Ilan, Y. Wu, F. Zhu, K. Schulten, and G. A. Voth, "Charge Delocalization in Proton Channels. I. The Aquaporin Channels and Proton Blockage," *Biophys. J.* **92**, 46-60 (2007).

240. Y. Wu, B. Ilan, and G. A. Voth, "Charge Delocalization in Proton Channels. II. The LS2 Channel and Proton Selectivity," *Biophys. J.* **92**, 61-69 (2007).
241. P. Liu and G. A. Voth, "Smart Resolution Exchange: An Efficient Algorithm for Exploring Complex Energy Landscapes," *J. Chem. Phys.* **126**, 045106(1-6) (2007).
242. S. Paramore, G. S. Ayton, and G. A. Voth, "Extending the Fluctuation Theorem to Describe Reaction Coordinates," *J. Chem. Phys.* **126**, 051102(1-4) (2007).
243. G. S. Ayton and G. A. Voth, "Multiscale Simulation of Transmembrane Proteins," *J. Struct. Biol.* **157**, 570-578 (2007).
244. J. Xu, M. A. Sharpe, L. Qin, S. Ferguson-Miller, and G. A. Voth, "Storage of an Excess Proton in the Hydrogen-bonded Network of the D-pathway of Cytochrome c Oxidase: Identification of a Protonated Water Cluster," *J. Am. Chem. Soc.* **129**, 2910-2913 (2007).
245. C. M. Maupin and G. A. Voth, "Preferred Orientation of His-64 in Human Carbonic Anhydrase II," *Biochem.* **46**, 2938-2947 (2007).
246. S. Z. Fisher, C. M. Maupin, L. Govindasamy, M. Budayova-Spano, C. Tu, M. Agbandje-McKenna, D. N. Silverman, G. A. Voth, and R. McKenna, "Atomic Crystal and Molecular Dynamics Simulation Structures of Human Carbonic Anhydrase II: Insights into the Proton Transfer Mechanism," *Biochem.* **46**, 2930-2937 (2007).
247. J.-W. Chu, S. Izvekov, G. S. Ayton, and G. A. Voth, "Emerging Methods for Multiscale Simulation of Biomolecular Systems," *Mol. Phys.* **105**, 167-175 (2007).
248. S. Iuchi, S. Izvekov, and G. A. Voth, "Are Many-body Electronic Polarization Effects Important in Liquid Water," *J. Chem. Phys.* **126**, 124505(1-13) (2007).
249. G. S. Ayton, W. G. Noid, and G. A. Voth, "Multiscale Modeling of Biomolecular Systems: In Serial and in Parallel," *Curr. Opin. Struct. Biol.* **17**, 192-198 (2007).
250. G. S. Ayton, P. D. Blood, and G. A. Voth, "Membrane Remodeling from N-BAR Domain Interactions: Insights from Multiscale Simulation," *Biophys. J.* **92**, 3595-3602 (2007).
251. W. G. Noid, J.-W. Chu, G. S. Ayton, and G. A. Voth, "Multiscale Coarse-graining and Structural Correlations: Connections to Liquid State Theory," *J. Phys. Chem. B* **111**, 4116-4127 (2007).
252. J. M. J. Swanson, C. M. Maupin, H. Chen, M. K. Petersen, J. Xu, Y. Wu, and G. A. Voth, "Proton Solvation and Transport in Aqueous and Biomolecular Systems: Insights from Computer Simulations," (Invited Feature Article) *J. Phys. Chem. B* **111**, 4300-4314 (2007).
253. Y. Wang, W. Jiang, and G. A. Voth, "Spatial Heterogeneity in Ionic Liquids," in *Ionic Liquids IV. Not Just Solvents Anymore*, Brennecke, J. F.; Rogers, R. D.; Seddon, K. R. (Eds.); ACS Symposium Series 975; American Chemical Society: Washington DC, 2007; pp. 272-307.
254. W. Jiang, Y. Wang, and G. A. Voth, "Molecular Dynamics Simulation of Nanostructural Organization in Ionic Liquid/Water Mixtures." *J. Phys. Chem. B* **111**, 4812-4818 (2007).
255. J. Zhou, I. F. Thorpe, S. Izvekov, and G. A. Voth, "Coarse-grained Peptide Modeling using a Systematic Force-matching Approach," *Biophys. J.* **92**, 4289-4303 (2007).

