

Publications of Gregory A. Voth

(As of 5/25/22: 582 total publications, Google Scholar h-index = 114; i10 index = 536; total citations = 53,131; 18,390 since 2017)

Submitted

1. M. Gupta, A. J. Pak, and G. A. Voth, “Critical Mechanistic Role of Inositol Hexakisphosphate (IP6) in HIV-1 Viral Capsid Assembly” *Science Adv.* (under review).
2. F.-C. Tsai, J. M. Henderson, Z. Jarin, E. Kremneva, Y. Senju¹, J. Pernier, O. Mikhajlov, J. Manzi, C. Le Clainche, G. A. Voth, P. Lappalainen, and Patricia Bassereau, “Activated IRSp53 Clustering Controls the Formation of VASP-Actin-Based Membrane Protrusions”, *Science Adv.* (in revision).

Accepted

3. A. J. Pak, M. Gupta, M. Yeager, and G. A. Voth, “Inositol Hexakisphosphate (IP6) Accelerates Immature HIV-1 Gag Protein Assembly Towards Kinetically-Trapped Morphologies”, *J. Am Chem. Soc.* (in press).
4. C. Li, Z. Yue, S. Newstead, and G. A. Voth, “Proton Coupling and the Multiscale Kinetic Mechanism of a Peptide Transporter”, *Biophys. J.* (in press).

Published

5. S. Kim, J. Chung, H. Arlt, A. J. Pak, R. V. Farese, Jr, T. C. Walther, and G. A. Voth, “Seipin Transmembrane Segments Critically Function in Triglyceride Nucleation and Lipid Droplet Budding from the Membrane”, *eLife* **11**, e75808 (2022).
6. C. Li, F. Paesani, and G. A. Voth, “Static and Dynamic Correlations in Water: Comparison of Classical *Ab Initio* Molecular Dynamics at Elevated Temperature With Path Integral Simulations at Ambient Temperature”, *J. Chem. Theory Comp.* **18**, 2124-2131 (2022). PMID: PMC9059465
7. Z. Yue,* Z. Wang,* and G. A. Voth, “Ion Permeation, Selectivity, and Electronic Polarization in Fluoride Channels”, *Biophys. J.* **121**, 1336–1347(2022). (*Authors contributed equally). PMID: PMC9034187
8. S. Kim, J. M. J. Swanson, and G. A. Voth, “Computational Studies of Lipid Droplets”, *J. Phys. Chem. B* **126**, 2145-2154 (2022). (Feature Article). PMID: PMC8957551
9. A. Yu, E. M.Y. Lee, J. A.G. Briggs, B. K. Ganser-Pornillos, O. Pornillos, and G. A. Voth, “Strain and Rupture of HIV-1 Capsids During Uncoating”, *Proc. Nat. Acad. Sci. USA* **119**, e2117781119(1-8) (2022). PMID: PMC8915963
10. A. J. Pak, A. Yu, Z. Ke, J. A. G. Briggs, and G. A. Voth, “Cooperative Multivalent Receptor Binding Promotes Exposure of the SARS-CoV-2 Fusion Machinery Core”, *Nature Comm.* **13**, 1002 (2022). PMID: PMC8863989
11. S. Kim, C. Li, R. V. Farese, Jr, T. C. Walther, and G. A. Voth, “Key Factors Governing Initial Stages of Lipid Droplet Formation”, *J. Phys. Chem. B* **126**, 453–462 (2022). PMID: PMC8922452

12. C. Li and G. A. Voth, “Using Machine Learning to Greatly Accelerate Path Integral *Ab Initio* Molecular Dynamics”, *J. Chem. Theory Comp.* **18**, 599-604 (2022). PMID: PMC8864787
13. L. C. Watkins, W. F. DeGrado, and G. A. Voth, “Multiscale Simulation of an Influenza A M2 Channel Mutant Reveals Key Features of Its Markedly Different Proton Transport Behavior”, *J. Am. Chem. Soc.* **144**, 769–776 (2022). PMID: PMC8834648
14. V. Monje-Galvan and G. A. Voth, “Molecular Interactions of the M and E Integral Membrane Proteins of SARS-CoV-2”, *Faraday Discussions* **232**, 49-67 (2021). PMID: PMC8712422
15. C. Li and G. A. Voth, “A Quantitative Paradigm for Water Assisted Proton Transport Through Proteins and Other Confined Spaces”, *Proc. Nat. Acad. Sci. USA* **118**, e2113141118(1-8) (2021). PMID: PMC8670507
16. A. J. Pak, M. D. Purdy, M. Yeager, and G. A. Voth, “Preservation of HIV-1 Gag Helical Bundle Symmetry by Bevirimat is Central to Maturation Inhibition”, *J. Am. Chem. Soc.* **143**, 19137-19148 (2021). PMID: PMC8610020
17. P. B. Calio, C. Li, and G. A. Voth, “Resolving the Structural Debate for the Hydrated Excess Proton in Water”, *J. Am. Chem. Soc.* **143**, 18672-18683 (2021).
18. T. Driscoll, T. C. Bidone, S. Ahn, A. Goisman, G. A. Voth, and M. A. Schwartz, “Integrin-Based Mechanosensing through Conformational Activation”, *Biophys. J.* **120**, 4349-4359 (2021). PMID: PMC8553792
19. C. Li and G. A. Voth, “Accurate and Transferable Reactive Molecular Dynamics Models from Constrained Density Functional Theory”, *J. Phys. Chem B* **125**, 10471-10480 (2021). PMID: PMC8480781
20. C. Li and G. A. Voth, “Using Constrained Density Functional Theory to Track Proton Transfers and to Sample Their Associated Free Energy Surface”, *J. Chem. Theory Comp.* **17**, 5759-5765 (2021). PMID: PMC8444337
21. K. E. Homa, V. Zsolnay, C. A. Anderson, M. E. O’Connell, E. M. Neidt, G. A. Voth, T. C. Bidone,* and D. R. Kovar,* “Formin Cdc12’s Specific Actin Assembly Properties are Tailored for Cytokinesis in Fission Yeast”, *Biophys. J.* **120**, 2984-2997 (2021). (*Co-corresponding authors) PMID: PMC8390969
22. S. Zhou, P. He, S. Dhindwal, V. L. Grum-Tokars, Y. Li, K. Parker, J. A. Modica, R. Bleher, R. dos Reis, J. Zuchniarz, V. P. Dravid, G. A. Voth, B. Roux, and M. Mrksich, “Synthesis, Characterization and Simulation of Four-Armed Megamolecules”, *Biomacromolecules* **22**, 2363–2372 (2021).
23. E. Barry, R. Burns, W. Chen, G. X. de Hoe, J. M. M. de Oca, J. J. de Pablo, J. Dombrowski, J. W. Elam, A. M. Felts, G. Galli, J. Hack, Q. He, X. He, E. Hoeng, A. Iscen, B. Kash, H. Kung, N. H. C. Lewis, C. Liu, X. Ma, A. Mane, A. B. F. Martinson, K. L. Mulfort, J. Murphy, K. Mølhave, P. Nealey, Y. Qiao, V. Rozyyev, G. C. Schatz, S. J. Sibener, D. Talapin, D. Tiede, M. V. Tirrell, A. Tokmakoff, G. A. Voth, Z. Wang, Z. Ye, M. Yesibolati, N. Zaluzec, and S. B. Darling, “Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport”, *Chem. Rev.* **121**, 9450–9501 (2021).

24. J. H. Hack,[‡] J. P. Dombrowski,[‡] X. Ma,[‡] Y. Chen, N. H. C. Lewis, W. B. Carpenter, C. Li, G. A. Voth,* H. H. Kung,* and A. Tokmakoff,* “Structural Characterization of Protonated Water Clusters Confined in HZSM-5 Zeolites”, *J. Am. Chem. Soc.* **143**, 10203-10213 (2021) ([‡]Authors contributed equally, *Co-corresponding authors)
25. S. Kim and G. A. Voth, “Physical Characterization of Triolein and Implications for Its Role in Lipid Droplet Biogenesis”, *J. Phys. Chem. B* **125**, 6872-6888 (2021). PMID: PMC8314861
26. Y. Liu, C. Li, M. Gupta, J. Finer-Moore, N. Verma, A. K. Johri, R. M. Stroud, and G. A. Voth, “Key Computational Findings Reveal Proton Transfer as Driving the Functional Cycle in the Phosphate Transporter PiPT”, *Proc. Nat. Acad. Sci. USA* **118**, e2101932118 (2021). PMID: PMC8237618
27. C. Arntsen,* C.Chen,* P. B. Calio, C. Li, and G. A. Voth, “The Hopping Mechanism of the Hydrated Excess Proton and Its Contribution to Proton Diffusion in Water”, *J. Chem. Phys.* **154**, 194506(1-11) (2021). (*Authors contributed equally)
28. S. Mani, H. H. Katkar, and G. A. Voth, “Compressive and Tensile Deformations Alter ATP Hydrolysis and Phosphate Release Rates in Actin Filaments”, *J. Chem. Theory Comp.* **17**, 1900-1913 (2021).
29. G. M. Hocky, C. V. Sindelar, W. Cao, G. A. Voth, and E. M. De La Cruz, “Structural Asymmetry in Fast- And Slow-Severing Actin-Cofilactin Boundaries”, *J. Biol. Chem.* **296**, 100337(1-9) (2021). PMID: PMC7961102
30. Y. Han,* J. Jin,* and G. A. Voth, “Constructing Many-Body Dissipative Particle Dynamics Models of Fluids from Bottom-up Coarse-Graining”, *J. Chem. Phys.* **154**, 084122(1-15) (2021). (*Authors contributed equally)
31. Z. Jarin, J. Newhouse, and G. A. Voth, “Coarse-grained Force Fields from the Perspective of Statistical Mechanics: Better Understanding the Origins of a MARTINI Hangover”, *J. Chem. Theory Comp.* **17**, 1170–1180 (2021). PMID: PMC7876797
32. J. Jin, Y. Han, A. J. Pak, and G. A. Voth, “A New One-Site Coarse-Grained Model for Water: Bottom-Up Many-body Projected Water (BUMPer). I. General Theory and Model”, *J. Chem. Phys.* **154**, 044104(1-22) (2021). PMID: PMC7826168
33. J. Jin, A. J. Pak, Y. Han, and G. A. Voth, “A New One-Site Coarse-Grained Model for Water: Bottom-Up Many-Body Projected Water (BUMPer). II. Temperature Transferability and Structural Properties at Low Temperature”, *J. Chem. Phys.* **154**, 044105(1-21) (2021). PMID: PMC7826166
34. A. Tan,# A. J. Pak,# D. R. Morado, G. A. Voth,* and J. A. G. Briggs,* “Immature HIV-1 Assembles From Gag Dimers Leaving Partial Hexamers at Lattice Edges as Substrates for Proteolytic Maturation”, *Proc. Nat. Acad. Sci. USA* **118**, e2020054118 (2021). (#Authors contributed equally, *Corresponding authors) PMID: PMC7826355
35. Z. Jarin, A. J. Pak, P. Bassereau, and G. A. Voth, “Lipid-Composition-Mediated Forces Can Stabilize Tubular Assemblies of I-BAR Proteins”, *Biophys. J.* **120**, 46–54 (2021). PMID: PMC7820731

