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CURRICULUM VITAE

Richard W. Pastor, Ph.D.

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Date of Birth: June 21, 1951

Citizenship: United States

Education:

1984	Ph.D. Harvard University, Biophysics Dissertation Title: <i>Topics in Stochastic Dynamics of Polymers.</i> Preceptor: Martin Karplus
1977	M.S. Syracuse University, Chemistry Thesis Title: <i>Surface Tension Calculations for Molten Salts: Critique and Modification of the Kirkwood-Buff Model</i> Preceptor: Jerry Goodisman
1973	B.A. Hamilton College, Major in Philosophy

Employment:

2017-present	Chief, Laboratory of Membrane Biophysics, NHLBI/NIH
2006-2016	Principal Investigator, Laboratory of Computational Biology, NHLBI/NIH
1996-2006	Chief, Biophysics Laboratory, CBER/FDA
1998	Acting Chief, Laboratory of Immunobiochemistry, CBER/FDA
1990-1996	Research Chemist, Biophysics Lab, CBER/FDA
1984-1990	Senior Staff Fellow, Biophysics Lab, CBER/FDA
1984	Staff Fellow, Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health

Awards:

2021	<i>Avanti Award in Lipids</i> Biophysical Society
2019	<i>Orloff Award (Basic Science)</i> National Heart Lung Blood Institute
2013	<i>Director's Outstanding Basic Science Award</i> National Heart Lung Blood Institute
1997	<i>Center Director's Public Health Achievement Award</i> Center for Biologics Evaluation and Research
1996	<i>Scientific Achievement - Senior Investigator</i> Center for Biologics Evaluation and Research

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1996 *Excellence in Science by a Group*
Food and Drug Administration

Research Area: The application of computer simulations and statistical mechanics to biophysics, with emphasis on membranes.

Scientific Review: Reviewer for numerous journals, including *Biophysical Journal*, *Journal of the American Chemical Society*, *Journal of Physical Chemistry*, *Journal of Chemical Physics*, *Journal of Computational Chemistry*, *Nature Communications*, and *Proceedings of the National Academy of Science*.

Guest editor for *Biophysical Journal*, and *PNAS*.

Ad Hoc reviewer for NIH (Biochemistry and Biophysics of Membranes Study Section, postdoctoral fellowships), NSF and PRF.

Publications (h=68, 33000+ citations, Google Scholar, April 2023)

1. Resonance Raman Studies of Macrocyclic Complexes. 1. Structural and Electronic Effects in Synthetic Metal (II) Porphrin Analogues. W.H. Woodruff, R.W. Pastor and J.C. Dabrowiak, *J. Am. Chem. Soc.* **98**, 7999-8006 (1976).
2. Resonance Raman Studies of Macrocyclic Complexes. 2. Antiresonance and Selective Intensity Enhancement in Synthetic Metal (II) Porphrin Analogues, L.A. Nafie, R.W. Pastor, J.C. Dabrowiak, and W.H. Woodruff, *J. Am. Chem. Soc.* **98**, 8007-8014 (1976).
3. Surface Tension Calculations for Molten Salts: Critique and Modification of the Kirkwood-Buff Model, R.W. Pastor and J. Goodisman, *J. Chem. Phys.* **68**, 3654-3666 (1978).
4. A Model for the Surface of a Molten Salt, J. Goodisman and R.W. Pastor, *J. Phys. Chem.* **82**, 2078-2081 (1978).
5. A Recognition Site in Synthetic Helical Oligonucleotides for Monoclonal Anti-Native DNA Autoantibody, David Stollar, Gerald Zon, and Richard W. Pastor, *Proc. Natl. Acad. Sci. USA* **83**, 4469-2273 (1986).
6. Local Sequence Patterns of Hydrophobicity and Solvent Accessibility in Soluble Globular Proteins, David J. Lipman, Richard W. Pastor, and B. Lee, *Biopolymers* **26**, 17-26 (1987).
7. A Theoretically Determined Three-Dimensional Structure for the Repeating Tetrapeptide Unit of the Circumsporozoite Coat Protein of the Malaria Parasite *Plasmodium falciparum*, Bernard R. Brooks, Richard W. Pastor, and Frederick W. Carson, *Proc. Natl. Acad. Sci. USA* **84**, 4470-4474 (1987).
8. The Parametrization of the Friction Constant for Stochastic Simulations of Polymers, Richard W. Pastor and Martin Karplus, *J. Phys. Chem.* **92**, 2636-2641 (1988).
9. Frictional Models for Stochastic Simulations of Proteins, Richard M. Venable and Richard W. Pastor, *Biopolymers* **27**, 1001-1014 (1988).
10. Brownian Dynamics Simulation of a Lipid Chain in a Membrane Bilayer, Richard W. Pastor, Richard M. Venable, and Martin Karplus, *J. Chem. Phys.* **89**, 1112-1127 (1988).
11. A Simulation Based Model of NMR T_1 Relaxation in Lipid Bilayer Vesicles, Richard W. Pastor, Richard M. Venable, Martin Karplus, and Attila Szabo, *J. Chem. Phys.* **89**, 1128-1140 (1988).

