Richard W Pastor

List of Publications by Year
in descending order

120 papers	20,252 citations	23567 58 h-index	18647 119 g-index
121 all docs	121 docs citations	121 times ranked	17239 citing authors

#	Article	IF	Citations
1	Constant pressure molecular dynamics simulation: The Langevin piston method. Journal of Chemical Physics, 1995, 103, 4613-4621.	3.0	3,818
2	Update of the CHARMM All-Atom Additive Force Field for Lipids: Validation on Six Lipid Types. Journal of Physical Chemistry B, 2010, 114, 7830-7843.	2.6	3,676
3	Langevin dynamics of peptides: The frictional dependence of isomerization rates ofN-acetylalanyl-N?-methylamide. Biopolymers, 1992, 32, 523-535.	2.4	922
4	An analysis of the accuracy of Langevin and molecular dynamics algorithms. Molecular Physics, 1988, 65, 1409-1419.	1.7	865
5	CHARMM Additive All-Atom Force Field for Glycosidic Linkages between Hexopyranoses. Journal of Chemical Theory and Computation, 2009, 5, 2353-2370.	5.3	578
6	Additive empirical force field for hexopyranose monosaccharides. Journal of Computational Chemistry, 2008, 29, 2543-2564.	3.3	483
7	Molecular Dynamics Studies of Polyethylene Oxide and Polyethylene Glycol: Hydrodynamic Radius and Shape Anisotropy. Biophysical Journal, 2008, 95, 1590-1599.	0.5	415
8	Effect of Electrostatic Force Truncation on Interfacial and Transport Properties of Water. The Journal of Physical Chemistry, 1996, 100, 17011-17020.	2.9	369
9	Computer simulation of liquid/liquid interfaces. I. Theory and application to octane/water. Journal of Chemical Physics, 1995, 103, 10252-10266.	3.0	341
10	A Coarse-Grained Model for Polyethylene Oxide and Polyethylene Glycol: Conformation and Hydrodynamics. Journal of Physical Chemistry B, 2009, 113, 13186-13194.	2.6	338
11	Importance of the CMAP Correction to the CHARMM22 Protein Force Field: Dynamics of Hen Lysozyme. Biophysical Journal, 2006, 90, L36-L38.	0.5	321
12	An ab Initio Study on the Torsional Surface of Alkanes and Its Effect on Molecular Simulations of Alkanes and a DPPC Bilayer. Journal of Physical Chemistry B, 2005, 109, 5300-5311.	2.6	303
13	Constant surface tension simulations of lipid bilayers: The sensitivity of surface areas and compressibilities. Journal of Chemical Physics, 1999, 111, 1281-1287.	3.0	277
14	Mechanical properties of lipid bilayers from molecular dynamics simulation. Chemistry and Physics of Lipids, 2015, 192, 60-74.	3.2	250
15	Additive and Classical Drude Polarizable Force Fields for Linear and Cyclic Ethers. Journal of Chemical Theory and Computation, 2007, 3, 1120-1133.	5.3	233
16	Simulation-Based Methods for Interpreting X-Ray Data from Lipid Bilayers. Biophysical Journal, 2006, 90, 2796-2807.	0.5	219
17	The Molecular Structure of the Liquid-Ordered Phase of Lipid Bilayers. Journal of the American Chemical Society, 2014, 136, 725-732.	13.7	217
18	Molecular Dynamics Simulations of Membrane Permeability. Chemical Reviews, 2019, 119, 5954-5997.	47.7	214