36. A. Yu, A. J. Pak, P. He, V. Monje-Galvan, L. Casalino, Z. Gaieb, A. C. Dommer, R. E. Amaro, and G. A. Voth, “A Multiscale Coarse-grained Model of the SARS-CoV-2 Virion”, *Biophys. J.* **120**, 1097–1104 (2021). PMID: PMC7695975
37. V. Zsolnay, H. H. Katkar, S. Z. Chou, T. D. Pollard, and G. A. Voth, “Structural Basis for Polarized Elongation of Actin Filaments”, *Proc. Nat. Acad. Sci. USA* **117**, 30458–30464 (2020). PMID: PMC7720195
38. J. Jin, A. Yu, and G. A. Voth, “Temperature and Phase Transferable Bottom-up Coarse-Grained Models”, *J. Chem. Theory Comp.* **16**, 6823–6842 (2020).
39. P. B. Calio, C. Li, and G. A. Voth, “Molecular Origins of the Barriers to Proton Transport in Acidic Aqueous Solutions”, *J. Phys. Chem. B* **124**, 8868–8876 (2020).
40. L. C. Watkins, W. F. DeGrado, and G. A. Voth, “Influenza A M2 Inhibitor Binding Understood through Mechanisms of Excess Proton Stabilization and Channel Dynamics”, *J. Am. Chem. Soc.* **142**, 17425–17433 (2020). PMID: PMC7564090
41. A. V. Mironenko and G. A. Voth, “Density Functional Theory-based Quantum Mechanics/Coarse-grained Molecular Mechanics: Theory and Implementation”, *J. Chem. Theory Comp.* **16**, 6329–6342 (2020).
42. A. Yu, E. M.Y. Lee, J. Jin, and Gregory A. Voth, “Atomic-scale Characterization of Mature HIV-1 Capsid Stabilization by Inositol Hexakisphosphate (IP₆)”, *Science Adv.* **6**, eabc645 (2020). PMID: PMC74944349
43. V. Monje-Galvan and G. A. Voth, “Binding Mechanism of the Matrix Domain of HIV-1 Gag to Lipid Membranes”, *eLife* **9**, e58621 (2020). PMID: PMC7476761
44. P. B. Calio, G. M. Hocky, and G. A. Voth, “Minimal Experimental Bias on the Hydrogen Bond Greatly Improves *Ab Initio* Molecular Dynamics Simulations of Water”, *J. Chem. Theory Comp.* **16**, 5675–5684 (2020).
45. C. Li, Z. Yue, L. M. Espinoza-Fonseca, and G. A. Voth, “Multiscale Simulation Reveals Passive Proton Transport Through SERCA on the Microsecond Timescale”, *Biophys. J.* **119**, 1033–1040 (2020). PMID: PMC7474205. [See also S. Khalid and S. Newstead, “New and Notable: A Computational Swiss Army Knife Approach to Unraveling the Secrets of Proton Movement through SERCA”, *Biophys. J.* **119**, 890–891 (2020).]
46. A. Martyna, B. Bahsoun, J. J. Madsen, L. A. Clifton, F. St. J. S. Jackson, M. D. Badham, G. A. Voth, and J. S. Rossman “Cholesterol Alters the Membrane Orientation and Activity of the Influenza Virus M2 Amphipathic Helix”, *J. Phys. Chem. B* **124**, 6738–6747 (2020). PMID: PMC7515559
47. X. Ma, C. Li, A. B. F. Martinson, and G. A. Voth, “Water Assisted Proton Transport in Confined Nanochannels”, *J. Phys. Chem. C* **124**, 16186–16201 (2020).
48. Z. Li, C. Li, Z. Wang, and G. A. Voth, “What Coordinate Best Describes the Affinity of the Hydrated Excess Proton for the Air-Water Interface?” *J. Phys. Chem. B*, **124**, 5039–5046 (2020).

49. D. Tong and G. A. Voth, “Microtubule Simulations in Different Nucleotide States Provide Insight into the Molecular Mechanism Underlying Dynamic Instability”, *Biophys. J.* **118**, 2938–2951 (2020). PMID: PMC7300308
50. T. G. Flower, Y. Takahashi, A. Hudait, K. Rose, N. Tjahjono, A. J. Pak, A. L. Yokom, X. Liang, H.-G. Wang, F. Bouamr, G. A. Voth, and J. H. Hurley, “A Helical Assembly of Human ESCRT-I Scaffolds Reverse-Topology Membrane Scission”, *Nat. Struct. Mol. Biol.* **27**, 570–580 (2020). PMID: PMC7339825
51. S. Mani, D. J. Cosgrove, and G. A. Voth, “Anisotropic Motions of Fibrils Dictated by Their Orientations in the Lamella: A Coarse-Grained Model of a Plant Cell Wall”, *J. Phys. Chem. B* **124**, 3527-3539 (2020).
52. Z. Li and G. A. Voth, “Interfacial Solvation and Slow Transport of Hydrated Excess Protons in Non-ionic Reverse Micelles”, *Phys. Chem. Chem. Phys.* **22**, 10753-10763 (2020).
53. T. Dannenhoffer-Lafage, and G. A. Voth, “Reactive Coarse-grained Molecular Dynamics”, *J. Chem. Theory Comp.* **16**, 2541-2549 (2020).
54. A. Yu, K. Skorupka, A. J. Pak, B. K. Ganser-Pornillos, O. Pornillos, and G. A. Voth, “TRIM5 α Self-Assembly and Compartmentalization of the HIV-1 Viral Capsid”, *Nature Comm.* **11**, 1307(1-10) (2020). PMID: PMC7066149
55. Z. Wang, J. M. J. Swanson, and G. A. Voth, “Local Conformational Dynamics Regulating Transport Properties of a Cl⁻/H⁺ Antiporter”, *J. Comput. Chem.* **41**, 513-519 (2020). PMID: PMC7184886
56. M. Bonomi, *et al.*, “Promoting Transparency and Reproducibility in Enhanced Molecular simulations”, *Nature Methods* **16**, 670-673 (2019).
57. T. Dannenhoffer-Lafage,* J. W. Wagner,* A. E. P. Durumeric, and G. A. Voth, “Compatible Observable Decompositions for Coarse-grained Representations of Real Molecular Systems”, *J. Chem. Phys.* **151**, 134115(1-14) (2019). (*Authors contributed equally)
58. A. E. P. Durumeric and G. A. Voth, “Adversarial-Residual-Coarse-Graining: Applying Machine Learning Theory to Systematic Molecular Coarse-Graining”, *J. Chem. Phys.* **151**, 124110(1-12) (2019).
59. J. Jin, A. J. Pak, and G. A. Voth, “Understanding Missing Entropy in Coarse-Grained Systems: Addressing Issues of Representability and Transferability”, *J. Chem. Phys. Lett.* **10**, 4549-4557 (2019). PMID: PMC6782054
60. Z. Yue, C. Li, G. A. Voth, and J. M. J. Swanson, “Dynamic Protonation Dramatically Affects the Membrane Permeability of Drug-like Molecules”, *J. Am. Chem. Soc.* **141**, 13421-13433 (2019). PMID: PMC6755907
61. S. L. Freedman, C. Suarez,* J. D. Winkelman,* D. R. Kovar, G.A. Voth, A. R. Dinner, and G.M. Hocky, “Mechanical and Kinetic Factors Drive Sorting of F-Actin Crosslinkers on Bundles”, *Proc. Nat. Acad. Sci. USA* **116**, 16192-16197 (2019). (*Authors contributed equally) PMID: PMC6697872