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12. An Analysis of the Accuracy of Langevin and Molecular Dynamics Algorithms, Richard W. Pastor, Bernard R. Brooks, and Attila Szabo, *Mol. Phys.* **65**, 1409-1419 (1988).
13. Theoretically Determined Three-Dimensional Structures for Amphipathic Segments of the HIV-1 gp41 Envelope Protein, Richard M. Venable, Richard W. Pastor, Bernard R. Brooks, and Frederick W. Carson, *AIDS Research and Human Retroviruses* **5**, 7-21 (1989).
14. Anisotropic Bead Models for Molecular Hydrodynamics, Richard W. Pastor and Robert Zwanzig, *J. Chem. Phys.* **90**, 5729-5734 (1989).
15. Inertial Effects in Butane Stochastic Dynamics, Richard W. Pastor and Martin Karplus, *J. Chem. Phys.* **91**, 211-218 (1989).
16. Determination of Chain Conformations in the Membrane Interior by Brownian Dynamics Simulations, Richard W. Pastor, in *Molecular Description of Biological Membrane Components by Computer Aided Conformational Analysis*, Vol. I, (ed. R. Brasseur, CRC Press, Boca Raton, 1990), pp. 171-201.
17. Model for the Structure of the Lipid Bilayer, Richard W. Pastor, Richard M. Venable, and Martin Karplus, *Proc. Natl. Acad. Sci. USA* **88**, 892-896 (1991).
18. Mean Field Stochastic Boundary Molecular Dynamics Simulation of a Phospholipid in a Membrane, Hans De Loof, Stephen C. Harvey, Jere P. Segrest, and Richard W. Pastor, *Biochemistry* **30**, 2099-2113 (1991).
19. Molecular Dynamics Simulation of Methyl Group Relaxation in Water, Goran Widmalm, Richard W. Pastor and Thomas E. Bull, *J. Chem. Phys.* **94**, 4097-4098 (1991).
20. Analyses of Statistical Errors in Dynamics Simulations, Richard W. Pastor, in *Proteins: Structure, Dynamics, Design* (ed. V. Renugopalakrishnan, P.R. Carey, I.C.P. Smith, S.G. Huang, and A.C. Storer, ESCOM Science Publishers, The Netherlands, 1991), pp. 229-233.
21. Synexin: Molecular Mechanism of Calcium-Dependent Membrane Fusion and Voltage-Dependent Calcium Channel Activity, Harvey B. Pollard, Eduardo Rojas, Richard W. Pastor, Eduardo M. Rojas, H. Robert Guy, and A. Lee Burns, *Ann. New York Acad. Sci.* **635**, 328-351 (1991).
22. Langevin Dynamics of Peptides: the Frictional Dependence of Isomerization Rates of N-Acetylalanyl-N'-Methylamide, Richard J. Loncharich, Bernard R. Brooks, and Richard W. Pastor, *Biopolymers* **32**, 523-535 (1992).
23. Backbone Dynamics of Calmodulin Studied by ¹⁵N Relaxation Using Inverse Detected Two-Dimensional NMR Spectroscopy: The Central Helix is Flexible, Gaetano Barbato, Mitsuhiro Ikura, Lewis E. Kay, Richard W. Pastor, and Ad Bax, *Biochemistry* **31**, 5269-5278 (1992).
24. Conformational States of a TT Mismatch from Molecular Dynamics Simulation of d(CGCGATTCGCG), Richard M. Venable, Goran Widmalm, Bernard R. Brooks, William Egan, and Richard W. Pastor, *Biopolymers* **32**, 783-794 (1992).
25. A Comparison of Langevin and Molecular Dynamics Simulations: Equilibrium and Dynamics of Ethylene Glycol in Water, Goran Widmalm and Richard W. Pastor, *J. Chem. Soc. Faraday Trans.* **88**, 1747-1754 (1992).
26. Langevin Dynamics of a Linear Rotor in a Maier-Saupe Potential: Kramers Turnover of the Flipping Rate, Richard W. Pastor and Attila Szabo, *J. Chem. Phys.* **97**, 5098-5100 (1992).
27. Positional Time Correlation Function for One-Dimensional Systems with Barrier Crossing: Memory Function Corrections to the Optimized Rouse-Zimm Approximation, Angelo Perico, Roberto Pratolongo, Karl F. Freed, Richard W. Pastor, and Attila Szabo, *J. Chem. Phys.* **98**, 564-573 (1993).

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28. Molecular Dynamics Simulations of a Lipid Bilayer and of Hexadecane: An Investigation of Membrane Fluidity, Richard M. Venable, Yuhong Zhang, Barry J. Hardy, and Richard W. Pastor, *Science* **262**, 223-226 (1993).
29. Molecular and Stochastic Dynamics Simulation of Lipid Membranes, Richard W. Pastor and Richard M. Venable, in *Computer Simulation of Biomolecular Systems: theoretical and experimental applications* (ed. Wilfred F. van Gunsteren, Paul K. Weiner, and Anthony K. Wilkinson, ESCOM Science Publishers, Leiden, 1993), pp. 443-463.
30. Conformational Sampling of Hydrocarbon and Lipid Chains in an Ordering Potential, Barry J. Hardy, and Richard W. Pastor, *J. Comput. Chem.* **15**, 208-226 (1994).
31. A Comparison of Methods for Computing Transition Rates from Molecular Dynamics Simulation, Yuhong Zhang and Richard W. Pastor, *Molecular Simulation*, **13**, 25-38 (1994).
32. Techniques and Applications of Langevin Dynamics Simulations, Richard W. Pastor, in *The Molecular Dynamics of Liquid Crystals* (eds. G.R. Luckhurst and C.A. Veracini, Kluwer Academic Publishers, The Netherlands, 1994), pp. 85-138.
33. Molecular Dynamics and Monte Carlo Simulations of Lipid Bilayers, Richard W. Pastor, *Current Opinion in Structural Biology* **4**, 486-492 (1994).
34. Method For Characterizing Transition Concertedness From Polymer Dynamics Computer Simulations, Michael L. Brown, Richard M. Venable, and Richard W. Pastor, *Biopolymers* **35**, 31-46 (1995).
35. Constant Pressure Molecular Dynamics Simulation: The Langevin Piston Method, Scott E. Feller, Yuhong Zhang, Richard W. Pastor, and Bernard R. Brooks, *J. Chem. Phys.* **103**, 4613-4621 (1995).
36. Computer Simulation of Liquid/Liquid Interfaces. I. Theory and Application to Octane/Water, Yuhong Zhang, Scott E. Feller, Bernard R. Brooks, and Richard W. Pastor, *J. Chem. Phys.* **103**, 10252-10266 (1995).
37. Computer Simulation of Liquid/Liquid Interfaces. II. Surface Tension-Area Dependence of a Bilayer and Monolayer, Scott E. Feller, Yuhong Zhang, and Richard W. Pastor *J. Chem. Phys.* **103**, 10267-10276 (1995).
38. Rotational Diffusion Anisotropy of Human Ubiquitin from ¹⁵N NMR Relaxation, Nico Tjandra, Scott E. Feller, Richard W. Pastor, and Ad Bax, *J. Am. Chem. Soc.* **117**, 12562-12566 (1995).
39. Molecular Dynamics Simulations of Neat Alkanes: the Viscosity Dependence of Rotational Relaxation, Yuhong Zhang, Richard M. Venable, and Richard W. Pastor, *J. Phys. Chem.* **100**, 2652-2660 (1996).
40. Time Scales of Lipid Dynamics and Molecular Dynamics, Richard W. Pastor and Scott E. Feller, in *Membrane Structure and Dynamics* (ed. K.M. Merz and B. Roux, Birkhauser, Boston, 1996), pp. 3-29.
41. On Simulating Lipid Bilayers with an Applied Surface Tension: Periodic Boundary Conditions and Undulations, Scott E. Feller and Richard W. Pastor, *Biophysical Journal* **71**, 1350-1355 (1996).
42. Diffusion Limited First Contact of the Ends of a Polymer: Comparison of Theory and Simulation, Richard W. Pastor, Robert Zwanzig, and Attila Szabo, *J. Chem. Phys.* **105**, 3878-3882 (1996).
43. The Effect of Electrostatic Force Truncation on Interfacial and Transport Properties of Water, Scott E. Feller, Richard W. Pastor, Atipat Rojnuckarin, Steven Bogusz, and Bernard R. Brooks, *J. Phys. Chem.* **100**, 17011-17020 (1996).
44. The Length Scales of Lipid Dynamics and Molecular Dynamics, Scott E. Feller and Richard W. Pastor, in *Proceedings of the 1997 Pacific Symposium in Biocomputing*, (ed. R.B. Altman, A.K. Dunker, L.Hunter, T.E. Klein, World Scientific, Singapore, 1997), pp. 142-150.