256. Z. Qin, H. L. Tepper, and G. A. Voth, "Effect of Membrane Environment on Proton Permeation through Gramicidin A Channels," *J. Phys. Chem. B* **111**, 9931-9939 (2007).
257. F. Paesani, S. Iuchi, and G. A. Voth, "Quantum Effects in Liquid Water from an *Ab Initio*-Based Polarizable Force Field," *J. Chem. Phys.* **127**, 074506(1-15) (2007).
258. S. Paramore, G. S. Ayton, and G. A. Voth, "Transient Violations of the Second Law of Thermodynamics Examined Using Synthetic Atomic Force Microscopy and the Fluctuation Theorem," *J. Chem. Phys.* **127**, 105105(1-11) (2007).
259. P. Liu, S. Izvekov, and G. A. Voth, "Multiscale Coarse-Graining of Monosaccharides," *J. Phys. Chem. B* **111**, 11566-11575 (2007).
260. H. Chen, Y. Wu, and G. A. Voth, "Proton Transport Behavior Through the Influenza A M2 Channel: Insights from Molecular Simulation," *Biophys. J.* **93**, 3470-3479 (2007).
261. J.-W. Chu and G. A. Voth, "Coarse-Grained Free Energy Functions for Studying Protein Conformational Changes: A Many-Basin Double Well Model," *Biophys. J.* **93**, 3860-3871 (2007).
262. G. S. Ayton, W. G. Noid, and G. A. Voth, "Systematic Coarse-graining of Biomolecular and Soft Matter Systems," *MRS Bulletin* **32**, 929-934 (2007).
263. Y. Wang, W. Jiang, T. Yan, and G. A. Voth, "Understanding Ionic Liquids through Atomistic and Coarse-Grained Molecular Dynamics Simulations," *Acc. Chem. Res.* **40**, 1193-1199 (2007).
264. Y. Wu, H. Chen, F. Wang, F. Paesani, and G. A. Voth, "An Improved Multistate Empirical Valence Bond Model for Aqueous Proton Solvation and Transport," *J. Phys. Chem. B* **112**, 467-482 (2008); **112**, 7146 (2008) (Addition and Correction).
265. F. Paesani and G. A. Voth, "Quantum Effects Strongly Influence the Surface Premelting of Ice", *J. Phys. Chem. C* **112**, 324-327 (2008).
266. W. Jiang, Y. Wang, T. Yan, and G. A. Voth, "A Multiscale Coarse-Graining Study of Liquid/Vacuum Interface of Room-Temperature Ionic Liquids with Alkyl Substituents of Different Lengths", *J. Phys. Chem. C* **112**, 1132-1139 (2008).
267. J. Xu and G. A. Voth, "Redox-Coupled Proton Pumping in Cytochrome *c* Oxidase: Further Insights from Computer Simulation," *Biochim. et Biophys. Acta-Bioenergetics* **1777**, 196-201 (2008).
268. D. T. Mirjianian and G. A. Voth, "Unique Elastic Properties of the Spectrin Tetramer as Revealed by Multiscale Coarse-Grained Modeling," *Proc. Natl. Acad. Sci. USA* **105**, 1204-1208 (2008).
269. W. Jiang, T. Yan, Y. Wang, and G. A. Voth, "Molecular Dynamics Simulation of the Energetic Room Temperature Ionic Liquid 1-Hydroxyethyl-4Amino-1, 2, 4-Triazolium Nitrate (HEATN)", *J. Phys. Chem. B* **112**, 3121-3131 (2008).
270. F. Wang, S. Izvekov, and G. A. Voth, "Unusual 'Amphiphilic' Association of Hydrated Protons in Strong Acid Solution", *J. Am. Chem. Soc.* **130**, 3120-3126 (2008).
271. S. Izvekov,* J. M. J. Swanson,* and G. A. Voth, "Coarse-graining in Interaction Space: A Systematic Approach for Replacing Long-ranged Electrostatics by Short-ranged Effective Potentials", *J. Phys. Chem. B* **112**, 4711-4724 (2008). (*Authors contributed equally).

272. M. Ceotto, G. S. Ayton, and G. A. Voth, "Accelerated Superposition State Molecular Dynamics for Condensed Phase Systems", *J. Chem. Theor. Comp.* **4**, 560-568 (2008).
273. J. Jeon and G. A. Voth, "Gating of the Mechanosensitive Channel Protein MscL: The Interplay of Membrane and Protein," *Biophys. J.* **94**, 3497-3511 (2008).
274. M. K. Petersen, A. J. Hatt, and G. A. Voth, "Orientational Dynamics of Water in the Nafion Polymer Electrolyte Membrane and Its Relationship to Proton Transport", *J. Phys. Chem. B* **112**, 7754–7761 (2008).
275. W. G. Noid, J.-W. Chu, G. S. Ayton, V. Krishna, S. Izvekov, G. A. Voth, A. Das, and H. C. Andersen, "The Multiscale Coarse-graining Method I: A Rigorous Bridge between Atomistic and Coarse-grained Models" *J. Chem. Phys.* **128**, 244114 (1-11) (2008).
276. W. G. Noid, P. Liu, Y. Wang, J.-W. Chu, G. S. Ayton, S. Izvekov, H. C. Andersen, and G. A. Voth, "The Multiscale Coarse-graining Method. II. Numerical Implementation for Coarse-grained Molecular Models", *J. Chem. Phys.* **128**, 244115 (1-20) (2008).
277. P. D. Blood, R. D. Swenson, and G. A. Voth, "Factors Influencing Local Membrane Curvature Induction by N-BAR Domains as Revealed by Molecular Dynamics Simulations," *Biophys. J.* **95**, 1866-1876 (2008).
278. O. Markovitch, H. Chen, S. Izvekov, F. Paesani, G. A. Voth, and N. Agmon, "Statistical Identification of the Mechanism of Proton Mobility", *J. Phys. Chem. B* **112**, 9456-9466 (2008).
279. Y. Gebremichael, J.-W. Chu, and G. A. Voth, "Intrinsic Bending and Structural Rearrangement of Tubulin Dimer: Molecular Dynamics Simulations and Coarse-grained Analysis", *Biophys. J.* **95**, 2487-2499 (2008).
280. C. M. Maupin, M. G. Saunders, I. F. Thorpe, R. McKenna, D. N. Silverman, and G. A. Voth, "Origins of Enhanced Proton Transport in the Y7F Mutant of Human Carbonic Anhydrase II", *J. Am. Chem. Soc.* **130**, 11399–11408 (2008).
281. G. S. Ayton, S. Izvekov, W.G. Noid and G. A. Voth, "Multiscale Simulation of Membranes and Membrane Proteins: Connecting Molecular Interactions to Mesoscopic Behavior," *Current Topics in Membranes*, **60**, 182-219 (2008).
282. E. Lyman, J. Pfaendtner, and G. A. Voth, "Systematic Multiscale Parameterization of Heterogeneous Elastic Network Models of Proteins", *Biophys. J.* **95**, 4183–4192 (2008).
283. I. F. Thorpe, J. Zhou, and G. A. Voth, "Peptide Folding Using Multiscale Coarse-grained Models", *J. Phys. Chem. B* **112**, 13079–13090 (2008).
284. P. Liu, Q. Shi, E. Lyman, and G. A. Voth, "Reconstructing Atomistic Detail from Coarse-grained Models with Resolution Exchange", *J. Chem. Phys.* **129**, 114103(1-8) (2008).
285. Z. Zhang, L. Lu, W. G. Noid, V. Krishna, J. Pfaendtner, and G. A. Voth, "A Systematic Methodology for Defining Coarse-grained Sites in Large Biomolecules", *Biophys. J.* **95**, 5073-5083 (2008).
286. F. Paesani and G. A. Voth, "Nonlinear Quantum Time Correlation Functions from Centroid Molecular Dynamics and the Maximum Entropy Method", *J. Chem. Phys.* **129**, 194113(1-10) (2008).