62. L. C. Watkins, R. Liang, J. M.J. Swanson,* W. F. DeGrado, and G. A. Voth,* “Proton Induced Conformational and Hydration Dynamics in the Influenza A M2 Channel”, *J. Am. Chem. Soc.* **141**, 11667-11676 (2019). (*Co-corresponding authors) PMID: PMC6768079
63. Z. Jarin, F.-C. Tsai, A. Davtyan, A. J. Pak, P. Bassereau, and G. A. Voth, “Unusual Organization of I-BAR Proteins on Tubular and Vesicular Membranes”, *Biophys. J.* **117**, 553-562 (2019). PMID: PMC6697384
64. A. C. Schramm, G. M. Hocky, G. A. Voth, J.-L. Martiel, and E. M. De La Cruz, “Plastic Deformation and Fragmentation of Strained Actin Filaments”, *Biophys. J.* **117**, 453-463 (2019). PMID: PMC6697348
65. T. C. Bidone, A. V. Skeeters, P. W. Oakes, and G. A. Voth, “Multiscale Model of Integrin Adhesion Assembly”, *PLOS Comp. Bio.* **15**, e1007077(1-20) (2019). PMID: PMC6568411
66. A. J. Pak, J. M. A. Grime, A. Yu, and G. A. Voth, “Off-Pathway Assembly: A Broad-Spectrum Mechanism of Action for Drugs That Undermine Controlled HIV-1 Viral Capsid Formation”, *J. Am. Chem. Soc.* **141**, 10214-10224 (2019). PMID: PMC6739737
67. W. H. Ryu, Y. Han, and G. A. Voth, “Coarse-graining of Many-body Path Integrals: Theory and Numerical Approximations”, *J. Chem. Phys.* **150**, 244103(1-11) (2019).
68. M. E. Sharp, F. X. Vázquez, J. W. Wagner, T. Dannenhoffer-Lafage, and G. A. Voth, “Multi-Configurational Coarse-Grained Molecular Dynamics”, *J. Chem. Theory Comp.* **15**, 3306-3315 (2019). PMID: PMC6660024
69. A. J. Harker , H. H. Katkar , T. C. Bidone , F. Aydin , G. A. Voth , D. A. Applewhite, and D. R. Kovar, “Ena/VASP Processive Elongation is Modulated by Avidity on Actin Filaments Bundled by the Filopodia Crosslinker Fascin”, *Mol. Biol. Cell* **30**, 851-862 (2019). PMID: PMC6589784
70. J. Jin,* Y. Han,* and G. A. Voth, “Coarse-Graining Involving Virtual Sites: Centers of Symmetry Coarse-Graining”, *J. Chem. Phys.* **150**, 154103(1-15) (2019). (*Authors contributed equally)
71. T. C. Bidone, A. Polley,* J. Jin,* T. Driscoll, D. Iwamoto, D. Calderwood, M. A. Schwartz, and G. A. Voth, “New Insights into the Conformational Activation of Full-Length Integrin”, *Biophys. J.* **116**, 1000-1010 (2019). (*Authors contributed equally)
72. A. J. Pak, T. Dannenhoffer-Lafage, J. J. Madsen, and G. A. Voth “Systematic Coarse-Grained Lipid Force Fields with Semiexplicit Solvation via Virtual Sites”, *J. Chem. Theory Comp.* **15**, 2087-2100 (2019). PMID: PMC6416712
73. G. A. Voth, “Simulations of N-BAR Protein Interactions with Membranes”, *J. Phys. D: Appl. Phys.* **51**, 343001 (35-36) (2018). PMID: PMC7111462
74. P. Bassereau *et al.*, “The 2018 Biomembrane Curvature and Remodeling Roadmap”, *J. Phys. D: Appl. Phys.* **51**, 343001 (2018). PMID: PMC6333427
75. Z. Wang, J. M. J. Swanson,* and G. A. Voth,* “Modulating the Chemical Transport Properties of a Transmembrane Antipporter via Alternative Anion Flux”, *J. Am. Chem. Soc.*, **140**, 16535–16543 (2018). (*Co-corresponding authors). PMID: PMC6379079

76. A. J. Pak and G. A. Voth “Advances In Coarse-Grained Modeling of Bio-Macromolecular Complexes”, *Curr. Opin. Struct. Biol.* **52**, 119-126 (2018). PMID: PMC6296860
77. F. Aydin,* H. H. Katkar,* and G. A. Voth, “Multiscale Simulation of Actin Filaments and Actin-Associated Proteins”, *Biophys. Rev.* **10**, 1521-1535 (2018). (*Authors contributed equally) PMID: PMC6297090
78. J. Jin, Y. Han, and G. A. Voth, “Ultra-Coarse-Grained Liquid State Models with Implicit Hydrogen Bonding”, *J. Chem. Theory Comp.* **14**, 6159-6174 (2018).
79. H. H. Katkar, A. Davtyan, A. E. P. Durumeric, G. M. Hocky, A. C. Schramm, E. M. De La Cruz, and G. A. Voth, “Insights into the Cooperative Nature of ATP Hydrolysis in Actin Filaments”, *Biophys. J.* **115**, 1589-1602 (2018). PMID: PMC6260209
80. J. J. Madsen, J. M. A. Grime, J. S. Rossman, and G. A. Voth, “Entropic Forces Drive Clustering and Spatial Localization of Influenza A M2 During Viral Budding”, *Proc. Nat. Acad. Sci. USA* **115**, E8595-E8603 (2018). PMID: PMC6140502.
81. Y. Han, J. F. Dama, and G. A. Voth, “Mesoscopic Coarse-grained Representations of Fluids Rigorously Derived from Atomistic Models”, *J. Chem. Phys.* **149**, 044104(1-20) (2018). PMID: 30068206
82. F. Aydin, N. Courtemanche, T. D. Pollard, and G. A. Voth, “Gating Mechanisms during Actin Filament Elongation by Formins”, *eLife* **7**, e37342 (2018). PMID: PMC6056239
83. R. Sun, Y. Han, J. M.J. Swanson, J. S. Tan, J. P. Rose, and G. A. Voth, “Molecular Transport through Membranes: Accurate Permeability Coefficients from Multidimensional Potentials of Mean Force and Local Diffusion Constants”, *J. Chem. Phys.* **149**, 072310(1-11) (2018). PMID: 30134730
84. J. Jin and G. A. Voth, “Ultra-Coarse-Grained Models Allow for an Accurate and Transferable Treatment of Interfacial Systems”, *J. Chem. Theory Comp.* **14**, 2180-2197 (2018). PMID: 29481754
85. M. Simunovic, P. Bassereau, and G. A. Voth, “Organizing Membrane-Curving Proteins: The Emerging Dynamical Picture”, *Curr. Opin. Struct. Biol.* **51**, 99-105 (2018). PMID: PMC6165709
86. P. W. Oakes, T. C. Bidone, Y. Beckham, A. V. Skeeters, G. R. Ramirez-San Juan, S. P. Winter, G. A. Voth, and M. L. Gardel, “The Lamellipodia is a Myosin Independent Mechanosensor”, *Proc. Nat. Acad. Sci. USA* **115**, 2646-2651 (2018). PMID: PMC5856528
87. H. B. Mayes,* S. Lee,* G.A. Voth,# and J.M.J. Swanson,# “Multiscale Kinetic Modeling Reveals Ensemble of Cl⁻/H⁺ Exchange Pathways in ClC-ec1 Antiporter”, *J. Am. Chem. Soc.* **140**, 1793–1804 (2018) (*Authors contributed equally, #Co-corresponding authors). PMID: PMC5812667
88. A. V. Sinitkiy and G. A. Voth, “Quantum Mechanics / Coarse-Grained Molecular Mechanics (QM/CG-MM)”, *J. Chem. Phys.* **148**, 014102(1-16) (2018). PMID: 29332400
89. C. Prévost,* M. E. Sharp,* N. Kory, Q. Lin, G. A. Voth,# and R. V. Farese Jr.,# and T. C. Walther,# “Mechanism and Determinants of Amphipathic Helix-Containing Proteins to Lipid Droplets”, *Dev. Cell.* **44**, 73-86 (2018). (*,#Authors contributed equally). PMID: PMC5764114

90. Y. Han, J. Jin, J. Wagner, and G. A. Voth, “Quantum Theory of Multiscale Coarse-graining”, *J. Chem. Phys.* **148**, 102335(1-15) (2018).
91. J. L. Parker, C. Li, A. Brinith, Z. Wang, L. Vogeley, N. Solcan, G. Ledderboge-Vucinic, J.M.J. Swanson, M. Caffrey, G. A Voth, and S. Newstead, “Proton Movement and Coupling in the POT Family of Peptide Transporters”, *Proc. Nat. Acad. Sci. USA* **114**, 13182–13187 (2017). PMID: PMC5740623
92. M. Simunovic, A. Šarić, J. M. Henderson, K-Y.C. Lee, and G. A. Voth, “Long-range Organization of Membrane-Curving Proteins”, *ACS Cen. Sci.* **3**, 1246-1253 (2017) PMID: PMC5746856
93. A. J. Pak, J. M. A. Grime, P. Sengupta, A. K. Chen, A. E. P. Durumeric, A. Srivastava, M. Yeager, J. A. G. Briggs, J. Lippincott-Schwartz, and G. A. Voth, “Immature HIV-1 Lattice Assembly Dynamics are Regulated by Scaffolding from Nucleic Acid and the Plasma Membrane” *Proc. Nat. Acad. Sci. USA* **114**, E10056-E10065 (2017). PMID: PMC5703280
94. W. A. Elam, W. Cao, H. Kang, A. Huehn, G. M. Hocky, E. Prochniewicz, A. C. Schramm, K. Negrón, J. Garcia, T. T. Bonello, P. W. Gunning, D. D. Thomas, G. A. Voth, C. V. Sindelar, and E. M. De La Cruz, “Phosphomimetic S3D-Cofilin Binds But Does Not Sever Actin Filaments”, *J. Biol. Chem.* **292**, 19565-19579 (2017). PMID: PMC5712599
95. G. M. Hocky, T. Dannenhoffer-Lafage, and G. A. Voth, “Coarse-grained Directed Simulation”, *J. Chem. Theory Comp.* **13**, 4593-4603 (2017). PMID: PMC5649387
96. W. B. Carpenter, J. A. Fournier, R. Biswas, and G. A. Voth, and A. Tokmakoff, “Delocalization and Stretch-Bend Mixing of the HOH Bend in Liquid Water”, *J. Chem. Phys.* **147**, 084503(1-10) (2017). PMID: 28863511
97. C. Chen, C.Arntsen, and G. A. Voth, “Development of Reactive Force Fields Using *Ab Initio* Molecular Dynamics Simulation Minimally Biased to Experimental Data”, *J. Chem. Phys.* **147**, 161719(1-7) (2017). PMID: PMC5584654
98. J. W. Wagner, T. Dannenhoffer-Lafage, J. Jin, and G. A. Voth, “Extending the Range and Physical Accuracy of Coarse-grained Models: Order Parameter Dependent Interactions”, *J. Chem. Phys.* **147**, 044113(1-13) (2017). PMID: 28764380
99. A. Davtyan, M. Simunovic, and G. A. Voth, “The Mesoscopic Membrane with Proteins Model (MesM-P)”, *J. Chem. Phys.* **147**, 044101(1-12) (2017). PMID: PMC5552407
100. D. Zimmermann, K. E. Homa,* G. M. Hocky,* L. W. Pollard, E. M. De La Cruz, G. A. Voth, K. M. Trybus, and D. R. Kovar “Mechanosensitive Inhibition of Formin Facilitates Contractile Actomyosin Ring Assembly”, *Nature Commun.* **8**, 703 (2017). (2017). (*Authors contributed equally). PMID: PMC5614989
101. A. C. Schramm, G. M. Hocky, G. A. Voth, L. Blanchoin, J.-L. Martiel, E. M. De La Cruz, “Actin Filament Strain Promotes Severing and Cofilin Dissociation”, *Biophys. J.* **112**, 2624-2633 (2017). PMID: PMC5479148
102. M. Simunovic, J.-B. Manneville, H.-F. Renard, E. Evergren, K. Raghunathan, A. K. Kenworthy, G. A. Voth, J. Prost, H. T. McMahon, L. Johannes, P. Bassereau, and A. Callan-Jones, “Friction