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45. Molecular Dynamics Simulation of Unsaturated Lipid Bilayers at Low Hydration: Parametrization and Comparison with Diffraction Studies, Scott E. Feller, Daxu Yin, Richard W. Pastor, and Alexander D. MacKerell, Jr. *Biophysical Journal*, **73**, 2269-2279 (1997).
46. Computer simulation of a DPPC phospholipid bilayer: Structural Changes as a Function of Molecular Surface area, Scott E. Feller, Richard M. Venable, and Richard W. Pastor, *Langmuir* **13**, 6555-6561 (1997).
47. Time Correlation Functions, Richard W. Pastor, in *Encyclopedia of Computational Chemistry* (ed. P.R. Schleyer, John Wiley & Sons, UK, 1998), pp. 3003-3011.
48. Solution Structure of the Linked Cell Attachment Modules of Mouse Fibronectin Containing the RGD and Synergy Regions: Comparison with the Human Fibronectin Crystal Structure, Valerie Copie, York Tomita, Steven K. Akiyama, Shin-ichi Aota, Kenneth M. Yamada, Richard M. Venable, Richard W. Pastor, Susan Krueger, and Dennis A. Torchia, *J. Mol. Biol.* **277**, 663-682 (1998).
49. Constant Surface Tension Simulations of Lipid Bilayers: The Sensitivity of Surface Areas and Compressibilities, Scott E. Feller, and Richard W. Pastor, *J. Chem. Phys.* **111**, 1281-1287 (1999).
50. Distinguishing Anisotropy and Flexibility of the Pentasaccharide LNF-1 in Solution by Carbon-13 NMR Relaxation and Hydrodynamic Modeling, Torgny Rundlöf, Richard M. Venable, Richard W. Pastor, Jozef Kowalewski, and Göran Widmalm, *J. Am. Chem. Soc.* **121**, 11847-11854 (1999).
51. Statistical Considerations in the Establishment of Release Criteria for Allergen Vaccines, Jay E. Slater, Albert A. Gam, Maneesha D. Solanki, Suzann H. Burk, Faith M. May, and Richard W. Pastor in *Proceedings of the 1999 Paul Ehrlich Symposium*, (ed. R. Kurth and D. Haustein, GIT VERLAG, Darmstadt, 2000), pp. 47-56.
52. The Determination of Equivalent Doses of Standardized Allergen Vaccines, Jay E. Slater and Richard W. Pastor, *J. Allergy and Clinical Immunology* **105**, 468-474 (2000)
53. The Stability of House Dust Mite Allergens in Glycerinated Extracts. Lyudmila N. Soldatova, Elizabeth J. Paupore, Suzann H. Burk, Richard W. Pastor, and Jay E. Slater, *J. Allergy and Clinical Immunology* **105**, 482-488 (2000).
54. Molecular Dynamics Simulations of Gel ($L_{\beta 1}$) Phase Lipid Bilayers in Constant Pressure and Constant Surface Tension Ensembles, Richard M. Venable, Bernard R. Brooks, and Richard W. Pastor, *J. Chem. Phys.* **112**, 4822-4832 (2000).
55. Molecular Dynamics Simulations of Octyl Glucoside Micelles: Structural Properties, Stephen Bogusz, Richard M. Venable, and Richard W. Pastor, *J. Phys. Chem. B* **104**, 5462-5470 (2000).
56. ICAM-1 Enhances MHC-peptide Activation of CD8⁺ T-cells without an Organized Immunological Synapse, Julia S. Goldstein, Trina Chen, Elena Gubina, Richard W. Pastor, and Steven Kozlowski, *European J. Immunology*, **30**, 3266-3279 (2000).
57. Molecular Dynamics Simulations of Octyl Glucoside Micelles: Dynamic Properties, Stephen Bogusz, Richard M. Venable, and Richard W. Pastor, *J. Phys. Chem. B* **105**, 8312-8321 (2001).
58. Molecular Dynamics Simulations of Water Wires and Water/Octane Model Systems, Richard M. Venable, and Richard W. Pastor, *J. Chem. Phys.* **116**, 2663-2664 (2002).
59. Simulations of Membranes and Other Interfacial Systems Using P2₁ and P₆ Periodic Boundary Conditions, Elizabeth A. Dolan, Richard M. Venable, Richard W. Pastor, and Bernard R. Brooks, *Biophysical Journal* **85**, 2317-2325 (2002).
60. Lipid Bilayers, NMR Relaxation, and Computer Simulations, Richard W. Pastor, Richard M. Venable, and Scott E. Feller, *Accounts of Chemical Research* **35**, 438-446 (2002).