287. J. Pfaendtner and G. A. Voth, “Molecular Dynamics Simulation and Coarse-grained Analysis of the Arp2/3 Complex”, *Biophys. J.* **95**, 5324-5333 (2008).
288. Q. Shi, P. Liu, and G. A. Voth, “Coarse-Graining in Interaction Space: An Analytical Approximation for the Effective Short-Ranged Electrostatics”, *J. Phys. Chem. B* **112**, 16230–16237 (2008).
289. P. Liu, H. Daumé III, and G. A. Voth, “A Bayesian Statistics Approach to Multiscale Coarse-graining”, *J. Chem. Phys.* **129**, 214114(1-11) (2008).
290. L. Lu and G. A. Voth, “Systematic Coarse-graining of a Multi-component Lipid Bilayer”, *J. Phys. Chem. B* **113**, 1501-1510 (2009).
291. Y. Wang, W. G. Noid, P. Liu, and G. A. Voth, “Effective Force Coarse-Graining”, *Phys. Chem. Chem. Phys.* **11**, 2002-2015 (2009).
292. S. Iuchi, H. Chen, F. Paesani, and G. A. Voth, “The Hydrated Excess Proton at Water-Hydrophobic Interfaces”, *J. Phys. Chem. B* **113**, 4017-4030 (2009).
293. S. S. Xantheas and G. A. Voth, “Aqueous Solutions and their Interfaces”, *J. Phys. Chem. B* **113**, 3997 (2009).
294. G. S. Ayton and G. A. Voth, “A Hybrid Coarse-graining Approach for Lipid Bilayers at Large Length and Time Scales”, *J. Phys. Chem. B* **113**, 4413-4424 (2009).
295. S. Izvekov and G. A. Voth, “A Solvent Free Lipid Bilayer Model Using Multiscale Coarse-graining”, *J. Phys. Chem. B* **113**, 4443-4455 (2009).
296. H. Chen, T. Yan, and G. A. Voth, “A Computer Simulation Model for Proton Transport in Liquid Imidazole”, *J. Phys. Chem. A* **113**, 4507-4517 (2009).
297. J. L. Sonnenberg, K. F. Wong, G. A. Voth, and H. B. Schlegel, “A Distributed Gaussian Valence Bond Surface Derived from *Ab Initio* Calculations”, *J. Chem. Theory. Comp.* **5**, 949-961 (2009).
298. Y. Wang, S. Feng, and G. A. Voth, “Transferable Coarse-Grained Models for Ionic Liquids”, *J. Chem. Theor. Comp.* **5**, 1091-1098 (2009).
299. F. Paesani and G. A. Voth, “The Properties of Water: Insights from Quantum Simulations”, *J. Phys. Chem. B* **113**, 5702–5719 (2009). (Invited ACS Physical Chemistry Division Centennial Feature Article)
300. G. S. Ayton and G. A. Voth, “Systematic Multiscale Simulation of Membrane Protein Systems”, *Curr. Opin. Struct. Biol.* **19**, 138-144 (2009).
301. H. Chen and G. A. Voth, “Unusual Hydrophobic Interactions in Acidic Aqueous Solutions”, *J. Phys. Chem. B* **113**, 7291-7297 (2009).
302. C. M. Maupin, R. McKenna, D. N. Silverman, and G. A. Voth, “Elucidation of the Proton Transport Mechanism in Human Carbonic Anhydrase II”, *J. Am. Chem. Soc.* **131**, 7598-7608 (2009).
303. D. Wang and G. A. Voth, “Proton Transport Pathway in the ClC Cl⁻/H⁺ Antiporter”, *Biophys. J.* **97**, 121-131 (2009).