- Mediates Scission of Tubular Membranes Scaffolded by BAR Proteins”, *Cell* **170**, 172–184 (2017). PMID: PMC5576516
103. R. Liang, J. M. J. Swanson, M. Wikström, and G. A. Voth, “Understanding the Essential Proton Pumping Kinetic Gates and Decoupling Mutations in Cytochrome *c* Oxidase”, *Proc. Nat. Acad. Sci. USA* **114**, 5924-5929 (2017). PMID: PMC5468613
 104. R. Biswas and G. A. Voth, “Role of Solvation Structure in the Shuttling of the Hydrated Excess Proton”, *J. Chem. Sci.* **129**, 1045–1051 (2017).
 105. C. Arntsen, C. Chen, and Gregory A. Voth, “Reactive Molecular Dynamics Models from *Ab Initio* Molecular Dynamics Data Using Relative Entropy Minimization”, *Chem. Phys. Lett.* **683**, 573-578 (2017). PMID: PMC5568817
 106. R. Sun, O. Sode, J. F. Dama, and G. A. Voth, “Simulating Protein Mediated Hydrolysis of ATP and Other Nucleoside Triphosphates by Combining QM/MM Molecular Dynamics with Advances in Metadynamics”, *J. Chem. Theory Comp.* **13**, 2332–2341 (2017). PMID: PMC5425946
 107. S. Jang and G. A. Voth, “Non-Uniqueness of Quantum Transition State Theory and General Dividing Surfaces in the Path Integral Space”, *J. Chem. Phys.* **146**, 174106(1-7) (2017).
 108. R. Biswas, W. Carpenter, J. A. Fournier, G. A. Voth, and A. Tokmakoff, “IR Spectral Assignments for the Hydrated Excess Proton in Liquid Water”, *J. Chem. Phys.* **146**, 154507(1-11) (2017). PMID: 28433032
 109. J. R. Christensen, G. M. Hocky, A. N. Morganthaler, K. E. Homa, S. E. Hitchcock-DeGregori, G. A. Voth, and D. R. Kovar, “Competition Between Tropomyosin, Fimbrin, and ADF/Cofilin Drives Their Sorting to Distinct Actin Filament Networks”, *eLife* **6**, e23152 (2017). PMID: PMC5404920
 110. G. A. Voth, “A Multiscale Description of Mechanobiology: The Chemistry Underlying Many Life Processes”, *Acc. Chem. Res.* **50**, 594–598 (2017). (“Holy Grails in Chemistry” Issue)
 111. J. F. Dama,* J. Jin,* and G. A. Voth, “The Theory of Ultra-Coarse-Graining. 3. Coarse-grained Sites with Rapid Local Equilibrium of Internal States”, *J. Chem. Theory Comp.* **13**, 1010–1022 (2017). (*Authors contributed equally). PMID: 28112956
 112. A. D. White, C. Knight, G. M. Hocky, G. A. Voth, “Improved *Ab Initio* Molecular Dynamics by Minimally Biasing with Experimental Data”, *J. Chem. Phys.* **146**, 041102(1-5) (2017). PMID: 28147531
 113. J. J. Madsen, A. V. Sinitskiy, J. Li, and G. A. Voth, “Highly Coarse-grained Representations of Transmembrane Proteins”, *J. Chem. Theory Comp.* **13**, 935–944 (2017). PMID: PMC5312841
 114. A. Davtyan, G. A. Voth, and H. C. Andersen, “Dynamic Force Matching: Construction of Dynamic Coarse-Grained Models with Realistic Short Time Dynamics and Accurate Long Time Dynamics”, *J. Chem. Phys.* **145**, 224107(1-16) (2016). PMID: 27984910
 115. S. Lee, H. B. Mayes, J. M. J. Swanson, and G. A. Voth, “The Origin of Coupled Chloride and Proton Transport in a Cl⁻/H⁺ Antiporter”, *J. Am. Chem. Soc.* **38**, 14923–14930 (2016). PMID: PMC5114699

116. R. Biswas, W. Carpenter, G. A. Voth, and A. Tokmakoff, “Molecular Modeling and Assignment of IR Spectra of the Hydrated Excess Proton in Isotopically Dilute Water”, *J. Chem. Phys.* **145**, 154504(1-12) (2016). PMID: 27782492
117. R. Liang, J. M. J. Swanson, J. J. Madsen, M. Hong, W. F. DeGrado, and G. A. Voth, “Acid Activation Mechanism of the Influenza A M2 Proton Channel”, *Proc. Nat. Acad. Sci. USA* **113**, E6955–E6964 (2016). PMCID: PMC5111692
118. R. Sun,* J. F. Dama,* J. S. Tan, J. P. Rose, and G. A. Voth, “Transition-Tempered Metadynamics is a Promising Tool for Studying the Permeation of Drug-like Molecules through Membranes”, *J. Chem. Theory Comp.* **12**, 5157–5169 (2016). (*Authors contributed equally)
119. M. Simunovic, E. Evergren, I. Golushko, C. Prévost, H.-F. Renard, L. Johannes, H. McMahon, V. Lorman, G. A. Voth, and P. Bassereau, “How Curvature-Generating Proteins Build Scaffolds on Membrane Nanotubes”, *Proc. Nat. Acad. Sci. USA* **113**, 11226–11231 (2016). PMCID: PMC5056078
120. J. D. Winkelman,* C. Suarez,* G. M. Hocky, A. J. Harker, A. N. Morganthaler, J. R. Christensen, G. A. Voth, J. R. Bartles, and D. R. Kovar, “Fascin and α -Actinin-bundled Networks Contain Intrinsic Structural Features That Drive Protein Sorting”, *Curr. Biol.* **26**, 2697–2706 (2016). (*Authors contributed equally). PMID: 27666967 PMCID: PMC5119644
121. J. W. Wagner,* J. F. Dama,* A. E. P. Durumeric, and G. A. Voth, “On the Representability Problem and the Physical Meaning of Coarse-Grained Models”, *J. Chem. Phys.* **145**, 044108(1-12) (2016). (*Authors contributed equally)
122. A. Davtyan, M. Simunovic, and G. A. Voth, “Multiscale Simulations of Protein Facilitated Membrane Remodeling”, *J. Struct. Biol.* **196**, 57-63 (2016). PMCID: PMC5031523
123. R. Liang, J. M. J. Swanson, Y. Peng, M. Wikström, and G. A. Voth, “Multiscale Simulations Reveal Key Features of the Proton Pumping Mechanism in Cytochrome c Oxidase”, *Proc. Nat. Acad. Sci. USA* **113**, 7420-7425 (2016). PMCID: PMC4941487
124. G. M. Hocky,* J. L. Baker,* M. J. Bradley, A. V. Sinitskiy, E. M. De La Cruz, and G. A. Voth, “Cations Stiffen Actin Filaments by Adhering a Key Structural Element to Adjacent Subunits”, *J. Phys. Chem. B* **120**, 4558–4567 (2016). (*Authors contributed equally). PMCID: PMC4959277
125. J. M. A. Grime, J. F. Dama, B. K. Ganser-Pornillos, C. L. Woodward, G. J. Jensen, M. Yeager, G. A. Voth, “Coarse-grained Simulation Reveals Key Features of HIV-1 Capsid Self-Assembly”, *Nature Comm.* **7**, 11568(1-11) (2016). PMCID: PMC4869257
126. S. Taraphder, C. M. Maupin, J. M.J. Swanson, and G. A. Voth, “Coupling Protein Dynamics with Proton Transport in Human Carbonic Anhydrase II”, *J. Phys. Chem. B* **120**, 8389–8404 (2016). PMCID: PMC5003118.
127. Y. Li, J. R. Christensen, K. E. Homa, G. M. Hocky, A. Fok, J. A. Sees, G. A. Voth, and D. R. Kovar, “The F-Actin Bundler α -Actinin Ain1 is Tailored for Ring Assembly and Constriction during Cytokinesis in Fission Yeast”, *Mol. Biol. Cell* **27**, 1821-1833 (2016). PMCID: PMC4884072

128. T. Dannenhoffer-Lafage, A. D. White, and G. A. Voth, “A Direct Method for Incorporating Experimental Data into Multiscale Coarse-grained Models”, *J. Chem. Theory Comp.* **12**, 2144–2153 (2016). PMID: 27045328
129. C. Arntsen, J. Savage, Y.-L. S. Tse, and G. A. Voth, “Simulation of Proton Transport in Proton Exchange Membranes with Reactive Molecular Dynamics”, *Fuel Cells*. **16**, 695-703 (2016).
130. S. Jang and G. A. Voth, “Can Quantum Transition State Theory be Defined as a $t = 0^+$ Limit?”, *J. Chem. Phys.* **144**, 084110(1-12) (2016).
131. S. Lee, J.M.J. Swanson, and G. A. Voth, “Multiscale Simulations Reveal Key Aspects of the Proton Transport Mechanism in the ClC-ec1 Antiporter”, *Biophys. J.* **110**, 1334–1345 (2016). PMCID: PMC4816718
132. J. Savage and G. A. Voth, “Proton Solvation and Transport in Realistic Proton Exchange Membrane Morphologies”, *J. Phys. Chem. C* **120**, 3176–3186 (2016).
133. S. Lee, R. Liang, G. A. Voth, and J.M.J. Swanson, “Computationally Efficient Multiscale Reactive Molecular Dynamics to Describe Amino Acid Deprotonation in Proteins”, *J. Chem. Theory Comp.* **12**, 879–891 (2016). PMCID: PMC4750100
134. C. Chen, Y.-L. S. Tse, G. E. Lindberg, C. Knight, and G. A. Voth, “Hydroxide Solvation and Transport in Anion Exchange Membranes”, *J. Am. Chem. Soc.* **38**, 991–1000 (2016).
135. R. Biswas, Y.-L. S. Tse, A. Tokmakoff, and G. A. Voth, “Role of Pre-Solvation and Anharmonicity in Aqueous Phase Hydrated Proton Solvation and Transport”, *J. Phys. Chem. B* **120**, 1793–1804 (2016). PMID: 26575795
136. M. Simunovic, G. A. Voth, A. Callan-Jones, and P. Bassereau, “When Physics Takes Over: BAR Proteins and Membrane Curvature”, *Trends Cell Biol.* **25**, 780-792 (2015). PMCID: PMC4831700
137. J. F. Dama, G. M. Hocky, R. Sun, and G. A. Voth, “Exploring Valleys Without Climbing Every Peak: More Efficient and Forgiving Metabasin Metadynamics via Robust On-the-Fly Bias Domain Restriction”, *J. Chem. Theory Comp.* **11**, 5638–5650 (2015). PMCID: PMC4675329
138. Z. Cao and G. A. Voth, “The Multiscale Coarse-Graining Method. XI. Accurate Interactions Based on the Centers of Charge of Coarse-Grained Sites”, *J. Chem. Phys.* **143**, 243116(1-11) (2015). PMID: 26723601
139. Y.-L. S. Tse, C. Chen, G. E. Lindberg, R. Kumar, and G. A. Voth, “Propensity of Hydrated Excess Protons and Hydroxide Anions for the Air-Water Interface”, *J. Am. Chem. Soc.* **137**, 12610–12616 (2015). PMID: 26366480
140. A. V. Sinitskiy and G. A. Voth, “A Reductionist Perspective on Quantum Statistical Mechanics: Coarse-Graining of Path Integrals”, *J. Chem. Phys.* **143**, 094104(1-10) (2015). PMID: 26342356
141. J. W. Wagner,* J. F. Dama,* and G. A. Voth, “Predicting the Sensitivity of Multiscale Coarse-grained Models to their Underlying Fine-grained Model Parameters”, *J. Chem. Theory Comp.* **11**, 3547-3560 (2015). (*Authors contributed equally) PMID: 26574440

