Richard W Pastor

List of Publications by Citations

119 papers	16,150 citations	55 h-index	121 g-index
121 ext. papers	18,544 ext. citations	5.3 avg, IF	6.5 L-index

#	Paper	IF	Citations
119	Constant pressure molecular dynamics simulation: The Langevin piston method. *Journal of Chemical Physics*, **1995**, 103, 4613-4621	3.9	3093
118	Update of the CHARMM all-atom additive force field for lipids: validation on six lipid types. *Journal of Physical Chemistry B*, **2010**, 114, 7830-43	3.4	2654
117	An analysis of the accuracy of Langevin and molecular dynamics algorithms. *Molecular Physics*, **1988**, 65, 1409-1419	1.7	668
116	Langevin dynamics of peptides: the frictional dependence of isomerization rates of N-acetylalanyl-NSmethylamide. *Biopolymers*, **1992**, 32, 523-35	2.2	663
115	CHARMM Additive All-Atom Force Field for Glycosidic Linkages between Hexopyranoses. *Journal of Chemical Theory and Computation*, **2009**, 5, 2353-2370	6.4	473
114	Additive empirical force field for hexopyranose monosaccharides. *Journal of Computational Chemistry*, **2008**, 29, 2543-64	3.5	421
113	Effect of Electrostatic Force Truncation on Interfacial and Transport Properties of Water. *The Journal of Physical Chemistry*, **1996**, 100, 17011-17020		351
112	Molecular dynamics studies of polyethylene oxide and polyethylene glycol: hydrodynamic radius and shape anisotropy. *Biophysical Journal*, **2008**, 95, 1590-9	2.9	347
111	A coarse-grained model for polyethylene oxide and polyethylene glycol: conformation and hydrodynamics. *Journal of Physical Chemistry B*, **2009**, 113, 13186-94	3.4	298
110	Computer simulation of liquid/liquid interfaces. I. Theory and application to octane/water. *Journal of Chemical Physics*, **1995**, 103, 10252-10266	3.9	293
109	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, 5300-11	3.4	279
108	Importance of the CMAP correction to the CHARMM22 protein force field: dynamics of hen lysozyme. *Biophysical Journal*, **2006**, 90, L36-8	2.9	263
107	Constant surface tension simulations of lipid bilayers: The sensitivity of surface areas and compressibilities. *Journal of Chemical Physics*, **1999**, 111, 1281-1287	3.9	256
106	Additive and Classical Drude Polarizable Force Fields for Linear and Cyclic Ethers. *Journal of Chemical Theory and Computation*, **2007**, 3, 1120-33	6.4	210
105	Simulation-based methods for interpreting x-ray data from lipid bilayers. *Biophysical Journal*, **2006**, 90, 2796-807	2.9	188
104	Computer Simulation of a DPPC Phospholipid Bilayer:Structural Changes as a Function of Molecular Surface Area. *Langmuir*, **1997**, 13, 6555-6561	4	179
103	Computer simulation of liquid/liquid interfaces. II. Surface tension-area dependence of a bilayer and monolayer. *Journal of Chemical Physics*, **1995**, 103, 10267-10276	3.9	174