304. V. Krishna, W. G. Noid, and G. A. Voth, “The Multiscale Coarse-graining Method. IV. Transferring Coarse-grained Potentials Between Temperatures”, *J. Chem. Phys.* **131**, 024103(1-12) (2009).
305. J. Pfaendtner, D. Branduardi, T. D. Pollard, M. Parrinello, and G. A. Voth, “Nucleotide-Dependent Conformational States of Actin”, *Proc. Natl. Acad. Sci. USA* **106**, 12723–12728 (2009).
306. C. M. Maupin, J. Zheng, C. Tu, R. McKenna, D. N. Silverman, and G. A. Voth, “Effect of Active-site Mutations at Asn67 on the Proton Transfer Mechanism of Human Carbonic Anhydrase II”, *Biochem.* **48**, 7996-8005 (2009).
307. G. S. Ayton, R. D. Swenson, C. Mim, V. Unger, and G. A. Voth, “New Insights into BAR Domain Induced Membrane Remodeling”, *Biophys. J.* **97**, 1616–1625 (2009).
308. F. Paesani, S. S. Xantheas, and G. A. Voth, “Infrared Spectroscopy and Hydrogen-Bond Dynamics in Liquid Water from Quantum Simulations”, *J. Phys. Chem. B* **113**, 13118–13130 (2009).
309. Z. Zhang, J. Pfaendtner, and G. A. Voth, “Defining Coarse-grained Representations of Large Biomolecules and Biomolecular Complexes from Elastic Network Models”, *Biophys. J.* **97**, 2327–2337 (2009).
310. H. Cui, G. S. Ayton and G. A. Voth, “Membrane Binding by the Endophilin N-BAR Domain”, *Biophys. J.* **97**, 2746-2753 (2009).
311. S. Izvekov and G. A. Voth, “Mixed Resolution Modeling of Interactions in Condensed Phase Systems”, *J. Chem. Theor. Comp.* **5**, 3232–3244 (2009).
312. E. Lyman, C. Higgs, B. Kim, D. Lupyán, J. C. Shelley, R. Farid, and G. A. Voth, “A Role for a Specific Cholesterol Interaction in Stabilizing the Apo Configuration of the Human A_{2A} Adenosine Receptor”, *Structure* **17**, 1660–1668 (2009).
313. C. M. Maupin and G. A. Voth, “Proton Transport in Carbonic Anhydrase: Insights from Molecular Simulation”, *Biochim. et Biophys. Acta - Proteins and Proteomics* **1804**, 332-341 (2010).
314. G. S. Ayton, E. Lyman, and G. A. Voth, “Hierarchical Coarse-graining Strategy for Protein-Membrane Systems to Access Mesoscopic Scales”, *Faraday Disc. Chem. Soc.* **144**, 347–357 (2010).
315. V. Krishna, G. S. Ayton, and G. A. Voth, “Role of Protein Interactions in Defining HIV-1 Viral Capsid Shape and Stability: A Coarse-grained Analysis”, *Biophys. J.* **98**, 18-26 (2010).
316. H. Chen, G. A. Voth, and N. Agmon, “The Kinetics of Proton Migration in Liquid Water”, *J. Phys. Chem. B* **114**, 333–339 (2010).
317. T. Yamashita and G. A. Voth, “Properties of Hydrated Excess Protons Near Phospholipid Bilayers”, *J. Phys. Chem. B.* **114**, 592–603 (2010).
318. F. Paesani and G. A. Voth, “A Quantitative Assessment of the Accuracy of Centroid Molecular Dynamics for the Calculation of the Infrared Spectrum of Liquid Water”, *J. Chem. Phys.* **132**, 014105(1-6) (2010).
319. J. Pfaendtner, E. Lyman, T. D. Pollard, and G. A. Voth, “Structure and Dynamics of the Actin Filament”, *J. Mol. Biol.* **396**, 252–263 (2010).

320. L. Lu, S. Izvekov, A. Das, H. C. Andersen, and G. A. Voth, “Efficient, Regularized, and Scalable Algorithms for Multiscale Coarse-Graining”, *J. Chem. Theor. Comp.* **6**, 954–965 (2010).
321. G. S. Ayton and G. A. Voth, “Multiscale Simulation of Protein Mediated Membrane Remodeling”, *Seminars in Cell and Developmental Biology* **21**, 357–362 (2010).
322. C. K. Knox and G. A. Voth, “Probing Selected Morphological Models of Hydrated Nafion Using Large Scale Molecular Dynamics Simulations”, *J. Phys. Chem. B* **114**, 3205–3218 (2010).
323. J. Pfaendtner, E. M. De La Cruz, and G. A. Voth, “Actin Filament Remodeling by Actin Depolymerization Factor/Cofilin”, *Proc. Natl. Acad. Sci. USA* **107**, 7299–7304 (2010).
324. S. Feng and G. A. Voth, “Molecular Dynamics Simulations of Ionic Liquid/Water Mixtures: Alkyl Side Chain Length and Anion Effects”, *Fluid Phase Equilibria* (Special Issue) **294**, 148–156 (2010).
325. L. Larini, L. Lu, and G. A. Voth, “The Multiscale Coarse-Graining Method. VI. Implementation of Three-Body Coarse-Grained Potentials”, *J. Chem. Phys.* **132**, 164107(1-10) (2010).
326. C. M. Maupin, B. Aradi, and G. A. Voth, “The Self-Consistent Charge Density Functional Tight Binding Method Applied to Liquid Water and the Hydrated Excess Proton: Benchmark Simulations”, *J. Phys. Chem. B* **114**, 6922–6931 (2010).
327. R. D. Hills Jr., L. Lu, and G. A. Voth, “Multiscale Coarse-Graining of the Protein Energy Landscape”, *PLoS Comp. Bio.* **6**, e1000827(1-12) (2010).
328. Y. Wang and G. A. Voth, “Molecular Dynamics Simulations of Polyglutamine Aggregation using Solvent-Free Multiscale Coarse-Grained Models”, *J. Phys. Chem. B* **114**, 8735–8743 (2010).
329. J. Xu, S. Izvekov, and G. A. Voth, “Structure and Dynamics of Concentrated Hydrochloric Acid Solutions”, *J. Phys. Chem. B* **114**, 9555–9562 (2010).
330. Z. Cao, Y. Peng, T. Yan, S. Li, A. Li, and G. A. Voth, “Mechanism of Fast Proton Transport in Water Filled Carbon Nanotubes”, *J. Am. Chem. Soc.* **132**, 11395–11397 (2010).
331. K. F. Wong, J. L. Sonnenberg, F. Paesani, T. Yamamoto, J. Vaníček, W. Zhang, H. B. Schlegel, D. A. Case, T. E. Cheatham, III, W. H. Miller, and G. A. Voth, “Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology”, *J. Chem. Theor. Comp.* **6**, 2566–2580 (2010).
332. C.-L. Lai, K. E. Landgraf, G. A. Voth, and J. J. Falke, “Membrane Docking Geometry and Target Lipid Stoichiometry of Membrane-Bound PKC α C2 Domain: A Combined Molecular Dynamics and Experimental Study”, *J. Mol. Bio.* **402**, 301–310 (2010).
333. E. Lyman, H. Cui, and G. A. Voth, “Water Under the BAR”, *Biophys. J.* **99**, 1783–1790, (2010).
334. Z. Zhang and G. A. Voth, “Coarse-Grained Representations of Large Biomolecular Complexes from Low Resolution Structural Data”, *J. Chem. Theor. Comp.* **6**, 2990–3002 (2010).
335. H. Chen, P. Liu, and G. A. Voth, “An Efficient Multi-State Reactive Molecular Dynamics Approach Based on Short-Ranged Effective Potentials”, *J. Chem. Theor. Comp.* **6**, 3039–3047 (2010).