142. Y. Peng, J. M. J. Swanson, S. Kang, R. Zhou, and G. A. Voth, “Hydrated Excess Protons Can Create Their Own Water Wires”, *J. Phys. Chem. B* **119**, 9212–9218 (2015). PMID: PMC4515783
143. Z. Cao, R. Kumar, Y. Peng, and G. A. Voth, “Hydrated Proton Structure and Diffusion at Platinum Surfaces”, *J. Phys. Chem. C* **119**, 14675–14682 (2015).
144. Z. Cao, Y. Peng, and G. A. Voth, “Ion Transport through Ultra-Thin Electrolyte under Applied Voltages”, *J. Phys. Chem. B* **119**, 7516–7521 (2015). PMID: 25556845
145. M. Simunovic and G. A. Voth, “Membrane Tension Controls the Assembly of Curvature-Generating Proteins”, *Nature Commun.* **6**, 7219(1-8) (2015). doi: 10.1038/ncomms8219. PMID: PMC4455092
146. A. D. White, J. F. Dama, and G. A. Voth, “Designing Free Energy Surfaces that Match Experimental Data with Metadynamics”, *J. Chem. Theory Comp.* **11**, 2451-2460 (2015).
147. Y.-L. S. Tse, G. A. Voth, and T. A. Witten, “Ion Mixing, Hydration, and Transport in Aqueous Ionic Systems”, *J. Chem. Phys.* **142**, 184905(1-7) (2015).
148. A. Davtyan, J. F. Dama, G. A. Voth, and H. C. Andersen, “Dynamic Force Matching: A Method for Constructing Dynamical Coarse-Grained Models with Realistic Time Dependence”, *J. Chem. Phys.* **142**, 154104(1-21) (2015).
149. S. Liu, J. Savage, and G. A. Voth, “Mesoscale Study of Proton Transport in Proton Exchange Membranes: Role of Morphology”, *J. Phys. Chem. C* **119**, 1753–1762 (2015).
150. Y.-L. S. Tse, C. Knight, and G. A. Voth, “An Analysis of Hydrated Proton Diffusion in *Ab Initio* Molecular Dynamics”, *J. Chem. Phys.* **142**, 014104(1-13) (2015).
151. 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* **23**, 68–79 (2015). PMID: PMC4286494
152. A. Davtyan, J. F. Dama, A. V. Sinitskiy, and G. A. Voth, “The Theory of Ultra-Coarse-Graining. 2. Numerical Implementation”, *J. Chem. Theory Comp.* **10**, 5265–5275 (2014).
153. O. Sode and G. A. Voth, “Electron Transfer Activation of a Second Water Channel for Proton Transport in [FeFe]-Hydrogenase”, *J. Chem. Phys.* **141**, 22D527(1-9) (2014).
154. A. Srivastava and G. A. Voth, “Solvent-Free Highly Coarse-Grained Models for Charged Lipid Systems”, *J. Chem. Theory Comp.* **10**, 4730–4744 (2014). PMID: PMC4196741
155. M. McCullagh, M. G. Saunders, and G. A. Voth, “Unraveling the Mystery of ATP Hydrolysis in Actin Filaments” *J. Am. Chem. Soc.* **136**, 13053–13058 (2014). PMID: PMC4183606
156. Y. Peng, Z. Cao, R. Zhou, and G. A. Voth, “Path Integral Coarse-graining Replica Exchange Method for Enhanced Sampling”, *J. Chem. Theory Comp.* **10**, 3634–3640 (2014).
157. J. F. Dama, G. Rotskoff, M. Parrinello, and G. A. Voth, “Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-The-Fly Transition Barrier Estimation”, *J. Chem. Theory Comp.* **10**, 3626–3633 (2014).

158. J. Li, B. P. Ziemba, 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.* **136**, 11757–11766 (2014). PMID: PMC4140453
159. J. Savage and G. A. Voth, “Persistent Subdiffusive Proton Transport in Perfluorosulfonic Acid Membranes”, *J. Phys. Chem. Lett.* **5**, 3037–3042 (2014).
160. J. Savage, Y.-L. S. Tse, and G. Voth, “The Proton Transport Mechanism of Perfluorosulfonic Acid Membranes”, *J. Phys. Chem. C* **118**, 17436–17445 (2014).
161. A. D. White and G. A. Voth, “An Efficient and Minimal Method to Bias Molecular Simulations with Experimental Data”, *J. Chem. Theory Comp.* **10**, 3023–3030 (2014).
162. J. F. Dama, M. Parrinello, and G. A. Voth, “Well-tempered Metadynamics Converges Asymptotically”, *Phys. Rev. Lett.* **112**, 240602(1-6) (2014).
163. J. A. McCammon, B. Roux, G. A. Voth, and W. Yang, “Special Issue on Free Energy”, *J. Chem. Theory Comp.*, **10**, 2631–2631 (2014).
164. 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). PMID: PMC4084430
165. Z. Cao, R. Kumar, Y. Peng, and G. A. Voth, “Proton Transport Under External Applied Voltage”, *J. Phys. Chem. B* **118**, 8090–8098 (2014).
166. S. Jang, A. V. Sinitskiy, 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).
167. 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). PMID: PMC4008840
168. B. P. Ziemba, 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- α ”, *Biochemistry* **53**, 1697–1713 (2014). PMID: PMC3971957
169. 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)
170. 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).
171. R. Liang, J. M. J. Swanson, and G. A. Voth, “Benchmark Study of the SCC-DFTB Approach for a Biomolecular Proton Channel”, *J. Chem. Theory Comp.* **10**, 451–462 (2014). PMID: PMC4120842

172. 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).
173. J. M. A. Grime and G. A. Voth, “Highly Scalable and Memory Efficient Ultra-Coarse-Grained Molecular Dynamics Simulations”, *J. Chem. Theory Comp.* **10**, 423–431 (2014).
174. 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).
PMCID: PMC3870675
175. R. Kumar, C. Knight, and G. A. Voth, “Exploring the Behaviour of the Hydrated Excess Proton at Hydrophobic Interfaces”, *Faraday Discussions* **167**, 263-278 (2013).
176. 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).
177. 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).
178. 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). PMCID: PMC3791303
179. A. W. Lange and G. A. Voth, “A Multi-state Approach to Chemical Reactivity in Fragment Based Quantum Chemistry Calculations”, *J. Chem. Theory Comp.* **9**, 4018–4025 (2013).
180. 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) PMCID: PMC3765055
181. C. L. Phillips and G. A. Voth, “Discovering Crystals Using Shape Matching and Machine Learning”, *Soft Matter* **9**, 8552–8568 (2013).
182. A. V. Sinitkiy and G. A. Voth, “Coarse-graining of Proteins Based on Elastic Network Models”, *Chem. Phys.* **422**, 165–174 (2013).
183. 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).
PMCID: PMC3736692
184. 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).
185. 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) PMCID: PMC4265004

186. J. Li, A. L. Jonsson, J. C. Shelley, T. Beuming, and G. A. Voth, "Ligand-Dependent Activation and Deactivation of the Human Adenosine A2A Receptor", *J. Am. Chem. Soc.* **135**, 8749–8759 (2013). PMID: PMC4120839
187. 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).
188. 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).
189. 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).
190. J. F. Dama, A. V. Sinitskiy, M. McCullagh, J. Weare, B. Roux, A. R. Dinner, and G. A. Voth, "The Theory of Ultra Coarse-Graining. I. General Principles", *J. Chem. Theory Comp.* **9**, 2466–2480 (2013).
191. A. Grafmüller, E. G. Noya, and G. A. Voth, "Nucleotide-dependent Lateral and Longitudinal Interactions in Microtubules", *J. Mol. Biol.* **425**, 2232–2246 (2013).
192. 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).
193. G. A. Voth, "New and Notable: Key New Insights into Membrane Targeting by Proteins", *Biophys. J.* **104**, 517-519 (2013). PMID: PMC3566443
194. 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).
195. 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).
196. 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). PMID: PMC3740545
197. M. G. Saunders and G. A. Voth, "Coarse-graining Methods for Computational Biology", *Annu. Rev. Biophys.* **42**, 73–93 (2013).
198. 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).
199. 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). PMID: PMC3552260

200. 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). PMID: PMC3552259
201. A. Srivastava and G. A. Voth, “A Hybrid Approach for Highly Coarse-grained Lipid Bilayer Models”, *J. Chem. Theory Comp.* **9**, 750-765 (2013). PMID: PMC4120858
202. Z. Cao, J. F. Dama, L. Lu, and G. A. Voth, “Solvent Free Ionic Solution Models from Multiscale Coarse-Graining”, *J. Chem. Theory Comp.* **9**, 172–178 (2013).
203. L. Lu and G. A. Voth, “The Multiscale Coarse-Graining Method” In *Adv. Chem. Phys.*, S. A Rice and A. R. Dinner Editors (Wiley-Interscience: New York, 2012) Vol. 149.
204. 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.
205. J. M. A. Grime and G. A. Voth, “Early Stages of the HIV-1 Capsid Protein Lattice Formation”, *Biophys. J.* **103**, 1774–1783 (2012). PMID: PMC3475334
206. T. Yamashita, Y. Peng, C. Knight, and G. A. Voth, “Computationally Efficient Multiconfigurational Reactive Molecular Dynamics”, *J. Chem. Theory Comp.* **8**, 4863–4875 (2012). PMID: PMC4120847
207. 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). PMID: PMC3682188
208. 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).
209. 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). PMID: PMC3446683
210. C. Knight, G. Lindberg, and G. A. Voth, “Multiscale Reactive Molecular Dynamics”, *J. Chem. Phys.* **137**, 22A525 (2012). PMID: PMC3432097
211. 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)
212. 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).
213. R. Jorn, J. Savage, and G. A. Voth, “Proton Conduction in Exchange Membranes Across Multiple Length Scales”, *Acc. Chem. Res.* **45**, 2002–2010 (2012).