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61. Micelle-Bound Conformation of a Hairpin-Forming Peptide: A Combined NMR and Molecular Dynamics Study, Ann M. Dixon, Richard M. Venable, Richard W. Pastor, and Thomas E. Bull, *Biopolymers* **65**, 284-298 (2002).
62. Application of NMR, Molecular Simulation and Hydrodynamics to Conformational Analysis of Trisaccharides, Ann M. Dixon, Richard M. Venable, Göran Widmalm, Thomas E. Bull, and Richard W. Pastor, *Biopolymers* **69**, 448-460 (2003).
63. Sample Size Considerations for Establishing Clinical Bioequivalence of Allergen Formulations, Ronald L. Rabin, Jay E. Slater, Peter Lachenbruch, and Richard W. Pastor in *Proceedings of the 2002 Paul Ehrlich Symposium*, (ed. J. Lower, W. Becker and S. Vieths, Druck und Verlagshaus Sperllich, Frankfurt, 2003), pp. 24-33.
64. A Pressure-Based Long-Range Correction for Lennard Jones Interactions In Molecular Dynamics Simulations: Application To Alkanes and Interfaces, Patrick Lague, Richard W. Pastor, Bernard Brooks, *J. Phys. Chem. B* **108**, 363-368 (2004).
65. Discriminating the Helical Forms of Peptides by NMR and Molecular Dynamics Simulation, Darón I. Freedberg, Richard M. Venable, Angelo Rossi, Thomas E. Bull, and Richard W. Pastor, *J. Am. Chem. Soc.* **126**, 10478-10484 (2004).
66. An Ab Initio Study on the Torsional Surface of Alkanes and its Effect on Molecular Simulations of Alkanes and a DPPC Bilayer, Jeffery B. Klauda, Bernard R. Brooks, Alexander D. MacKerell, Jr., Richard M. Venable, and Richard W. Pastor, *J. Phys. Chem. B.* **109**, 5300-5311 (2005).
67. Adjacent Gauche Stabilization in Linear Alkanes: Implications for Polymer Models and Conformational Analysis, Jeffery B. Klauda, Richard W. Pastor, and Bernard R. Brooks, *J. Phys. Chem B.* **109**, 16584-15686 (2005).
68. A Molecular Dynamics Study of the Response of Lipid Bilayers and Monolayers to Trehalose. Anna Skibinsky, Richard M. Venable, and Richard W. Pastor, *Biophysical Journal*, **89**, 4111-4121 (2005).
69. Molecular Dynamics Simulations of the Influenza Hemagglutinin Fusion Peptide in Micelles and Bilayers: Conformational Analysis of Peptide and Lipids. Patrick Lagüe, Benoît Roux, and Richard W. Pastor, *J. Mol. Biol.*, **354**, 1129-1141 (2005).
70. Importance of the CMAP Correction to the CHARMM22 Protein Force Field. Dynamics of Hen Lysozyme, Matthias Buck, Sabine Bouguet-Bonnet, Richard W. Pastor, and Alexander D. MacKerell, Jr, *Biophysical Journal*, **90**, L36-L38 (2006).
71. Simulation-based Methods for Interpreting X-ray Data from Lipid Bilayers, Jeffery B. Klauda, Norbert Kučerka, Bernard R. Brooks, Richard W. Pastor, and John F. Nagle, *Biophysical Journal*, **90**, 2796-2807 (2006).
72. Constant Surface Tension Molecular Dynamics Simulations of Lipid Bilayers with Trehalose, Richard M. Venable, Anna Skibinsky, and Richard W. Pastor, *Molecular Simulation*, **32**, 849-855 (2006).
73. Dynamical Motions of Lipids and a Finite Size Effect in Simulations of Bilayers, Jeffery B. Klauda, Bernard R. Brooks, and Richard W. Pastor, *J. Chem. Phys.*, **125**, 144710-144718 (2006).
74. Long-range Lennard-Jones and Electrostatic Interactions in Interfaces: Application of the Isotropic Periodic Sum Method, Jeffery B. Klauda, Xiongwu Wu, Richard W. Pastor, and Bernard R. Brooks, *J. Phys. Chem., B*, **111**, 4393-4400 (2007).
75. Additive and Classical Drude Polarizable Force Fields for Linear and Cyclic Ethers, Igor Vorobyov, Victor M. Anisimov, Shannon Greene, Richard M. Venable, Adam Moser, Richard W. Pastor, and Alexander D. MacKerell, Jr., *J. Chemical Theory and Computation*, **3**, 1120-1133 (2007).

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76. Ab initio Modeling of Glycosyl Torsions and Anomeric Effects in a Model Carbohydrate: 2- Ethoxy Tetrahydropyran, H. Lee Woodcock, Damian Moran, Richard W. Pastor, Alexander D. MacKerell Jr., and Bernard R. Brooks, *Biophysical Journal*, **93**, 1-10 (2007).
77. Rotation of Lipids in Membranes: MD Simulation,³¹P Spin-Lattice Relaxation, and Rigid-Body Dynamics, Jeffrey B. Klauda, Mary F. Roberts, Alfred G. Redfield, Bernard R. Brooks, and Richard W. Pastor, *Biophysical Journal*, **94**, 3074-3083 (2008).
78. Collective and Noncollective Models of NMR Relaxation in Lipid Vesicles and Multilayers, Jeffery B. Klauda, Nadukkudy V. Eldho, Klaus Gawrisch, Bernard R. Brooks, and Richard W. Pastor. *J. Phys. Chem. B*, **112**, 5924-5929 (2008).
79. Langevin Network Model of Myosin, Benjamin T. Miller, Wenjun Zheng, Richard M. Venable, Richard W. Pastor, and Bernard R. Brooks, *J. Phys. Chem. B.*, **112**, 6274-6281 (2008).
80. Pathways and Populations of the 5-hydroxy-methyl-tetrahydropyran Exocyclic Torsion: Stereoelectronic Insights from a Computational Perspective, H. Lee Woodcock, Bernard R. Brooks, and Richard W. Pastor, *J. Am. Chem. Soc.*, **130**, 6345-6347 (2008).
81. Considerations for Lipid Force Field Development, Jeffery B. Klauda, Richard M. Venable, Alexander D. MacKerell, Jr., and Richard W. Pastor. In *Computational Modeling of Membrane Bilayers* (ed. Scott E. Feller), *Current Topics in Membranes*, **60** (Elsevier, San Diego), 1-48 (2008).
82. Molecular Dynamics Studies of Polyethylene Oxide and Polyethylene Glycol: Hydrodynamic Radius and Shape Anisotropy, Hwanky Lee, Richard M. Venable, Alexander D. MacKerell, Jr., and Richard W. Pastor, *Biophysical Journal*, **95**, 1590-1599 (2008).
83. Additive Empirical Force Field for Hexopyranose Monosaccharides, Olgun Guvench, Shannon N. Greene, Ganesh Kamath, John W. Brady, Richard M. Venable, Richard W. Pastor, and Alexander D. MacKerell, Jr., *J. Comp. Chem.*, **29**, 2543-2564 (2008).
84. Structure and Dynamics of Helix-0 of the N-BAR Domain in Lipid Micelles and Bilayers, Christian Löw, Ulrich Weininger, Hwanky Lee, Kristian Schweimer, Ines Neundorf, Annette G. Beck-Sickinger, Richard W. Pastor, and Jochen Balbach, *Biophysical Journal*, **95**, 4315-4323 (2008).
85. Comparison of the Extended Isotropic Periodic Sum and Particle Mesh Ewald Methods for Simulations of Lipid Bilayers and Monolayers, Richard M. Venable, Linda E. Chen, and Richard W. Pastor, *J. Phys. Chem. B.*, **113**, 5855-5862 (2009).
86. CHARMM: The Biomolecular Simulation Program, B.R. Brooks, C.L. Brooks III, A.D. MacKerell, Jr., L. Nilsson, R.J. Petrella, B. Roux, Y. Won, G. Archontis, C. Bartels, S. Boresch, A. Caffisch, L. Caves, Q. Cui, A.R. Dinner, M. Feig, S. Fischer, J. Gao, M. Hodoscek, W. Im, K. Kuczera, T. Lazaridis, J. Ma, V. Ovchinnikov, E. Paci, R.W. Pastor, C.B. Post, J.Z. Pu, M. Schaefer, B. Tidor, R. M. Venable, H. L. Woodcock, X. Wu, W. Yang, D.M. York, and M. Karplus, *J. Comp. Chem.*, **30**, 1545-1614 (2009).
87. Molecular Dynamics Simulations of PIP₂ and PIP₃ in Lipid Bilayers: Determination of Ring Orientation, and the Effects of Surface Roughness on a Poisson-Boltzmann Description, Zheng Li, Richard M. Venable, Laura A. Rogers, Diana Murray, and Richard W. Pastor, *Biophysical Journal*, **97**, 155-163 (2009).
88. CHARMM Additive All-Atom Force Field for Glycosidic Linkages between Hexopyranoses, Olgun Guvench, Elizabeth R. Hatcher, Richard M. Venable, Richard W. Pastor, and Alexander D. MacKerell, Jr. *J. Chemical Theory and Computation*, **5**, 2353-2370 (2009).
89. A Coarse-Grained Model for Polyethylene Oxide and Polyethylene Glycol: Conformation and Hydrodynamics, Hwanky Lee, Alex H. de Vries, Siewert-Jan Marrink, and Richard W. Pastor, *J. Phys. Chem. B.*, **113**, 13186-13194 (2009).