336. C. Knight, C. M. Maupin, S. Izvekov, and G. A. Voth, “Defining Condensed Phase Reactive Force Fields From Ab Initio Molecular Dynamics Simulations: The Case of the Hydrated Excess Proton”, *J. Chem. Theor. Comp.* **6**, 3223–3232 (2010).
337. G. S. Ayton and G. A. Voth “Multiscale Computer Simulation of the Immature HIV-1 Virion”, *Biophys. J.* **99**, 2757–2765 (2010).
338. H.-J. Lee,* E. Svahn,* J. M. J. Swanson,* H. Lepp, G. A. Voth, P. Brzezinski, and R. B. Gennis, “The Intricate Role of Water in Proton Transport through Cytochrome *c* Oxidase”, *J. Am. Chem. Soc.* **132**, 16225–16239 (2010). (*Authors contributed equally)
339. S. Bagchi, D. G. Thorpe, I. F. Thorpe, G. A. Voth, and M. D. Fayer, “Conformational Switching Between Protein Substates Studied with 2D IR Vibrational Echo Spectroscopy and Molecular Dynamics Simulations”, *J. Phys. Chem. B* **114**, 17187–17193 (2010).
340. J. Xu, Y. Zhang, and G. A. Voth, “Infrared Spectrum of the Hydrated Proton in Water”, *J. Phys. Chem. Lett.* **2**, 81–86 (2011).
341. H. Cui, E. Lyman, and G. A. Voth, “Mechanism of Membrane Curvature Sensing by Amphipathic Helix Containing Proteins”, *Biophys. J.* **100**, 1271–1279 (2011).
342. H. Li, H. Chen, T. Zeuthen, C. Conrad, B. Wu, E. Beitz, and G. A. Voth, “Enhancement of Proton Conductance by Mutations of the Selectivity Filter of Aquaporin-1”, *J. Mol. Biol.* **407**, 607–620 (2011).
343. A. Grafmüller and G. A. Voth, “Intrinsic Bending of Microtubule Protofilaments”, *Structure* **19**, 409–417 (2011).
344. C. M. Maupin, N. Castillo, S. Taraphder, C. Tu, R. McKenna, D. N. Silverman, and G. A. Voth, “Chemical Rescue of Enzymes: Proton Transfer in Mutants of Human Carbonic Anhydrase II”, *J. Am. Chem. Soc.* **133**, 6223–6234 (2011).
345. E. Lyman, H. Cui, and G. A. Voth, “Reconstructing Protein Remodeled Membranes in Molecular Detail From Mesoscopic Models”, *Phys. Chem. Chem. Phys.* **13**, 10430–10436 (2011).
346. S. Feng and G. A. Voth, “Proton Solvation and Transport in Hydrated Nafion”, *J. Phys. Chem. B* **115**, 5903–5912 (2011); Addition and Correction, *J. Phys. Chem. B* **115**, 10570 (2011).
347. D. Xiao, L. G. Hines, Jr., R. A. Bartsch, E. L. Quitevis, P. Yang, and G. A. Voth, “Nanostructural Organization in Carbon Disulfide/Ionic Liquid Mixtures: Optical Kerr Effect Spectroscopy and Molecular Dynamics Simulations”, *J. Chem. Phys.* **135**, 034502(1-12) (2011).
348. L. Lu and G. A. Voth, “The Multiscale Coarse-Graining Method. VII. Free Energy Decomposition of Coarse-Grained Effective Potentials”, *J. Chem. Phys.* **134**, 224107 (2011).
349. Y. Zhang and G. A. Voth, “A Combined Metadynamics and Umbrella Sampling Method for the Calculation of Ion Permeation Free Energy Profiles”, *J. Chem. Theor. Comp.* **7**, 2277–2283 (2011).
350. M. G. Saunders and G. A. Voth, “Water Molecules in the Nucleotide Binding Cleft of Actin: Effects on Subunit Conformation and Implications for ATP Hydrolysis”, *J. Mol. Biol.* **413**, 279–291 (2011).
351. Z. Zhang, K. Y. Sanbonmatsu, and G. A. Voth, “Key Inter-molecular Interactions in the *E. Coli* 70S Ribosome Revealed by Coarse-Grained Analysis”, *J. Am. Chem. Soc.* **133**, 16828–16838 (2011).