214. M. Simunovic and G. A. Voth, "Molecular and Thermodynamic Insights Into the Conformational Transitions of Hsp90", *Biophys. J.* **103**, 284-292 (2012). PMID: PMC3400771
215. 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", *Chem. Phys. Chem* **13**, 1687-1700 (2012).
216. 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).
217. R. Jorn and G. A. Voth, "Mesoscale Simulation of Proton Transport in Proton Exchange Membranes", *J. Phys. Chem. C* **116**, 10476-10489 (2012).
218. M. G. Saunders and G. A. Voth, "Comparison Between Actin Filament Models: Coarse-graining Reveals Essential Differences", *Structure* **20**, 641-653 (2012).
219. 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).
220. I. Sumner and G. A. Voth, "Proton Transport Pathways in [NiFe]-Hydrogenase", *J. Phys. Chem. B* **116**, 2917-2926 (2012).
221. A. V. Sinitskiy, 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).
222. M. G. Saunders and G. A. Voth, "Coarse-graining of Multi-Protein Assemblies", *Curr. Opin. Struct. Biol.* **22**, 144-150 (2012).
223. 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). PMID: PMC3319357
224. 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).
225. J. Pfaendtner, N. Volkman, 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). PMID: PMC3423189
226. 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). PMID: PMC4120846
227. 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). PMID: PMC4120843
228. C. Knight and G. A. Voth, "The Curious Case of the Hydrated Proton", *Acc. Chem. Res.* **45**, 101-109 (2012).

229. Y. Zhang and G. A. Voth, “The Coupled Proton Transport in the ClC-ec1 Cl⁻/H⁺ Antiporter”, *Biophys. J.* **101**, L47–L49 (2011). PMCID: PMC3218320
230. 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).
231. 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). PMCID: PMC3641354
232. 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).
233. Y. Zhang and G. A. Voth, “A Combined Metadynamics and Umbrella Sampling Method for the Calculation of Ion Permeation Free Energy Profiles”, *J. Chem. Theory Comp.* **7**, 2277–2283 (2011). PMCID: PMC4120845
234. 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). PMCID: PMC4120858
235. 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).
236. 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).
237. 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). PMCID: PMC4149255
238. 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). PMCID: PMC4120857
239. Grafmüller and G. A. Voth, “Intrinsic Bending of Microtubule Protofilaments”, *Structure* **19**, 409–417 (2011).
240. 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).
241. H. Cui, E. Lyman, and G. A. Voth, “Mechanism of Membrane Curvature Sensing by Amphipathic Helix Containing Proteins”, *Biophys. J.* **100**, 1271–1279 (2011). PMCID: PMC3043213.
242. J. Xu, Y. Zhang, and G. A. Voth, “Infrared Spectrum of the Hydrated Proton in Water”, *J. Phys. Chem. Lett.* **2**, 81–86 (2011).

243. 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). PMCID: PMC3033731
244. 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) PMCID: PMC3005615
245. G. S. Ayton and G. A. Voth, “Multiscale Computer Simulation of the Immature HIV-1 Virion”, *Biophys. J.* **99**, 2757–2765 (2010). PMCID: PMC2966041
246. 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. Theory Comp.* **6**, 3223–3232 (2010).
247. H. Chen, P. Liu, and G. A. Voth, “An Efficient Multi-State Reactive Molecular Dynamics Approach Based on Short-Ranged Effective Potentials”, *J. Chem. Theory Comp.* **6**, 3039–3047 (2010).
248. Z. Zhang and G. A. Voth, “Coarse-Grained Representations of Large Biomolecular Complexes from Low Resolution Structural Data”, *J. Chem. Theory Comp.* **6**, 2990–3002 (2010).
249. E. Lyman, H. Cui, and G. A. Voth, “Water Under the BAR”, *Biophys. J.* **99**, 1783–1790, (2010). PMCID: PMC2941004
250. 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). PMCID: PMC3602446
251. K. F. Wong, J. L. Sonnenberg, F. Paesani, T. Yamamoto, J. Vaniček, 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. Theory Comp.* **6**, 2566–2580 (2010). PMCID: PMC2992356
252. Z. Cao, Y. Peng, T. Yan, S. Li, A. Li, and G. A. Voth, “Mechanism of Fast Proton Transport along One-Dimensional Water Chains Confined in Carbon Nanotubes”, *J. Am. Chem. Soc.* **132**, 11395–11397 (2010).
253. J. Xu, S. Izvekov, and G. A. Voth, “Structure and Dynamics of Concentrated Hydrochloric Acid Solutions”, *J. Phys. Chem. B* **114**, 9555–9562 (2010).
254. 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).
255. 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). PMCID: PMC2891700
256. 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).

257. 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).
258. S. Feng and G. A. Voth, "Molecular Dynamics Simulations of Imidazolium-Based Ionic Liquid/Water Mixtures: Alkyl Side Chain Length and Anion Effects", *Fluid Phase Equilibria (Special Issue)* **294**, 148–156 (2010).
259. J. Pfandtner, 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). PMID: PMC2867716
260. 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).
261. G. S. Ayton and G. A. Voth, "Multiscale Simulation of Protein Mediated Membrane Remodeling", *Seminars in Cell and Developmental Biology* **21**, 357-362 (2010). PMID: PMC2855739
262. L. Lu, S. Izvekov, A. Das, H. C. Andersen, and G. A. Voth, "Efficient, Regularized, and Scalable Algorithms for Multiscale Coarse-Graining", *J. Chem. Theory Comp.* **6**, 954-965 (2010).
263. J. Pfandtner, E. Lyman, T. D. Pollard, and G. A. Voth, "Structure and Dynamics of the Actin Filament", *J. Mol. Biol.* **396**, 252–263 (2010). PMID: PMC2815099
264. 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).
265. T. Yamashita and G. A. Voth, "Properties of Hydrated Excess Protons Near Phospholipid Bilayers", *J. Phys. Chem. B.* **114**, 592–603 (2010).
266. H. Chen, G. A. Voth, and N. Agmon, "The Kinetics of Proton Migration in Liquid Water", *J. Phys. Chem. B* **114**, 333–339 (2010).
267. 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). PMID: PMC2800964
268. 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). PMID: PMC4153359
269. 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). PMID: PMC2818142
270. 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). PMID: PMC2796422
271. S. Izvekov and G. A. Voth, "Mixed Resolution Modeling of Interactions in Condensed Phase Systems", *J. Chem. Theory Comp.* **5**, 3232–3244 (2009).

272. H. Cui, G. S. Ayton and G. A. Voth, “Membrane Binding by the Endophilin N-BAR Domain”, *Biophys. J.* **97**, 2746-2753 (2009). PMID: PMC2776271
273. 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). PMID: PMC2764101
274. F. Paesani, S. S. Xantheas, and G. A. Voth, “Infrared Spectroscopy and Hydrogen-Bond Dynamics of Liquid Water from Centroid Molecular Dynamics with an *Ab Initio*-Based Force Field”, *J. Phys. Chem. B* **113**, 13118–13130 (2009).
275. 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). PMID: PMC2749773
276. 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). PMID: PMC2739621
277. 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). PMID: PMC2722336
278. 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). PMID: PMC2721766
279. D. Wang and G. A. Voth, “Proton Transport Pathway in the ClC Cl⁻/H⁺ Antiporter”, *Biophys. J.* **97**, 121-131 (2009). PMID: PMC2711357
280. 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). PMID: PMC2774804
281. H. Chen and G. A. Voth, “Unusual Hydrophobic Interactions in Acidic Aqueous Solutions”, *J. Phys. Chem. B* **113**, 7291-7297 (2009).
282. G. S. Ayton and G. A. Voth, “Systematic Multiscale Simulation of Membrane Protein Systems”, *Curr. Opin. Struct. Biol.* **19**, 138-144 (2009). PMID: PMC4693605
283. 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)
284. Y. Wang, S. Feng, and G. A. Voth, “Transferable Coarse-Grained Models for Ionic Liquids”, *J. Chem. Theory Comp.* **5**, 1091-1098 (2009).
285. 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).
286. 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).