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19	CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature. Biophysical Journal, 2014, 107, 134-145.	0.5	192
20	Computer Simulation of a DPPC Phospholipid Bilayer:Â Structural Changes as a Function of Molecular Surface Area. Langmuir, 1997, 13, 6555-6561.	3.5	189
21	Computer simulation of liquid/liquid interfaces. II. Surface tensionâ€area dependence of a bilayer and monolayer. Journal of Chemical Physics, 1995, 103, 10267-10276.	3.0	184
22	Simulations of Anionic Lipid Membranes: Development of Interaction-Specific Ion Parameters and Validation Using NMR Data. Journal of Physical Chemistry B, 2013, 117, 10183-10192.	2.6	181
23	Molecular dynamics and Monte Carlo simulations of lipid bilayers. Current Opinion in Structural Biology, 1994, 4, 486-492.	5.7	179
24	Single Molecule Diffusion of Membrane-Bound Proteins: Window into Lipid Contacts and Bilayer Dynamics. Biophysical Journal, 2010, 99, 2879-2887.	0.5	161
25	Solution structure and dynamics of linked cell attachment modules of mouse fibronectin containing the RGD and synergy regions: comparison with the human fibronectin crystal structure 1 1Edited by P. E. Wright. Journal of Molecular Biology, 1998, 277, 663-682.	4.2	146
26	Diffusion limited first contact of the ends of a polymer: Comparison of theory with simulation. Journal of Chemical Physics, 1996, 105, 3878-3882.	3.0	143
27	Molecular Dynamics Simulations of Octyl Glucoside Micelles:Â Structural Properties. Journal of Physical Chemistry B, 2000, 104, 5462-5470.	2.6	135
28	Brownian dynamics simulation of a lipid chain in a membrane bilayer. Journal of Chemical Physics, 1988, 89, 1112-1127.	3.0	129
29	Lipid Bilayers, NMR Relaxation, and Computer Simulations. Accounts of Chemical Research, 2002, 35, 438-446.	15.6	129
30	Frictional models for stochastic simulations of proteins. Biopolymers, 1988, 27, 1001-1014.	2.4	123
31	Hexagonal Substructure and Hydrogen Bonding in Liquid-Ordered Phases Containing Palmitoyl Sphingomyelin. Biophysical Journal, 2015, 109, 948-955.	0.5	121
32	Dynamical motions of lipids and a finite size effect in simulations of bilayers. Journal of Chemical Physics, 2006, 125, 144710.	3.0	117
33	Theoretically Determined Three-Dimensional Structures for Amphipathic Segments of the HIV-1 gp41 Envelope Protein. AIDS Research and Human Retroviruses, 1989, 5, 7-22.	1.1	113
34	A simulation based model of NMRT1relaxation in lipid bilayer vesicles. Journal of Chemical Physics, 1988, 89, 1128-1140.	3.0	112
35	Positional time correlation function for oneâ€dimensional systems with barrier crossing: Memory function corrections to the optimized Rouseâ€“Zimm approximation. Journal of Chemical Physics, 1993, 98, 564-573.	3.0	112
36	Coarse-Grained Model for PEGylated Lipids: Effect of PEGylation on the Size and Shape of Self-Assembled Structures. Journal of Physical Chemistry B, 2011, 115, 7830-7837.	2.6	104

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37	Mean field stochastic boundary molecular dynamics simulation of a phospholipid in a membrane. Biochemistry, 1991, 30, 2099-2113.	2.5	102
38	Parametrization of the friction constant for stochastic simulations of polymers. The Journal of Physical Chemistry, 1988, 92, 2636-2641.	2.9	101
39	Molecular dynamics simulations of gel (LÎ²I) phase lipid bilayers in constant pressure and constant surface area ensembles. Journal of Chemical Physics, 2000, 112, 4822-4832.	3.0	98
40	Pressure-Based Long-Range Correction for Lennard-Jones Interactions in Molecular Dynamics Simulations:Â Application to Alkanes and Interfaces. Journal of Physical Chemistry B, 2004, 108, 363-368.	2.6	96
41	A Molecular Dynamics Study of the Response of Lipid Bilayers and Monolayers to Trehalose. Biophysical Journal, 2005, 89, 4111-4121.	0.5	94
42	Rotation of Lipids in Membranes: Molecular Dynamics Simulation, 31P Spin-Lattice Relaxation, and Rigid-Body Dynamics. Biophysical Journal, 2008, 94, 3074-3083.	0.5	94
43	Depth of Î±-Synuclein in a Bilayer Determined by Fluorescence, Neutron Reflectometry, and Computation. Biophysical Journal, 2012, 102, 613-621.	0.5	94
44	Influence of Hydrophobic Mismatch on Structures and Dynamics of Gramicidin A and Lipid Bilayers. Biophysical Journal, 2012, 102, 1551-1560.	0.5	92
45	Determination of Biomembrane Bending Moduli in Fully Atomistic Simulations. Journal of the American Chemical Society, 2014, 136, 13582-13585.	13.7	92
46	Lipid and Peptide Diffusion in Bilayers: The Saffmanâ€“DelbrÃ¼ck Model and Periodic Boundary Conditions. Journal of Physical Chemistry B, 2017, 121, 3443-3457.	2.6	91
47	Molecular Dynamics Simulations of the Influenza Hemagglutinin Fusion Peptide in Micelles and Bilayers: Conformational Analysis of Peptide and Lipids. Journal of Molecular Biology, 2005, 354, 1129-1141.	4.2	83
48	Molecular Dynamics Simulations of Octyl Glucoside Micelles:â€‰ Dynamic Properties. Journal of Physical Chemistry B, 2001, 105, 8312-8321.	2.6	79
49	Long-Range Lennard-Jones and Electrostatic Interactions in Interfaces:Â Application of the Isotropic Periodic Sum Method. Journal of Physical Chemistry B, 2007, 111, 4393-4400.	2.6	78
50	Molecular Dynamics Studies of Ion Permeation in VDAC. Biophysical Journal, 2011, 100, 602-610.	0.5	78
51	High-Resolution Structures and Orientations of Antimicrobial Peptides Piscidin 1 and Piscidin 3 in Fluid Bilayers Reveal Tilting, Kinking, and Bilayer Immersion. Journal of the American Chemical Society, 2014, 136, 3491-3504.	13.7	78
52	Permeability of membranes in the liquid ordered and liquid disordered phases. Nature Communications, 2019, 10, 5616.	12.8	78
53	Evidence for a fence that impedes the diffusion of phosphatidylinositol 4,5-bisphosphate out of the forming phagosomes of macrophages. Molecular Biology of the Cell, 2011, 22, 3498-3507.	2.1	71
54	Strong influence of periodic boundary conditions on lateral diffusion in lipid bilayer membranes. Journal of Chemical Physics, 2015, 143, 243113.	3.0	70