352. I. F. Thorpe, D. P. Goldenberg, and G. A. Voth, “An Exploration of Transferability in Multiscale Coarse-grained Peptide Models”, *J. Phys. Chem. B* **115**, 11911–11926 (2011).
353. Y. Zhang and G. A. Voth, “The Coupled Proton Transport in the ClC-ec1 Cl⁻/H⁺ Antiporter”, *Biophys. J.* **101**, L47–L49 (2011).
354. C. Knight and G. A. Voth, “The Curious Case of the Hydrated Proton”, *Acc. Chem. Res.* **45**, 101–109 (2012).
355. T. Yamashita and G. A. Voth, Insights into the Mechanism of Proton Transport in Cytochrome *c* Oxidase,” *J. Am. Chem. Soc.* **134**, 1147–1152 (2012).
356. Y. Peng and G. A. Voth, “Expanding the View of Proton Pumping in Cytochrome *c* Oxidase through Computer Simulation,” *Biochim. et Biophys. Acta-Bioenergetics* **1817**, 518–525 (2012).
357. J. Pfaendtner, N. Volkmann, D. Hanein, P. Dalhaimer, T. D. Pollard, and G. A. Voth, “Key Structural Features of the Actin Filament Arp2/3 Complex Branch Junction Revealed by Molecular Simulation”, *J. Mol. Biol.* **416**, 148–161 (2012).
358. M. K. Petersen, R. Kumar, H. S. White, and G. A. Voth, “A Computationally Efficient Treatment of Polarizable Electrochemical Cells Held at a Constant Potential”, *J. Phys. Chem. C* **116**, 4903–4912 (2012).
359. C. Mim, H. Cui, J. A. Gawronski-Salerno, A. Frost, E. Lyman, G. A. Voth, and V. M Unger, “Structural Basis of Membrane Bending by the N-BAR Protein Endophilin”, *Cell* **149**, 137–145 (2012).
360. M. G. Saunders and G. A. Voth, “Coarse-graining of Multi-Protein Assemblies”, *Curr. Opin. Struct. Biol.* **22**, 144–150 (2012).
361. A. V. Sinit斯基, M. G. Saunders, and G. A. Voth, “Optimal Number of Coarse-Grained Sites in Different Components of Large Biomolecular Complexes”, *J. Phys. Chem. B* **116**, 8363–8374 (2012).
362. I. Sumner and G. A. Voth, “Proton Transport Pathways in [NiFe]-Hydrogenase”, *J. Phys. Chem. B* **116**, 2917–2926 (2012).
363. A. Das, L. Lu, H. C. Andersen, and G. A. Voth, “The Multiscale Coarse-Graining Method. X. Improved Algorithms for Constructing Coarse-grained Potentials for Molecular Systems”, *J. Chem. Phys.* **136**, 194115(1-12) (2012).
364. M. G. Saunders and G. A. Voth, “Comparison Between Actin Filament Models: Coarse-graining Reveals Essential Differences”, *Structure* **20**, 641–653 (2012).
365. R. Jorn and G. A. Voth, “Mesoscale Simulation of Proton Transport in Proton Exchange Membranes”, *J. Phys. Chem. C* **116**, 10476–10489 (2012).
366. C. Knight and G. A. Voth, “Coarse-graining Away Electronic Structure: A Rigorous Route to Accurate Condensed Phase Interaction Potentials”, *Mol. Phys.* **110**, 935–944 (2012).

367. F. Bardak, D. Xiao, L. G. Hines Jr., P. Son, R. A. Bartsch, E. L. Quitevis, P. Yang, and G. A. Voth, “Nanostructural Organization in Acetonitrile/Ionic Liquid Mixtures: Molecular Dynamics Simulations and Optical Kerr Effect Spectroscopy”, *ChemPhysChem* **13**, 1687–1700 (2012).
368. M. Simunovic and G. A. Voth, “Molecular Insights Into the Conformational Transitions of Hsp90”, *Biophys. J.* **103**, 284–292 (2012).
369. R. Jorn, J. Savage, and G. A. Voth, “Proton Conduction in Exchange Membranes Across Multiple Length Scales”, *Acc. Chem. Res.* **45**, 2002–2010 (2012).
370. A. Chaudhri, I. E. Zarraga, T. J. Kamerzell, J. P. Brandt, T. W. Patapoff, S. J. Shire, and G. A. Voth, “Coarse-Grained Modeling of the Self-Association of Therapeutic Monoclonal Antibodies”, *J. Phys. Chem. B* **116**, 8045–8057 (2012).
371. Y. Peng, C. Knight, P. Blood, L. Crosby, and G. A. Voth, “Extending Parallel Scalability of LAMMPS and Multiscale Reactive Molecular Simulations”, *XSEDE’12: Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the Campus and Beyond*, Article No. 37 (ACM, New York, 2012). (Peer Reviewed)
372. C. Knight, G. Lindberg, and G. A. Voth, “Multiscale Reactive Molecular Dynamics”, *J. Chem. Phys.* **137**, 22A525 (2012).
373. J. Fan, M. G. Saunders, and G. A. Voth, “Coarse-Graining Provides Insight on the Essential Nature of Heterogeneity In Actin Filaments”, *Biophys. J.* **103**, 1334–1342 (2012).
374. S. Feng, J. Savage, and G. A. Voth, “Effect of Polymer Morphology on Proton Solvation and Transport in Proton Exchange Membranes”, *J. Phys. Chem C* **116**, 19104–19116 (2012).
375. C-L. Lai, C. C. Jao, E. Lyman, J. L. Gallop, B. J. Peter, H. T. McMahon, R. Langen, and G. A. Voth, “Membrane Binding and Self-Association of the Epsin N-Terminal Homology Domain”, *J. Mol. Biol.* **423**, 800–817 (2012).
376. T. Yamashita, Y. Peng, C. Knight, and G. A. Voth, “Computationally Efficient Multiconfigurational Reactive Molecular Dynamics”, *J. Chem. Theor. Comp.* **8**, 4863–4875 (2012).
377. J. M. A. Grime and G. A. Voth, “Early Stages of the HIV-1 Capsid Protein Lattice Formation”, *Biophys. J.* **103**, 1774–1783 (2012).
378. E. L. Quitevis, F. Bardak, D. Xiao, L. G. Hines, Jr., P. Son, R. A. Bartsch, P. Yang, and G. A. Voth, “OKE Spectroscopy and Molecular Dynamics Simulations of Polar and Nonpolar Molecules in Ionic Liquids” in *Ionic Liquids: Science and Applications*; Visser, A. E., Bridges, N. J., Rogers, R. D., Eds.; ACS Symposium Series 1117; American Chemical Society, Washington, DC, 2012; Chap. 13, pp. 271–287.
379. Z. Cao, J. F. Dama, L. Lu, and G. A. Voth, “Solvent Free Ionic Solution Models from Multiscale Coarse-Graining”, *J. Chem. Theor. Comp.* **9**, 172–178 (2013).
380. A. Srivastava and G. A. Voth, “A Hybrid Approach for Highly Coarse-grained Lipid Bilayer Models”, *J. Chem. Theor. Comp.* **9**, 750–765 (2013).
381. F. X. Vázquez, V. M. Unger, and G. A. Voth, “Autoinhibition of Endophilin in Solution via Inter-domain Interactions”, *Biophys. J.* **104**, 396–403 (2013).