287. S. Izvekov and G. A. Voth, "A Solvent Free Lipid Bilayer Model Using Multiscale Coarse-graining", *J. Phys. Chem. B* **113**, 4443-4455 (2009). PMID: PMC2666921
288. 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). PMID: PMC2689158
289. S. S. Xantheas and G. A. Voth, "Aqueous Solutions and their Interfaces", *J. Phys. Chem. B* **113**, 3997 (2009).
290. 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).
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. L. Lu and G. A. Voth, "Systematic Coarse-graining of a Multi-component Lipid Bilayer", *J. Phys. Chem. B* **113**, 1501-1510 (2009). PMID: PMC2633031
293. W. G. Noid, G. S. Ayton, S. Izvekov, and G. A. Voth, "The Multiscale Coarse-Graining Method: A Systematic Approach to Coarse Graining". In *Coarse-Graining of Condensed Phase and Biomolecular Systems*, G. A. Voth, Editor (CRC Press/Taylor and Francis Group, Boca Raton, FL, 2009).
294. 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).
295. 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).
296. J. Pfaendtner and G. A. Voth, "Molecular Dynamics Simulation and Coarse-grained Analysis of the Arp2/3 Complex", *Biophys. J.* **95**, 5324-5333 (2008). PMID: PMC2586551
297. 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).
298. 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). PMID: PMC2586547
299. 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).
300. I. F. Thorpe, J. Zhou, and G. A. Voth, "Peptide Folding Using Multiscale Coarse-grained Models", *J. Phys. Chem. B* **112**, 13079-13090 (2008).
301. E. Lyman, J. Pfaendtner, and G. A. Voth, "Systematic Multiscale Parameterization of Heterogeneous Elastic Network Models of Proteins", *Biophys. J.* **95**, 4183-4192 (2008). PMID: PMC2567941

302. 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).
303. 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). PMID: PMC2562593
304. 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). PMID: PMC2517022
305. O. Markovitch, H. Chen, S. Izvekov, F. Paesani, G. A. Voth, and N. Agmon, “Special Pair Dance and Partner Selection: Elementary Steps in Proton Transport in Liquid Water”, *J. Phys. Chem. B* **112**, 9456-9466 (2008).
306. 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). PMID: PMC2483763
307. 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). PMID: PMC2671180
308. 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). PMID: PMC2671183
309. 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).
310. 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). PMID: PMC2292381
311. M. Ceotto, G. S. Ayton, and G. A. Voth, “Accelerated Superposition State Molecular Dynamics for Condensed Phase Systems”, *J. Chem. Theory Comp.* **4**, 560-568 (2008).
312. 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).
313. 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).
314. W. Jiang, T. Yan, Y. Wang, and G. A. Voth, “Molecular Dynamics Simulation of the Energetic Room Temperature Ionic Liquid 1-Hydroxyethyl-4-Amino-1, 2, 4-Triazolium Nitrate (HEATN)”, *J. Phys. Chem. B* **112**, 3121-3131 (2008).

315. D. T. Mirijanian 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).
PMCID: PMC2234116
316. 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).
PMCID: PMC2254171
317. 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).
318. F. Paesani and G. A. Voth, "Quantum Effects Strongly Influence the Surface Premelting of Ice", *J. Phys. Chem. C* **112**, 324-327 (2008).
319. 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).
320. 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).
321. 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).
322. 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).
PMCID: PMC2084241
323. 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).
PMCID: PMC2072055
324. P. Liu, S. Izvekov, and G. A. Voth, "Multiscale Coarse-Graining of Monosaccharides," *J. Phys. Chem. B* **111**, 11566-11575 (2007).
325. S. Paramore, G. S. Ayton, and G. A. Voth, "Transient Violations of the Second Law of Thermodynamics in Protein Unfolding Examined Using Synthetic Atomic Force Microscopy and the Fluctuation Theorem," *J. Chem. Phys.* **127**, 105105(1-11) (2007).
326. 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).
327. 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).
328. J. Zhou, I. F. Thorpe, S. Izvekov, and G. A. Voth, "Coarse-grained Peptide Modeling using a Systematic Multiscale Approach," *Biophys. J.* **92**, 4289-4303 (2007).
PMCID: PMC1877786
329. 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).

330. 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.
331. 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). PMID: PMC2548316
332. 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). PMID: PMC2642678
333. 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). PMID: PMC1853153
334. 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).
335. 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). PMID: PMC17411142
336. 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).
337. 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).
338. C. M. Maupin and G. A. Voth, "Preferred Orientation of His-64 in Human Carbonic Anhydrase II," *Biochem.* **46**, 2938-2947 (2007). PMID: PMC2569863
339. 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). PMID: PMC2556150
340. G. S. Ayton and G. A. Voth, "Multiscale Simulation of Transmembrane Proteins," *J. Struct. Biol.* **157**, 570-578 (2007).
341. 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).
342. 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).
343. 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). PMID: PMC1697870

344. 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). PMID: PMC1697834
345. 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).
346. 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).
347. Y. Gebremichael, G. S. Ayton, and G. A. Voth, "Mesoscopic Modeling of Bacterial Flagellar Microhydrodynamics" *Biophys. J.* **91**, 3640–3652 (2006). PMID: PMC1630491
348. 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). PMID: PMC4129643
349. 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).
350. 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). PMID: PMC1614492
351. D. Blood and G. A. Voth, "Direct Observation of Bin/amphiphysin/Rvs (BAR) Domain-Induced Membrane Curvature by Means of Molecular Dynamics Simulations," *Proc. Natl. Acad. Sci. USA* **103**, 15068-15072 (2006). PMID: PMC1622778
352. Y. Wang and G. A. Voth, "Tail Aggregation and Domain Diffusion in Ionic Liquids," *J. Phys. Chem B* **110**, 18601-18608 (2006).
353. 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).
354. 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).
355. 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).
356. 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).
357. J.-W. Chu, S. Izvekov, and G. A. Voth, "The Multiscale Challenge for Biomolecular Systems: Coarse-grained Modeling," *Mol. Sim.* **32**, 211-218 (2006).
358. 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). PMID: PMC1440765

359. 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).
360. G. A. Voth, "Computer Simulation of Proton Solvation and Transport in Aqueous and Biomolecular Systems," *Acc. Chem. Res.* **39**, 143-150 (2006). PMID: PMC2548316
361. 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).
362. S. Izvekov and G. A. Voth, "Multiscale Coarse-graining of Mixed Phospholipid/Cholesterol Bilayer," *J. Chem. Theory Comp.* **2**, 637-648 (2006).
363. 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).
364. 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).
365. 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). PMID: PMC1367308
366. Y. Wang, S. Izvekov, T. Yan, and G. A. Voth, "Multiscale Coarse-Graining of Ionic Liquids," *J. Phys. Chem. B* **110**, 3564-3575 (2006).
367. 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).
368. 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).
369. 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).
370. S. Paramore, G. S. Ayton, and G. A. Voth, "Extending a Spectrin Repeat Unit II. Rupture Behavior," *Biophys. J.* **90**, 101-111 (2006). PMID: PMC1367010
371. 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). PMID: PMC1367040
372. 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).
373. 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).
374. S. Izvekov and G. A. Voth, "Multiscale Coarse-Graining of Liquid State Systems," *J. Chem. Phys.* **123**, 134105(1-13) (2005).

375. 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).
376. Q. Shi and G. A. Voth, "Multiscale Modeling of Phase Separation in Mixed Lipid Bilayers," *Biophys. J.* **89**, 2385-2394 (2005). PMID: PMC1366738
377. 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). PMID: PMC1366740
378. 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).
379. J.-W. Chu and G. A. Voth, "Allostery of Actin Filaments: Molecular Dynamics Simulations and Coarse-Grained Analysis," *Proc. Natl. Acad. Sci. USA* **102**, 13111-13116 (2005). PMID: PMC1201585
380. Y. Wang and G. A. Voth, "Unique Spatial Heterogeneity in Ionic Liquids," *J. Am. Chem. Soc.* **127**, 12192-12193 (2005).
381. 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).
382. 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).
383. 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).
384. 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). PMID: PMC1305619
385. 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). PMID: PMC1100745
386. 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).
387. 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).
388. H. L. Tepper and G. A. Voth, "Protons May Leak Through Pure Lipid Bilayers via a Concerted Mechanism," *Biophys. J.* **88**, 3095-3108 (2005). PMID: PMC1305461

389. 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).
390. 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).
391. 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).
392. 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).
393. S. Izvekov and G. A. Voth, "A Multiscale Coarse-Graining Method for Biomolecular Systems," *J. Phys. Chem. B* **109**, 2469-2473 (2005).
394. J. Jeon and G. A. Voth, "The Dynamic Stress Responses to Area Change in Planar Lipid Bilayer Membranes," *Biophys. J.* **88**, 1104-1119 (2005). PMID: PMC1305116
395. 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).
396. A. Venkatnathan and G. A. Voth, "Superposition State Molecular Dynamics," *J. Chem. Theory Comp.* **1**, 36-40 (2005).
397. 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).
398. 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, 2005), Chap. 10.
399. G. S. Ayton and G. A. Voth, "Mesoscopic Lateral Diffusion in Lipid Bilayers," *Biophys. J.* **87**, 3299-3311 (2004). PMID: PMC1304798
400. 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). PMID: PMC1304794
401. 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).
402. 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).
403. 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).

404. 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).
405. 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).
406. B. J. Ka and G. A. Voth, "Combining the Semiclassical Initial Value Representation with Centroid Dynamics," *J. Phys. Chem. B* **108**, 6883-6892 (2004).
407. 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).
408. 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).
409. 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).
410. G. Ayton, H. L. Tepper, D. T. Mirijanian, and G. A. Voth, "A New Perspective on the Coarse-grained Dynamics of Fluids," *J. Chem. Phys.* **120**, 4074-4088 (2004).
411. M. G. Del Popolo and G. A. Voth, "On the Structure and Dynamics of Ionic Liquids," *J. Phys. Chem. B* **108**, 1744-1752 (2004).
412. 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).
413. G. A. Voth, "The Computer Simulation of Proton Transport in Biomolecular Systems," *Frontiers in Bioscience* **8**, 1384-1397 (2003).
414. 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). PMID: PMC1303208
415. Y. Wu and G. A. Voth, "Computational Studies of Proton Transport through the M2 Channel", *FEBS Letters* **552**, 23-27 (2003).
416. 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)
417. 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).
418. S. D. Shellman, J. P. Lewis, K. R. Glaesemann, K. Sikorski, and G. A. Voth, "Massively Parallel Linear-Scaling Algorithm in an *Ab Initio* Local-Orbital Total-Energy Method," *J. Comp. Phys.* **188**, 1-15 (2003).

419. J. Jeon, A. E. Lefohn, and G. A. Voth, "An Improved Polarflex Water Model," *J. Chem. Phys.* **118**, 7504-7518 (2003).
420. 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).
421. 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.
422. D. T. Mirijanian, 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).
423. G. Ayton and G. A. Voth, "Bridging Microscopic and Mesoscopic Simulations of Lipid Bilayers," *Biophys. J.* **83**, 3357-3370 (2002). PMID: PMC1302411
424. 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).
425. 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).
426. 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).
427. 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). PMID: PMC1302288
428. 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). PMID: PMC1302206
429. 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).
430. J.-L. Liao and G. A. Voth, "Numerical Approaches for Computing Nonadiabatic Electron Transfer Rate Constants," *J. Chem. Phys.* **116**, 9174-9187 (2002).
431. S. Izvekov and G. A. Voth, "Car-Parrinello Molecular Dynamics Simulation of Liquid Water: New Results," *J. Chem. Phys.* **116**, 10372-10376 (2002).
432. 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). PMID: PMC1301947
433. 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). PMID: PMC1301926

434. 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).
435. G. A. Voth, "Feynman Path Centroid Dynamics," in *Progress in Theoretical Chemistry and Physics, Vol. 5*, S. D. Schwartz, Ed. (Kluwer, Dordrecht, 2002), Chap. 2, pp. 47-65.
436. 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).
437. 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).
438. 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).
439. S. Izvekov and G. A. Voth, "Ab initio Molecular Dynamics Simulation of the Ag(111)–Water Interface," *J. Chem. Phys.* **115**, 7196-7206 (2001).
440. 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).
441. 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).
442. 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).
443. 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).
444. 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).
445. 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).
446. 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).
447. 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).
448. 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).