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90. Molecular Dynamics Studies of the Conformation of Sorbitol, Adrian Lerbret, P.E. Mason, Richard M. Venable, A. Cesàro, M.-L. Saboungi, Richard W. Pastor, and John W. Brady, *Carbohydrate Research*, **344**, 2229-2235 (2009).
91. Update of the CHARMM all-atom additive force field for lipids: Validation on six lipid types, Jeffery B. Klauda, Richard M. Venable, J. Alfredo Freites, Joseph W. O'Connor, Douglas J. Tobias, Carlos Mondragon-Ramirez, Igor Vorobyov, Alexander D. MacKerell, Jr., and Richard W. Pastor, *J. Phys. Chem. B.*, **114**, 7830-7843 (2010).
92. Comparing Simulated and Experimental Translation and Rotation Constants: Range of Validity for Viscosity Scaling. Richard M. Venable, Elizabeth Frush, Olgun Guvench, Alexander D. MacKerell, Jr., and Richard W. Pastor, *J. Phys. Chem. B.*, **114**, 12501-12507 (2010).
93. Single molecule diffusion of membrane-bound proteins: A window into lipid contacts and bilayer dynamics, Jefferson D. Knight, Michael G. Lerner, Joan G. Marcano-Velázquez, Richard W. Pastor, and Joseph J. Falke, *Biophysical Journal*, **99**, 2879-2887 (2010).
94. Molecular Dynamics Studies of Ion Permeation in VDAC, Huan Rui, Kyu Il Lee, Richard W. Pastor, and Wonpil Im, *Biophysical Journal*, **100**, 602-610 (2011).
95. Brownian Dynamics Simulations of Ion Transport through VDAC, Kyu Il Lee, Huan Rui, Richard W. Pastor, and Wonpil Im, *Biophysical Journal*, **100**, 611-619 (2011).
96. A coarse-grained model for PEGylated lipids: the effect of PEGylation on size and shape of self-assembled structures, Hwankyu Lee, and Richard W. Pastor, *J. Phys. Chem. B.*, **115**, 7830-7837 (2011).
97. Development of the CHARMM Force Field for Lipids, R.W. Pastor, and A.D. MacKerell, Jr., *J. Phys. Chem. Letters*, **2**, 1526-1532 (2011).
98. Evidence for a fence that impedes the diffusion of phosphatidylinositol 4,5-bisphosphate (PIP₂) out of the forming phagosomes of macrophages, Urszula Golebiewska, Jason G. Kay, Thomas Masters, Sergio Grinstein, Wonpil Im, Richard W. Pastor, Suzanne Scarlata, and Stuart McLaughlin, *Molecular Biology of the Cell*, **22**, 3498-3507 (2011).
99. Web Interface for Brownian Dynamics Simulation of Ion Transport and Its Applications to Beta-Barrel Pores, Kyu Il Lee, Sunhwan Jo, Huan Rui, Bernhard Egwolf, Benoit Roux, Richard W. Pastor, and Wonpil Im, *J. Comp. Chem.*, **33**, 331-339 (2012).
100. Molecular Insights into α -Synuclein and its N-terminal Peptides at the Membrane Interface, Candace M. Pfeifferkorn, Frank Heinrich, Alexander J. Sodt, Alexander S. Maltsev, Richard W. Pastor, and Jennifer C. Lee, *Biophysical Journal*, **102**, 613-621 (2012).
101. Structure and Elasticity of Lipid Membranes with Genistein and Daidzein Bioflavonoids Using X-Ray Scattering and MD Simulations, Mohit Raghunathan, Yuriy Zubovski, Richard M. Venable, Richard W. Pastor, John Nagle, and Stephanie Tristram-Nagle, *J. Phys. Chem. B.*, **116**, 3928-3927 (2012).
102. Influence of Hydrophobic Mismatch on Structures and Dynamics of Gramicidin A and Lipid Bilayers, Taehoon Kim, Kyu Il Lee, Phillip Morris, Richard W. Pastor, Olaf S. Andersen, and Wonpil Im, *Biophysical Journal*, **102**, 1551-1560 (2012).
103. The Tension of a Curved Surface from Simulation, Alexander J. Sodt and Richard W. Pastor, *J. Chem. Phys.*, **137**, 243101-234113 (2012).
104. Prediction, Refinement and Persistency of Transmembrane Helix Dimers in Lipid Bilayers using Implicit and Explicit Solvent/Lipid Representations: Microsecond Molecular Dynamics Simulations of ErbB1/B2 and EphA1. Liqun Zhang, Alexander J. Sodt, Richard M. Venable, Richard W. Pastor, and Matthias Buck, *Proteins: Structure, Function, and Bioinformatics*, **81**, 365-376 (2013).

Richard W. Pastor, Ph.D.