382. H. Cui, C. Mim, F. X. Vázquez, E. Lyman, V. M. Unger, and G. A. Voth, “Understanding the Role of Amphipathic Helices in N-BAR Domain Driven Membrane Remodeling”, *Biophys. J.* **104**, 404–411 (2013).
383. A. Chaudhri, I. E. Zarraga, S. Yadav, T. W. Patapoff, S. J. Shire, and G. A. Voth, “The Role of Amino Acid Sequence in the Self-Association of Therapeutic Monoclonal Antibodies: Insights from Coarse-Grained Modeling”, *J. Phys. Chem. B* **117**, 1269–1279 (2013).
384. M. G. Saunders and G. A. Voth, “Coarse-graining Methods for Computational Biology”, *Annu. Rev. Biophys.* **42**, 73–93 (2013).
385. J. Fan, M. G. Saunders, E. J. Haddadian, K. F. Freed, E. M. De La Cruz, and G. A. Voth, “Molecular Origins of Cofilin-linked Changes in Actin Filament Mechanics”, *J. Mol. Biol.* **425**, 1225–1240 (2013).
386. N. Guttenberg, J. F. Dama, M. G. Saunders, G. A. Voth, J. Weare, and A. R. Dinner, “Minimizing Memory as an Objective for Coarse-graining”, *J. Chem. Phys.* **138**, 094111(1-10) (2013).
387. R. Jorn, R. Kumar, D. P. Abraham, and G. A. Voth, “Atomistic Modeling of the Electrode-Electrolyte Interface in Li-ion Energy Storage Systems: Electrolyte Structuring”, *J. Phys. Chem. C* **117**, 3747–3761 (2013).
388. G. A. Voth, “New and Notable: Key New Insights into Membrane Targeting by Proteins”, *Biophys. J.* **104**, 517–519 (2013).
389. M. McCullagh and G. A. Voth, “Unraveling the Role of the Protein Environment for [FeFe]-Hydrogenase Charge Transfer: A New Application of Coarse-Graining”, *J. Phys. Chem. B* **117**, 4062–4071 (2013).
390. A. Grafmüller, E. G. Noya, and G. A. Voth, “Nucleotide-dependent Lateral and Longitudinal Interactions in Microtubules”, *J. Mol. Biol.* **425**, 2232–2246 (2013).
391. J. F. Dama, A. V. Sinitskiy, M. McCullagh, J. Weare, B. Roux, A. R. Dinner, and G. A. Voth, “Theory of Ultra Coarse-Graining. I. General Principles”, *J. Chem. Theor. Comp.* **9**, 2466–2480 (2013).
392. Y.-L. S. Tse, A. M. Herring, K. Kim, G. A. Voth, “Molecular Dynamics Simulations of Proton Transport in 3M and Nafion Perfluorosulfonic Acid Membranes”, *J. Phys. Chem. C* **117**, 8079–8091 (2013).
393. G. Saielli, G. A. Voth, and Y. Wang, “Diffusion Mechanisms in Smectic Ionic Liquid Crystals: Insights from Coarse-grained MD Simulations”, *Soft Matter* **9**, 5716–5725 (2013).
394. T. H. Choi, R. Liang, C. M. Maupin, and G. A. Voth, “Application of the SCC-DFTB Method to Hydroxide Water Clusters and Aqueous Hydroxide Solutions”, *J. Phys. Chem. B* **117**, 5165–5179 (2013).
395. J. Li, A. L. Jonsson, J. C. Shelley, T. Beuming, and G. A. Voth, “Ligand-Dependent Activation and Deactivation of a G Protein-Coupled Receptor”, *J. Am. Chem. Soc.* **135**, 8749–8759 (2013).
396. C.-L. Lai,* A. Srivastava,* C. Pilling, A. R. Chase, J. J. Falke, and G.A. Voth, “Molecular Mechanism of Membrane Binding of the GRP1 PH Domain”, *J. Mol. Biol.* **425**, 3073–3090 (2013). (*Contributed Equally)

397. L. Lu, J. F. Dama, and G. A. Voth, “Fitting Coarse-grained Distribution Functions Through An Iterative Force-Matching Method”, *J. Chem. Phys.* **139**, 121906(1-10) (2013).
398. M. Simunovic, C. Mim, T. C. Marlovits, G. Resch, V. M. Unger, and G. A. Voth, “Protein-mediated Transformation of Lipid Vesicles into Tubular Networks”, *Biophys. J.* **105**, 711–719 (2013).
399. A. V. Sinit斯基 and G. A. Voth, “Coarse-graining of Proteins Based on Elastic Network Models”, *Chem. Phys.* **422**, 165–174 (2013).
400. C. L. Phillips and G. A. Voth, “Discovering Crystals Using Shape Matching and Machine Learning”, *Soft Matter* **9**, 8552–8568 (2013).
401. Y. Chen, J. Aardema, S. Kale, Z. L. Whichard, A. Awomolo, E. Blanchard, B. Chang, D. R. Myers, L. Ju, R. Tran, D. Reece, H. Christensen, S. Boukour, N. Debili, T. S. Strom, D. Rawlings, F. X. Vázquez, G. A. Voth, C. Zhu, W. H. A. Kahr, W. A. Lam, and S. J. Corey, “Loss of the F-BAR Protein CIP4 Reduces Platelet Production by Impairing Membrane-Cytoskeleton Remodeling”, *Blood* **122**, 1695-1706 (2013)
402. A. W. Lange and G. A. Voth, “A Multi-state Approach to Chemical Reactivity in Fragment Based Quantum Chemistry Calculations”, *J. Chem. Theor. Comp.* **9**, 4018–4025 (2013).
403. J. L. Baker and G. A. Voth, “Effects of ATP and Actin-Filament Binding on the Dynamics of the Myosin II S1 Domain”, *Biophys. J.* **105**, 1624-1634 (2013).
404. J. Li, O. Sode, G. A. Voth and S. Hirata, “A Solid-Solid Phase Transition in Carbon Dioxide at High Pressures and Intermediate Temperatures”, *Nature Communications* **4**, 2647(1-7) (2013).
405. J. Xu, T. Yamashita, N. Agmon, and G. A. Voth, “On the Origin of Proton Mobility Suppression in Aqueous Solutions of Amphiphiles”, *J. Phys. Chem. B* **117**, 15426–15435 (2013).
406. R. Kumar, C. Knight, and G. A. Voth, “Exploring the Behavior of the Hydrated Excess Proton at Hydrophobic Interfaces”, *Faraday Discussion* **167**, 263-278 (2013).
407. M. Simunovic, A. Srivastava, and G. A. Voth, “Linear Aggregation of Proteins on the Membrane: A Prelude to Membrane Remodeling”, *Proc. Nat. Acad. Sci. USA* **110**, 20396–20401 (2013).
408. J. M. A. Grime and G. A. Voth, “Highly Scalable and Memory Efficient Ultra-coarse-grained Molecular Dynamics Simulations”, *J. Chem. Theor. Comp.* **10**, 423–431 (2014).
409. C. J. Bruns, J. Li, M. Frasconi, S. T. Schneebeli, J. Iehl, H.-P. Jacquot de Rouville, S. I. Stupp, G. A. Voth, J. F. Stoddart, “An Electrochemically and Thermally Switchable Donor-Acceptor [c2]Daisy Chain Rotaxane”, *Angewandte Chemie (Int. Ed.)* **53**, 1953-1958 (2014).
410. R. Liang, J. M. J. Swanson, and G. A. Voth, “Benchmark Study of the SCC-DFTB Approach for a Biomolecular Proton Channel”, *J. Chem. Theor. Comp.* **10**, 451–462 (2014).
411. Y.-L. S. Tse, H. N. Sarode, G. E. Lindberg, T. A. Witten, A. M. Herring, and G. A. Voth, “Chloride Enhances Fluoride Mobility in Anion Exchange Membrane/Polycationic Systems”, *J. Phys. Chem. C* **118**, 845–853 (2014).