449. 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). PMID: PMC1301359
450. 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)
451. 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).
452. J. P. Lewis, K. R. Glaesemann, R. B. Evans, K. VanOpdorp, and G. A. Voth, "*Ab Initio* Calculations of Reactive Pathways for Gas-Phase Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (-HMX)" *J. Phys. Chem. A* **104**, 11384-11389 (2000).
453. U. W. Schmitt and G. A. Voth, "The Isotope Substitution Effect on the Hydrated Proton," *Chem. Phys. Lett.* **329**, 36-41 (2000).
454. D. Matyushov and G. A. Voth, "Modeling the Free Energy Surfaces of Electron Transfer in Condensed Phases," *J. Chem. Phys.* **113**, 5413-5424 (2000).
455. 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).
456. G. K. Schenter, B. C. Garrett, and G. A. Voth, "The Quantum Vibrational Dynamics of $\text{Cl}^-(\text{H}_2\text{O})_n$ Clusters," *J. Chem. Phys.* **113**, 5171 (2000).
457. 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).
458. 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).
459. 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).
460. 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).
461. 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).
462. 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).
463. 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).

464. 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).
465. 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).
466. 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).
467. 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).
468. 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).
469. S. Jang, S. Jang, and G. A. Voth, "Quantum Molecular Dynamics Simulations of Low Temperature High Energy Density Matter: Solid $p\text{-H}_2/\text{Li}$ and $p\text{-H}_2/\text{B}$," *J. Phys. Chem. A* **103**, 9512-9520 (1999).
470. 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).
471. U. W. Schmitt and G. A. Voth, "The Computer Simulation of Proton Transport in Water," *J. Chem. Phys.* **111**, 9361-9381 (1999).
472. U. W. Schmitt and G. A. Voth, "Quantum Properties of the Excess Proton in Liquid Water," *Israeli J. Chem.* **39**, 483-492 (1999).
473. P.-N. Roy, S. Jang, and G. A. Voth, "Feynman Path Centroid Dynamics for Fermi-Dirac Statistics," *J. Chem. Phys.* **111**, 5303-5305 (1999).
474. 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).
475. 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).
PMCID: PMC1300517
476. D. V. Matyushov and G. A. Voth, "A Perturbation Theory for Solvation Thermodynamics: Dipolar-Quadrupolar Liquids," *J. Chem. Phys.* **111**, 3630-3638 (1999).
477. 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).
478. 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).

479. 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).
480. C. D. Schwieters 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).
481. 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).
482. 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).
483. 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).
484. 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).
485. 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).
486. 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).
487. 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).
488. 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).
489. 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).
490. 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).
491. 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).
492. M. Pavese and G. A. Voth, "Quantum and Classical Simulations of an Excess Proton in Water", Ber. Bunsenges. Phys. Chem. **102**, 527-532 (1998).
493. 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).
494. R. Hernandez and G. A. Voth, "Quantum Time Correlation Functions and Classical Coherence," Chem. Phys. **233**, 243-256 (1998).

495. 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).
496. 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).
497. 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).
498. 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).
499. C. D. Schwieters and G. A. Voth, "A Semiclassical Method for the Calculation of Nonadiabatic Tunneling Rates," *J. Chem. Phys.* **108**, 1055-1062 (1998).
500. 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).
501. S. Jang and G. A. Voth, "Simple Reversible Molecular Dynamics Algorithms for Nosé-Hoover Chain Dynamics," *J. Chem. Phys.* **107**, 9514-9526 (1997).
502. 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).
503. 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).
504. 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).
505. 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).
506. 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).
507. J. Lobaugh and G. A. Voth, "A Quantum Model for Water: Equilibrium and Dynamical Properties", *J. Chem. Phys.* **106**, 2400-2410 (1997).
508. 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). PMID: PMC1184292
509. J. Cao and G. A. Voth, "A Unified Framework for Quantum Activated Rate Processes: I. General Theory", *J. Chem. Phys.* **105**, 6856-6870 (1996).
510. 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).

511. J. Cao and G. A. Voth, "A Theory for the Quantum Activated Rate Constant in Dissipative Systems", Chem. Phys. Lett. **261**, 111-116 (1996).
512. 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).
513. 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).
514. D. E. Sagnella and G. A. Voth, "The Structure and Dynamics of Hydronium in the Ion Channel Gramicidin A.", Biophys. J. **70**, 2043-2051 (1996). PMID: PMC1225180
515. 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).
516. 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).
517. G. A. Voth, "Path Integral Centroid Methods in Quantum Statistical Mechanics and Dynamics", Adv. Chem. Phys. **93**, 135-218 (1996). (Invited)
518. J. Cao, L. W. Ungar, and G. A. Voth, "A Novel Method for Simulating Quantum Dissipative Systems", J. Chem. Phys. **104**, 4189-4197 (1996).
519. J. Lobaugh and G. A. Voth, "The Quantum Dynamics of an Excess Proton in Water", J. Chem. Phys. **104**, 2056-2069 (1996).
520. J. Cao and G. A. Voth, "Semiclassical Approximations to Quantum Dynamical Time Correlation Functions" J. Chem. Phys. **104**, 273-285 (1996).
521. 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).
522. 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).
523. 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).
524. 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).
525. J. Cao and G. A. Voth, "A Theory for Time Correlation Functions in Liquids", J. Chem. Phys. **103**, 4211-4220 (1995).
526. 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)

527. 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).
528. J. Cao and G. A. Voth, "Modeling Physical Systems by Effective Harmonic Oscillators: The Optimized Quadratic Approximation", *J. Chem. Phys.* **102**, 3337-3348 (1995).
529. 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).
530. 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).
531. 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).
532. 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).
533. 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).
534. 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).
535. 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).
536. 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).
537. 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).
538. 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).
539. 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)1x1 Surface", *J. Chem. Phys.* **100**, 3247-3252 (1994).
540. 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).

541. 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.
542. J. Cao and G. A. Voth, "A New Perspective on Quantum Time Correlation Functions", *J. Chem. Phys.* **99**, 10070-10073 (1993).
543. 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).
544. 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).
545. 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).
546. G. A. Voth, "Feynman Path Integral Formulation of Quantum Mechanical Transition State Theory", *J. Phys. Chem.* **97**, 8365-8377 (1993). (Invited Feature Article)
547. 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).
548. H. Gai and G. A. Voth, "Vibrational Energy Relaxation Dynamics of Si-H Stretching Modes on the H/Si(111)1x1 Surface", *J. Chem. Phys.* **99**, 740-743 (1993).
549. 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).
550. Y.-C. Sun and G. A. Voth, "Path Integral Calculation of Hydrogen Diffusion Rates on Metal Surfaces", *J. Chem. Phys.* **98**, 7451-7458 (1993).
551. 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).
552. 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).
553. G. A. Voth, "A Theory for Treating Spatially-Dependent Friction in Classical Activated Rate Processes", *J. Chem. Phys.* **97**, 5908-5910 (1992).
554. 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).
555. A. L. R. Bug, A. Wilson, and G. A. Voth, "Nonlinear Vibrational Dynamics of a Neon Atom in C₆₀", *J. Phys. Chem.* **96**, 7864-7869 (1992).
556. 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).

557. 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).
558. G. R. Haynes and G. A. Voth, "Effect of Nonlinear Dissipation on Quantum Activated Rate Processes in Condensed Phases ", *Phys. Rev. A* **46**, 2143-2146 (1992).
559. 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).
560. 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).
561. 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).
562. G. A. Voth, "Calculation of Equilibrium Averages with Feynman-Hibbs Effective Classical Potentials and Similar Variational Approximations", *Phys. Rev. A* **44**, 5302-5305 (1991).
563. 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).
564. 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).
565. G. A. Voth, "A Feynman Path Integral Approach for Calculating Quantum Rate Constants in Complex Systems", *Ber. Bunsenges. Phys. Chem.* **95**, 393-399 (1991).
566. 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).
567. 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).
568. G. A. Voth, "Analytic Expression for the Transmission Coefficient in Quantum Mechanical Transition State Theory", *Chem. Phys. Lett.* **170**, 289-296 (1990).
569. 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.
570. 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).
571. 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).
572. 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).
573. G. A. Voth, "An Effective Golden Rule Decay Rate Expression for Quasidissipative IVR Processes", *J. Chem. Phys.* **88**, 5547-5552 (1988).

574. G. A. Voth, "Quasidissipative Intramolecular Dynamics: An Adiabatically Reduced Coupled Equations Approach", *J. Chem. Phys.* **87**, 5272-5279 (1987).
575. 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).
576. G. A. Voth, "Approximate Coupled Equations for Multiphoton Processes Induced by One or More Lasers", *Chem. Phys. Lett.* **129**, 315-320 (1986).
577. G. A. Voth, "On the Relationship of Classical Resonances to the Quantum Mechanics of Coupled Oscillator Systems", *J. Phys. Chem.* **90**, 3624-3629 (1986).
578. G. A. Voth and R. A. Marcus, "Adiabatically Reduced Coupled Equations for Intramolecular Dynamics Calculations", *J. Chem. Phys.* **84**, 2254-2261 (1986).
579. 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).
580. 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).
581. 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).
582. G. A. Voth, R. A. Marcus, and A. H. Zewail, "The Highly Excited C-H Stretching States of CHD₃, CHT₃, and CH₃D", *J. Chem. Phys.* **81**, 5494-5507 (1984).

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).
2. *Methods in Enzymology Volume 577: Computational Approaches for Studying Enzyme Mechanism Part A*, G. A. Voth, Editor (Academic Press/Elsevier, Oxford, United Kingdom, 2016).
3. *Methods in Enzymology Volume 578: Computational Approaches for Studying Enzyme Mechanism Part B*, G. A. Voth, Editor (Academic Press/Elsevier, Oxford, United Kingdom, 2016).