105. Assessing Smectic Liquid-Crystal Continuum Models for Elastic Bilayer Deformations. Kyu Il Lee, Richard W. Pastor, Wonpil Im, and Olaf S. Andersen, *Chemistry and Physics of Lipids*, **169**, 19-26 (2013).
106. Theory of Polymer-Nanopore Interactions Refined Using Molecular Dynamics Simulations. Arvind Balijepalli, Joseph W. F. Robertson, Joseph E. Reiner, John J. Kasianowicz, and Richard W. Pastor, *J. Am. Chem. Soc.*, **135**, 7064-7072 (2013).
107. Bending free energy from simulation: Correspondence of planar and inverse hexagonal lipid phases. Alexander J. Sodt and Richard W. Pastor, *Biophysical Journal*, **104**, 2202-2211 (2013).
108. Simulations of Anionic Lipid Membranes: Development of Interaction-Specific Ion Parameters and Validation using NMR Data. Richard M. Venable, Yun Luo, Klaus Gawrisch, Benoît Roux, and Richard W. Pastor, *J. Phys. Chem. B*, **117**, 10183-10192 (2013).
109. The Molecular Structure of the Liquid Ordered Phase of Lipid Bilayers. Alexander J. Sodt, Michael Logan Sandar, Klaus Gawrisch, Richard W. Pastor, and Edward Lyman, *J. Am. Chem. Soc.* **136**, 725-732 (2014).
110. High-Resolution Structures and Orientations of Antimicrobial Peptides Piscidin 1 and Piscidin 3 in Fluid Bilayers Reveal Tilting, Kinking, and Bilayer Immersion. B. Scott Perrin Jr., Ye Tian, Riqiang Fu, Christopher V. Grant, Eduard Y. Chekmenev, William E. Wiczorek, Alexander E. Dao, Robert M. Hayden, Caitlin M. Burzynski, Richard M. Venable, Mukesh Sharma, Stanley J. Opella, Richard W. Pastor, and Myriam L. Cotten, *J. Am. Chem. Soc.* **136**, 3321-3712 (2014).
111. Combining NMR Spectroscopic Measurements and Molecular Dynamics Simulations to Determine the Orientation of Amphipathic Peptides in Lipid Bilayers. B. Scott Perrin Jr, Richard W. Pastor, and Myriam Cotten. In *Advances in Biological Solid-State NMR: Proteins and Membrane-Active Peptides* (Eds. F. Separovic and A. Naito). New Developments in NMR (Editor in Chief W.S. Price), Royal Society of Chemistry 18- 35 (2014).
112. Molecular Modeling of Lipid Membrane Curvature Induction by a Peptide: More than Simply Shape. Alexander J. Sodt and Richard W. Pastor, *Biophysical Journal*, **106**, 1958-1969 (2014).
113. CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature. Richard M. Venable, Alexander J. Sodt, Brent Rogaski, Huan Rui, Elizabeth Hatcher, Alexander D. MacKerell, Jr., Richard W. Pastor, and Jeffery B. Klauda, *Biophysical Journal*, **107**, 134-145 (2014).
114. Determination of Biomembrane Bending Moduli in Fully Atomistic Systems, Zachery A. Levine, Richard M. Venable, Max C. Watson, Michael G. Lerner, Joan-Emma Shea, Richard W. Pastor, and Frank L.H. Brown, *J. Am. Chem. Soc.* **136**, 13582-13585 (2014).
115. Langevin Dynamics Simulations of Charged Model Phosphatidylinositol Lipids in the Presence of Diffusion Barriers: Toward an Atomic Level Understanding of Corraling of PIP₂ by Protein Fences in Biological Membranes. Kyu Il Lee, Wonpil Im, and Richard W. Pastor, *BMC Biophysics*, **7** (2014).
116. The Curvature Induction of Surface-Bound Antimicrobial Peptides Piscidin 1 and Piscidin 3 Varies with Lipid Chain Length. B. Scott Perrin Jr., Alexander J. Sodt, Myriam Cotten, and Richard W. Pastor, *J. Membrane Biology*, **248**, 455-467 (2015).
117. Hexagonal Substructure and Hydrogen Bonding in Liquid Ordered Phases of Palmitoyl Sphingomyelin. Alexander J. Sodt, Richard W. Pastor, and Edward Lyman, *Biophysical Journal*, **109** 948-955 (2015).
118. Mechanical Properties of Lipid Bilayers from Molecular Dynamics Simulation. Richard M. Venable, Frank L.H. Brown, and Richard W. Pastor, *Chemistry and Physics of Lipids*, **192**, 60-74 (2015).

Richard W. Pastor, Ph.D.