412. H. N. Sarode,* G. E. Lindberg,* Y. Yang, L. E. Felberg, G. A. Voth, and A. M. Herring, “Insights Into the Transport of Aqueous Quaternary Ammonium Cations: A Combined Experimental and Computational Study”, *J. Phys. Chem. B* **118**, 1363–1372 (2014). (*Authors contributed equally)
413. B. P. Ziembra, J. Li, K. E. Landgraf, J. D. Knight, G. A. Voth, and J. J. Falke, “Single Molecule Studies Reveal a Hidden Key Step in the Activation Mechanism of Membrane-Bound Protein Kinase C alpha”, *Biochemistry* **53**, 1697–1713 (2014).
414. M. G. Saunders, J. Tempkin, J. Weare, A. R. Dinner, B. Roux, and G. A. Voth “Nucleotide Regulation of the Structure and Dynamics of G-actin”, *Biophys. J.* **106**, 1710–1720 (2014).
415. S. Jang, A. V. Sinit斯基, and G. A. Voth, “Can the Ring Polymer Molecular Dynamics Method be Interpreted as Real Time Quantum Dynamics?”, *J. Chem. Phys.* **140**, 154103(1-11) (2014).
416. Z. Cao, R. Kumar, Y. Peng, and G. A. Voth, “Proton Transport Under External Applied Voltage”, *J. Phys. Chem. B* (2014) Online: DOI: 10.1021/jp501130m.
417. R. Liang, H. Li, J. M. J. Swanson, and G. A. Voth, “Multiscale Simulation Reveals a Multifaceted Mechanism of Proton Permeation through the Influenza A M2 Proton Channel”, *Proc. Nat. Acad. Sci. USA* **111**, 9396–9401 (2014).
418. J. F. Dama, M. Parrinello, and G. A. Voth, “Well-tempered Metadynamics Converges Asymptotically”, *Phys. Rev. Lett.* **112**, 240602(1-6) (2014).
419. A. D. White and G. A. Voth, “An Efficient and Minimal Method to Bias Molecular Simulations with Experimental Data”, *J. Chem. Theor. Comp.* (in press).
420. J. Savage, Y.-L. S. Tse, and G. Voth, “The Proton Transport Mechanism of Perfluorosulfonic Acid Membranes”, *J. Phys. Chem. C* (in press).

Submitted

421. Y. Peng, Z. Cao, R. Zhou, and G. A. Voth, “Path Integral Coarse-graining Replica Exchange Method for Enhanced Sampling”, *J. Chem. Theor. Comp.* (submitted).
422. J. F. Dama, M. Parrinello, and G. A. Voth, “Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-The-Fly Transition Barrier Estimation”, *J. Chem. Theor. Comp.* (submitted).
423. J. Li, B. P. Ziembra, J. J. Falke, and G. A. Voth, “Interactions of Protein Kinase C- α C1A and C1B Domains with Membranes: A Combined Computational and Experimental Study”, *J. Am. Chem. Soc.* (submitted).
424. A. Srivastava and G. A. Voth, “Solvent-Free Highly Coarse-Grained Models for Charged Lipid Systems”, *J. Chem. Theor. Comp.* (submitted).
425. J. L. Baker, N. Courtemanche, D. L. Parton, M. McCullagh, T. D. Pollard, and G. A. Voth, “Electrostatic Interactions Between the Bni1p Formin FH2 Domain and Actin Influence Actin Filament Nucleation”, *Structure* (submitted).
426. J. Savage and G. A. Voth, “Persistent Sub-diffusive Proton Transport in Perfluorosulfonic Acid Membranes”, *J. Phys. Chem. Lett.* (submitted).

427. M. McCullagh, M. G. Saunders, and G. A. Voth, "Unraveling the Mystery of ATP Hydrolysis in Actin Filaments" J. Am. Chem. Soc. (submitted).

Books Written or Edited

1. "Coarse-Graining of Condensed Phase and Biomolecular Systems", G. A. Voth, Editor (CRC Press/Taylor and Francis Group, Boca Raton, FL, 2009).