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55	Bending Free Energy from Simulation: Correspondence of Planar and Inverse Hexagonal Lipid Phases. Biophysical Journal, 2013, 104, 2202-2211.	0.5	69
56	Simulations of Membranes and Other Interfacial Systems Using P21 and Pc Periodic Boundary Conditions. Biophysical Journal, 2002, 82, 2317-2325.	0.5	66
57	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. Biophysical Journal, 2009, 97, 155-163.	0.5	66
58	Theory of Polymerâ€“Nanopore Interactions Refined Using Molecular Dynamics Simulations. Journal of the American Chemical Society, 2013, 135, 7064-7072.	13.7	65
59	Molecular Modeling of Lipid Membrane Curvature Induction by a Peptide: More than Simply Shape. Biophysical Journal, 2014, 106, 1958-1969.	0.5	64
60	Structure and Elasticity of Lipid Membranes with Genistein and Daidzein Bioflavinoids Using X-ray Scattering and MD Simulations. Journal of Physical Chemistry B, 2012, 116, 3918-3927.	2.6	61
61	Structure and Function in Antimicrobial Piscidins: Histidine Position, Directionality of Membrane Insertion, and pH-Dependent Permeabilization. Journal of the American Chemical Society, 2019, 141, 9837-9853.	13.7	60
62	Brownian Dynamics Simulations of Ion Transport through the VDAC. Biophysical Journal, 2011, 100, 611-619.	0.5	56
63	Simulations of Membrane-Disrupting Peptides II: AMP Piscidin 1 Favors Surface Defects over Pores. Biophysical Journal, 2016, 111, 1258-1266.	0.5	56
64	A dual apolipoprotein C-II mimeticâ€“apolipoprotein C-III antagonist peptide lowers plasma triglycerides. Science Translational Medicine, 2020, 12, .	12.4	56
65	Chapter 1 Considerations for Lipid Force Field Development. Current Topics in Membranes, 2008, , 1-48.	0.9	54
66	Adjacent Gauche Stabilization in Linear Alkanes:Â Implications for Polymer Models and Conformational Analysis. Journal of Physical Chemistry B, 2005, 109, 15684-15686.	2.6	53
67	Collective and Noncollective Models of NMR Relaxation in Lipid Vesicles and Multilayers. Journal of Physical Chemistry B, 2008, 112, 5924-5929.	2.6	53
68	Position-Dependent Diffusion Tensors in Anisotropic Media from Simulation: Oxygen Transport in and through Membranes. Journal of Chemical Theory and Computation, 2017, 13, 2962-2976.	5.3	52
69	Distinguishing Anisotropy and Flexibility of the Pentasaccharide LNF-1 in Solution by Carbon-13 NMR Relaxation and Hydrodynamic Modeling. Journal of the American Chemical Society, 1999, 121, 11847-11854.	13.7	51
70	Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. Journal of Chemical Theory and Computation, 2018, 14, 948-958.	5.3	50
71	Synexin: Molecular Mechanism of Calcium-Dependent Membrane Fusion and Voltage-Dependent Calcium-Channel Activity.. Annals of the New York Academy of Sciences, 1991, 635, 328-351.	3.8	49
72	Comparing Simulated and Experimental Translation and Rotation Constants: Range of Validity for Viscosity Scaling. Journal of Physical Chemistry B, 2010, 114, 12501-12507.	2.6	49