119. Strong Influence of Periodic Boundary Conditions on Lateral Diffusion in Lipid Bilayer Membranes. Brian A. Camley, Michael G. Lerner, Richard W. Pastor, and Frank L.H. Brown, *J. Chem. Phys.*, **143**, 243113-243124 (2015).
120. Simulations of Membrane Disrupting Peptides I: Alamethicin Pore Stability and Spontaneous Insertion. B. Scott Perrin Jr. and Richard W. Pastor. *Biophysical Journal*, **111**, 1248-1257 (2016).
121. Simulations of Membrane Disrupting Peptides II: AMP Piscidin 1 Favors Surface Defects Over Pores. B. Scott Perrin Jr., Riqiang Fu, Myriam L. Cotten, M. and Richard W. Pastor, *Biophysical Journal*, **111**, 1258-1266 (2016).
122. Nonadditive Compositional Curvature Energetics of Lipid Bilayers. Alexander J. Sodt, Richard M. Venable, Edward Lyman, and Richard W. Pastor, *Phys. Rev. Lett.*, **117**, 138104 (2016).
123. Identification of a Novel Lipid Binding Motif in Apolipoprotein B by the Analysis of Hydrophobic Cluster Domains. Scott M. Gordon, Mohsen Pourmoussa, Maureen Sampson, Denis Sviridov, Rafique M. Islam, B. Scott Perrin Jr., Georgina Kemeh, Richard W. Pastor, and Alan T. Remaley, *BBA – Biomembranes* **1859**, 135-145 (2017).
124. Gramicidin A Channel Formation Induces Local Lipid Redistribution I: Simulation and Experiment. Andrew H. Beaven, Andria M. Maer, Alexander J. Sodt, Huan Rui, Richard W. Pastor, Olaf S. Andersen, and Wonpil Im, *Biophysical Journal*, **112**, 1185-1197 (2017).
125. Gramicidin A Channel Formation Induces Local Lipid Redistribution II: a 3D Continuum Elastic Model. Alexander J. Sodt, Andrew H. Beaven, Olaf S. Andersen, Wonpil Im, and Richard W. Pastor, *Biophysical Journal*, **112**, 1198-1213 (2017).
126. Lipid and Peptide Diffusion in Bilayers: the Saffman-Delbrück Model and Periodic Boundary Conditions. Richard M. Venable, Helgi I. Ingólfsson, Michael G. Lerner, B. Scott Perrin, Jr., Brian A. Camley, Siewert J. Marrink, Frank L.H. Brown, and Richard W. Pastor, *J. Phys. Chem. B.*, **121**, 3443-3457 (2017).
127. Position Dependent Diffusion Tensors in Anisotropic Media from Simulation: Oxygen Transport In and Through Membranes. An Ghysels, Richard M. Venable, Richard W. Pastor, and Gerhard Hummer, *J. Chem. Theory and Computation*, **13**, 2962-2976 (2017).
128. Characterizing Residue-Bilayer Interactions Using Gramicidin A As a Scaffold and Tryptophan Substitutions as Probes. Andrew H. Beaven, Alexander J. Sodt, Richard W. Pastor, Roger E. Koeppe II, Olaf S. Andersen, and Wonpil Im, *J. Chem. Theory and Computation*, **13**, 5054-5064 (2017).
129. Graph-Theoretic Analysis of Monomethyl Phosphate Clustering in Ionic Solutions. Kyungreem Han, Richard M. Venable, Anne-Marie Bryant, Christopher J. Legacy, Rong Shen, Hui Li, Benoît Roux, Arne Gericke, and Richard W. Pastor, *J. Phys. Chem. B.*, **122**, 1484-1494 (2018).
130. Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. Alison Leonard, Andrew C. Simmonett, Frank Pickard IV, Jing Huang, Richard M. Venable, Jeffery B. Klauda, Bernard R. Brooks, and Richard W. Pastor, *J. Chem. Theory and Computation*, **14**, 948-958 (2018).
131. Structural Properties of Apolipoprotein A-I Mimetic Peptides That Promote ABCA1-1 Dependent Cholesterol Efflux. Rafique M. Islam, Mohsen Pourmoussa, Denis Sviridov, Scott M. Gordon, Edward B. Neufeld, Lita A. Freeman, B. Scott Perrin Jr., Richard W. Pastor, and Alan T. Remaley, *Scientific Reports*, **8**, 2956 (2018).
132. Tertiary Structure of Apolipoprotein A-I in Nascent High-Density Lipoproteins. Mohsen Pourmoussa, Hyun D. Song, Yi He, Jay W. Heinecke, Jere P. Segrest, Richard W. Pastor, *Proc. Natl. Acad. Sci. U.S.A.*, **115**, 5163-5168 (2018).
133. Parameterization of the CHARMM All-Atom Force Field for Ether Lipids and Model Linear Ethers. Alison N. Leonard, Richard W. Pastor, and Jeffery B. Klauda, *J. Phys. Chem. B.*, **122**, 6744-6754 (2018).

Richard W. Pastor, Ph.D.

134. Membrane Permeability: Characteristic Times and Lengths for Oxygen, and a Simulation-Based Test of the Inhomogeneous Solubility-Diffusion Model. Oriana De Vos, Richard M. Venable, Tanja Van Hecke, Gerhard Hummer, Richard W. Pastor, and An Ghysels, *J. Chem. Theory and Computation*, **14**, 3811-3824 (2018).
135. Molecular Dynamics Simulation of Lipid Nanodiscs. Mohsen Pourmoussa and Richard W. Pastor, *BBA – Biomembranes*, **1860**, 2094-2107 (2018).
136. Mannobiose-Grafting Shifts PEI Charge and Biphasic Dependence on pH. Saswati Basu, Richard M. Venable, Bria Rice, Eric Ogharandunkun, Jeffery B. Klauda, Richard W. Pastor, and Preethi L. Chandran, *Macromolecular Chemistry and Physics*, **220**, 1800423 (2019).
137. Revisiting Volumes of Lipid Components in Bilayers. John F. Nagle, Richard M. Venable, Ezekiel Maroclo-Kemmerling, Stephanie Tristram-Nagle, Paul E. Harper, and Richard W. Pastor, *J. Phys. Chem. B*, **123**, 2697-2709 (2019).
138. Molecular Dynamics Simulations of Membrane Permeability. Richard M. Venable, Andreas Krämer, and Richard W. Pastor, *Chemical Reviews*, **119**, 5954-5997 (2019).
139. Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarizability. Andreas Krämer, Frank C. Pickard IV, Jing Huang, Richard M. Venable, Andrew C. Simmonett, Dirk Reith, Karl N. Kirschner, Richard W. Pastor, and Bernard R. Brooks, *J. Chem. Theory and Computation*, **15**, 3854-3867 (2019).
140. Structure and Function in Antimicrobial Piscidins: Histidine Position, Directionality of Membrane Insertion, and pH-dependent Permeabilization. Mihaela Mihailescu, Mirco Sorci, Jolita Seckute, Vitalii I. Silin, Janet Hammer, B. Scott Perrin, Jr., Jorge I. Hernandez, Nedzada Smajic, Akritee Shrestha, Kimberly A. Bogardus, Alexander I. Greenwood, Riqiang Fu, Jack Blazyk, Richard W. Pastor, Linda K. Nicholson, Georges Belfort, and Myriam L. Cotten, *J. Am. Chem. Soc.*, **141**, 9837-9853 (2019).
141. Nonequilibrium Calculation of Surface Shear Viscosity and Interleaflet Friction for the Martini and CHARMM36 Force Field. Andrew Zgorski, Richard W. Pastor, and Edward Lyman, *J. Chem. Theory and Computation*, **15**, 6471-6481 (2019).
142. Quantitative Characterization of Protein-Lipid Interactions by Free Energy Simulation Between Binary Bilayers. Soohyung Park, Min Sun Yeom, Olaf S. Andersen, Richard W. Pastor, and Wonpil Im, *J. Chem. Theory and Computation*, **15**, 6491-6503 (2019).
143. Permeability of Membranes in the Liquid Ordered and Liquid Disordered Phases. An Ghysels, Andreas Krämer, Richard M. Venable, Walter E. Teague Jr., Edward Lyman, Klaus Gawrisch, and Richard W. Pastor, *Nature Communications*, **10**, 5616 (2019).
144. A Dual ApoC-II Mimetic-ApoC-III Antagonist Peptide for Lowering Plasma Triglycerides. Anna Wolska, Larry Lo, Denis O. Sviridov, Mohsen Pourmoussa, Milton Pryor, Soumitra S. Ghosh, Rahul Kakkar, Michael Davidson, Sierra Wilson, Richard W. Pastor, Ira Goldberg, Debapriya Basu, Steven K. Drake, Antony Cougnoux, Ming Jing Wu, Saskia Neher, Lita A. Freeman, Jingrong Tang, Marcelo Amar, Matt Devalaraja, and Alan T. Remaley, *Science Translational Medicine*, **12**, eaaw7905 (2020). DOI: 10.1126/scitranslmed.aaw7905.
145. Characterization of Specific Ion Effects on PI(4,5)P₂ Clustering: Molecular Dynamics Simulations and Graph-Theoretic Analysis. Kyungreem Han, Arne Gericke, and Richard W. Pastor, *J. Phys. Chem. B*, **124**, 1183-1196 (2020).
146. Incorporation of α -Methylated Amino Acids into Apolipoprotein A-I Mimetic Peptides Improves their Helicity and Cholesterol Efflux Potential. Rafique Islam, Denis O. Sviridov, Steven K. Drake, Jude Tunyi, Galina Abdoulaeva, Lita A. Freeman, Richard W. Pastor, and Alan T. Remaley, *Biochemical and Biophysical Research Communications*, **526**, 349-354 (2020).