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73	Comparison of Langevin and molecular dynamics simulations. Equilibrium and dynamics of ethylene glycol in water. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 1747.	1.7	48
74	Molecular Dynamics Simulations of Neat Alkanes:Â The Viscosity Dependence of Rotational Relaxation. The Journal of Physical Chemistry, 1996, 100, 2652-2660.	2.9	48
75	Ab Initio Modeling of Glycosyl Torsions and Anomeric Effects in a Model Carbohydrate: 2-Ethoxy Tetrahydropyran. Biophysical Journal, 2007, 93, 1-10.	0.5	48
76	Gramicidin A Channel Formation Induces Local Lipid Redistribution I: Experiment and Simulation. Biophysical Journal, 2017, 112, 1185-1197.	0.5	48
77	Structure and Dynamics of Helix-0 of the N-BAR Domain in Lipid Micelles and Bilayers. Biophysical Journal, 2008, 95, 4315-4323.	0.5	47
78	Comparison of the Extended Isotropic Periodic Sum and Particle Mesh Ewald Methods for Simulations of Lipid Bilayers and Monolayers. Journal of Physical Chemistry B, 2009, 113, 5855-5862.	2.6	47
79	Graphâ€"Theoretic Analysis of Monomethyl Phosphate Clustering in Ionic Solutions. Journal of Physical Chemistry B, 2018, 122, 1484-1494.	2.6	46
80	CHARMM36 Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Phosphatidylethanolamine, Phosphatidylglycerol, and Ether Lipids. Journal of Chemical Theory and Computation, 2021, 17, 1581-1595.	5.3	45
81	Simulations of Membrane-Disrupting Peptides I: Alamethicin Pore Stability and Spontaneous Insertion. Biophysical Journal, 2016, 111, 1248-1257.	0.5	44
82	Inertial effects in butane stochastic dynamics. Journal of Chemical Physics, 1989, 91, 211-218.	3.0	43
83	Web interface for brownian dynamics simulation of ion transport and its applications to betaâ€barrel pores. Journal of Computational Chemistry, 2012, 33, 331-339.	3.3	43
84	Membrane permeability of small molecules from unbiased molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 124107.	3.0	42
85	Resonance Raman studies of macrocyclic complexes. 2. Antiresonance and selective intensity enhancement in synthetic metal(II) porphyrin analogs. Journal of the American Chemical Society, 1976, 98, 8007-8014.	13.7	41
86	The Curvature Induction of Surface-Bound Antimicrobial Peptides Piscidin 1 and Piscidin 3 Varies with Lipid Chain Length. Journal of Membrane Biology, 2015, 248, 455-467.	2.1	40
87	Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. Journal of Chemical Theory and Computation, 2021, 17, 1562-1580.	5.3	39
88	Resonance Raman studies of macrocyclic complexes. 1. Structural and electronic effects in synthetic metal(II) porphyrin analogs. Journal of the American Chemical Society, 1976, 98, 7999-8006.	13.7	36
89	Tertiary structure of apolipoprotein A-I in nascent high-density lipoproteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5163-5168.	7.1	35
90	Parameterization of the CHARMM All-Atom Force Field for Ether Lipids and Model Linear Ethers. Journal of Physical Chemistry B, 2018, 122, 6744-6754.	2.6	28

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91	Structural properties of apolipoprotein A-I mimetic peptides that promote ABCA1-dependent cholesterol efflux. Scientific Reports, 2018, 8, 2956.	3.3	27
92	Surface Shear Viscosity and Interleaflet Friction from Nonequilibrium Simulations of Lipid Bilayers. Journal of Chemical Theory and Computation, 2019, 15, 6471-6481.	5.3	27
93	Conformational sampling of hydrocarbon and lipid chains in an orienting potential. Journal of Computational Chemistry, 1994, 15, 208-226.	3.3	25
94	Discriminating the Helical Forms of Peptides by NMR and Molecular Dynamics Simulation. Journal of the American Chemical Society, 2004, 126, 10478-10484.	13.7	25
95	Membrane Permeability: Characteristic Times and Lengths for Oxygen and a Simulation-Based Test of the Inhomogeneous Solubility-Diffusion Model. Journal of Chemical Theory and Computation, 2018, 14, 3811-3824.	5.3	25
96	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. Journal of Chemical Theory and Computation, 2019, 15, 3854-3867.	5.3	25
97	Molecular dynamics simulations of lipid nanodiscs. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 2094-2107.	2.6	24
98	Molecular Structure of Sphingomyelin in Fluid Phase Bilayers Determined by the Joint Analysis of Small-Angle Neutron and X-ray Scattering Data. Journal of Physical Chemistry B, 2020, 124, 5186-5200.	2.6	24
99	Molecular dynamics simulations of water wires in a lipid bilayer and water/octane model systems. Journal of Chemical Physics, 2002, 116, 2663-2664.	3.0	22
100	Gramicidin A Channel Formation Induces LocalÂLipid Redistribution II: A 3D Continuum Elastic Model. Biophysical Journal, 2017, 112, 1198-1213.	0.5	22
101	Revisiting Volumes of Lipid Components in Bilayers. Journal of Physical Chemistry B, 2019, 123, 2697-2709.	2.6	21
102	Assessing smectic liquid-crystal continuum models for elastic bilayer deformations. Chemistry and Physics of Lipids, 2013, 169, 19-26.	3.2	20
103	The tension of a curved surface from simulation. Journal of Chemical Physics, 2012, 137, 234101.	3.0	18
104	Characterization of Specific Ion Effects on PI(4,5)P₂ Clustering: Molecular Dynamics Simulations and Graph-Theoretic Analysis. Journal of Physical Chemistry B, 2020, 124, 1183-1196.	2.6	18
105	Anisotropic bead models for molecular hydrodynamics. Journal of Chemical Physics, 1989, 90, 5729-5734.	3.0	15
106	Langevin dynamics of a linear rotor in a Maierâ€“Saupe potential: Kramers turnover of the flipping rate. Journal of Chemical Physics, 1992, 97, 5098-5100.	3.0	15
107	A Comparision of Methods for Computing Transition Rates from Molecular Dynamics Simulation. Molecular Simulation, 1994, 13, 25-38.	2.0	15
108	Characterizing Residue-Bilayer Interactions Using Gramicidin A as a Scaffold and Tryptophan Substitutions as Probes. Journal of Chemical Theory and Computation, 2017, 13, 5054-5064.	5.3	14

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109	Developing initial conditions for simulations of asymmetric membranes: a practical recommendation. Biophysical Journal, 2021, 120, 5041-5059.	0.5	14
110	Identification of a novel lipid binding motif in apolipoprotein B by the analysis of hydrophobic cluster domains. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 135-145.	2.6	13
111	Langevin dynamics simulations of charged model phosphatidylinositol lipids in the presence of diffusion barriers: toward an atomic level understanding of corralling of PIP2 by protein fences in biological membranes. BMC Biophysics, 2014, 7, 13.	4.4	10
112	Location and Conformational Ensemble of Menaquinone and Menaquinol, and Proteinâ€“Lipid Modulations in Archaeal Membranes. Journal of Physical Chemistry B, 2021, 125, 4714-4725.	2.6	10
113	Molecular dynamics simulation of methyl group relaxation in water. Journal of Chemical Physics, 1991, 94, 4097-4098.	3.0	9
114	Mannobioseâ€Grafting Shifts PEI Charge and Biphasic Dependence on pH. Macromolecular Chemistry and Physics, 2019, 220, 1800423.	2.2	9
115	Quantitative Characterization of Proteinâ€“Lipid Interactions by Free Energy Simulation between Binary Bilayers. Journal of Chemical Theory and Computation, 2019, 15, 6491-6503.	5.3	7
116	Functional Group Distributions, Partition Coefficients, and Resistance Factors in Lipid Bilayers Using Site Identification by Ligand Competitive Saturation. Journal of Chemical Theory and Computation, 2021, 17, 3188-3202.	5.3	6
117	Design principles of PI(4,5)P₂clustering under protein-free conditions: Specific cation effects and calcium-potassium synergy. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	6
118	PLD2â€“PI(4,5)P2 interactions in fluid phase membranes: Structural modeling and molecular dynamics simulations. PLoS ONE, 2020, 15, e0236201.	2.5	5
119	Incorporation of Î±-methylated amino acids into Apolipoprotein A-I mimetic peptides improves their helicity and cholesterol efflux potential. Biochemical and Biophysical Research Communications, 2020, 526, 349-354.	2.1	5
120	Development of CHARMM Additive Potential Energy Parameters for Î±-Methyl Amino Acids. Journal of Physical Chemistry B, 2021, 125, 11687-11696.	2.6	0