Richard W. Pastor, Ph.D.

147. The Molecular Structure of Sphingomyelin in Fluid Phase Bilayers Determined by the Joint Analysis of Small-Angle X-Ray and Neutron Scattering Data. Milka Doktorova, Norbert Kučerka, Jacob J. Kinnun, Jianjun Pan, Drew Marquardt, Richard M. Venable, Richard W. Pastor, Stephen R. Wassall, John Katsaras, and Frederick A. Heberle, *J. Phys. Chem. B.*, **124**, 5186-5200 (2020).
148. PLD2–PI(4,5)P₂ Interactions in Fluid Phase Membranes: Structural Modeling and Molecular Dynamics Simulations. Kyungreem Han, Richard W. Pastor, and Cristina Fenollar–Ferrer, *PLOS One*, **15**, e0236201 (2020). <https://doi.org/10.1371/journal.pone.0236201>.
149. Membrane Permeability of Small Molecules from Unbiased Molecular Dynamics Simulations. Andreas Krämer, An Ghysels, Eric Z. Wang, Richard M. Venable, Jeffery B. Klauda, Bernard R. Brooks, and Richard W. Pastor. *J. Chem. Phys.*, **153**, 124107 (2020).
150. Semi-Automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. Yalun Yu, Andreas Krämer, Richard M. Venable, Andrew C. Simmonett, Alexander D. MacKerell, Jr., Jeffery B. Klauda, Richard W. Pastor, and Bernard R. Brooks, *J. Chem. Theory and Computation*, **17**, 1562-1580 (2021).
151. CHARMM36 Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for PE, PG, and Ether Lipids. Yalun Yu, Andreas Krämer, Richard M. Venable, Bernard R. Brooks, Jeffery B. Klauda, and Richard W. Pastor, *J. Chem. Theory and Computation*, **17**, 1581-1595 (2021).
152. Functional Group Distributions, Partition Coefficients, and Resistance Factors in Lipid Bilayers Using Site-Identification by Ligand Competitive Saturation (SILCS). Christoffer Lind, Poonam Pandey, Richard W. Pastor & Alexander D. MacKerell Jr, *J. Chem. Theory and Computation*, **17**, 3188-3202 (2021)
153. Location and Conformational Ensemble of Menaquinone and Menaquinol, and Protein-Lipid Modulations in Archaeal Membranes. Shasha Feng, Ruixing Wang, Richard W. Pastor, Jeffery B. Klauda, Wonpil Im, *J. Phys. Chem. B*, **125**, 4714-4725 (2021).
154. Development of CHARMM Additive Potential Energy Parameters for α -Methyl Amino Acids. Anthony J. Pane, Wenbo Yu, Asaminew Aytenfisu, Jude Tunyi, Richard M. Venable, Alexander D. MacKerell, Jr., and Richard W. Pastor, *J. Phys. Chem. B*, **125**, 11687-11696 (2021).
155. Developing Initial Conditions for Simulations of Asymmetric Membranes: A Practical Recommendation. Soohyung Park, Wonpil Im, and Richard W. Pastor, *Biophysical Journal*, **120**, 5041-5019 (2021).
156. Design Principles of PI(4,5)P₂ Clustering Under Protein-Free Conditions: Specific Cation Effects and Calcium-Potassium Synergy. Kyungreem Han, Soon Ho Kim, Richard M. Venable, and Richard W. Pastor, *Proc. Natl. Acad. Sci. U.S.A.*, **119**, e22022647119 (2022).
157. Finite-Size Effects in Simulations of Peptide/Lipid Assembly, Zack Jarin, Olivia Agolini, Richard W. Pastor, *Journal of Membrane Biology* **255**, 439-449 (2022)
158. Planar Aggregation of the Influenza Viral Fusion Peptide Alters Membrane Structure and Hydration. Amy Rice, Sourav Halder, Eric Wang, Paul S. Blank, Sergey A. Akimov, Timur R. Galimzyanov, Richard W. Pastor, Joshua Zimmerberg, *Nature Communications*, **13**, 7336 (2022).
159. Editorial: Special Issue for Klaus Gawrisch, Joshua Zimmerberg, Olivier Soubias, and Richard W. Pastor, *Biophysical Journal*, **122**, E01-E08 (2023).
160. Initiation and Evolution of Pores Formed by Influenza Fusion Peptides Probed by Lysolipid Inclusion. Amy Rice, Joshua Zimmerberg, and Richard W. Pastor, *Biophysical Journal*, **122**, 1018-1032 (2023).

Richard W. Pastor, Ph.D.

161. Surface Viscosities of Lipid Bilayers Determined from Equilibrium Molecular Dynamics Simulations. James E. Fitzgerald III, Richard M. Venable, Richard W. Pastor, and Edward Lyman, *Biophysical Journal*, **122**, 1094-1104 (2023).
162. Drude Polarizable Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Saturated and Mono-unsaturated Zwitterionic Lipids. Yalun Yu, Richard M. Venable, Jonathan Thirman, Payal Chatterjee, Anmol Kumar, Richard W. Pastor, Benoit Roux, Alexander. D. MacKerell Jr., and Jeffery B. Klauda, *J. Chem. Theory and Computation*, *in press*.
163. Toward Establishing the Correspondence of Liquid Ordered Phases and Cellular Rafts: Lipid Unsaturation and Peptide Affinity. Soohyung Park, Ilya Levental, Richard W. Pastor, and Wonpil Im, *J. Chem. Theory and Computation*, *in revision*.
164. Extra-small and small HDL particles are key mediators of ABCA1-dependent cholesterol efflux in both control and LCAT-deficient humans. Yi He, Patrick M. Hutchins, Mohsen Pourmousa, Hyun D. Song, Chiara Pavenello, Richard W. Pastor, W. Sean Davidson, Karin E. Bornfeldt, Laura Calabresi, Jere P. Segrest, and Jay W. Heinecke, *Circulation*, *in revision*.