102	The molecular structure of the liquid-ordered phase of lipid bilayers. *Journal of the American Chemical Society*, **2014**, 136, 725-32	16.4	164
101	Mechanical properties of lipid bilayers from molecular dynamics simulation. *Chemistry and Physics of Lipids*, **2015**, 192, 60-74	3.7	162
100	Molecular dynamics and Monte Carlo simulations of lipid bilayers. *Current Opinion in Structural Biology*, **1994**, 4, 486-492	8.1	161
99	CHARMM all-atom additive force field for sphingomyelin: elucidation of hydrogen bonding and of positive curvature. *Biophysical Journal*, **2014**, 107, 134-45	2.9	138
98	Diffusion limited first contact of the ends of a polymer: Comparison of theory with simulation. *Journal of Chemical Physics*, **1996**, 105, 3878-3882	3.9	136
97	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. *Journal of Molecular Biology*, **1998**, 277, 663-82	6.5	135
96	Single molecule diffusion of membrane-bound proteins: window into lipid contacts and bilayer dynamics. *Biophysical Journal*, **2010**, 99, 2879-87	2.9	131
95	Simulations of anionic lipid membranes: development of interaction-specific ion parameters and validation using NMR data. *Journal of Physical Chemistry B*, **2013**, 117, 10183-92	3.4	130
94	Molecular Dynamics Simulations of Octyl Glucoside Micelles: Structural Properties. *Journal of Physical Chemistry B*, **2000**, 104, 5462-5470	3.4	125
93	Frictional models for stochastic simulations of proteins. *Biopolymers*, **1988**, 27, 1001-14	2.2	119
92	Molecular Dynamics Simulations of Membrane Permeability. *Chemical Reviews*, **2019**, 119, 5954-5997	68.1	117
91	Lipid bilayers, NMR relaxation, and computer simulations. *Accounts of Chemical Research*, **2002**, 35, 438-46	24.3	117
90	Dynamical motions of lipids and a finite size effect in simulations of bilayers. *Journal of Chemical Physics*, **2006**, 125, 144710	3.9	106
89	Brownian dynamics simulation of a lipid chain in a membrane bilayer. *Journal of Chemical Physics*, **1988**, 89, 1112-1127	3.9	106
88	Positional time correlation function for one-dimensional systems with barrier crossing: Memory function corrections to the optimized Rouse–Zimm approximation. *Journal of Chemical Physics*, **1993**, 98, 564-573	3.9	102
87	A simulation based model of NMR T1 relaxation in lipid bilayer vesicles. *Journal of Chemical Physics*, **1988**, 89, 1128-1140	3.9	102
86	Molecular dynamics simulations of gel (L$_{\beta'}$) phase lipid bilayers in constant pressure and constant surface area ensembles. *Journal of Chemical Physics*, **2000**, 112, 4822-4832	3.9	95
85	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, 7830-7	3.4	93

84	Parametrization of the friction constant for stochastic simulations of polymers. *The Journal of Physical Chemistry*, **1988**, 92, 2636-2641		93
83	A molecular dynamics study of the response of lipid bilayers and monolayers to trehalose. *Biophysical Journal*, **2005**, 89, 4111-21	2.9	92
82	Mean field stochastic boundary molecular dynamics simulation of a phospholipid in a membrane. *Biochemistry*, **1991**, 30, 2099-113	3.2	92
81	Pressure-Based Long-Range Correction for Lennard-Jones Interactions in Molecular Dynamics Simulations: Application to Alkanes and Interfaces. *Journal of Physical Chemistry B*, **2004**, 108, 363-368	3.4	90
80	Hexagonal Substructure and Hydrogen Bonding in Liquid-Ordered Phases Containing Palmitoyl Sphingomyelin. *Biophysical Journal*, **2015**, 109, 948-55	2.9	89
79	Theoretically determined three-dimensional structures for amphipathic segments of the HIV-1 gp41 envelope protein. *AIDS Research and Human Retroviruses*, **1989**, 5, 7-22	1.6	89
78	Rotation of lipids in membranes: molecular dynamics simulation, 31P spin-lattice relaxation, and rigid-body dynamics. *Biophysical Journal*, **2008**, 94, 3074-83	2.9	81
77	Depth of □synuclein in a bilayer determined by fluorescence, neutron reflectometry, and computation. *Biophysical Journal*, **2012**, 102, 613-21	2.9	78
76	Influence of hydrophobic mismatch on structures and dynamics of gramicidin a and lipid bilayers. *Biophysical Journal*, **2012**, 102, 1551-60	2.9	78
75	Molecular Dynamics Simulations of Octyl Glucoside Micelles: Dynamic Properties. *Journal of Physical Chemistry B*, **2001**, 105, 8312-8321	3.4	73
74	Long-range Lennard-Jones and electrostatic interactions in interfaces: application of the isotropic periodic sum method. *Journal of Physical Chemistry B*, **2007**, 111, 4393-400	3.4	71
73	Lipid and Peptide Diffusion in Bilayers: The Saffman-Delbr□k Model and Periodic Boundary Conditions. *Journal of Physical Chemistry B*, **2017**, 121, 3443-3457	3.4	69
72	Molecular dynamics studies of ion permeation in VDAC. *Biophysical Journal*, **2011**, 100, 602-610	2.9	68
71	Determination of biomembrane bending moduli in fully atomistic simulations. *Journal of the American Chemical Society*, **2014**, 136, 13582-5	16.4	67
70	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, 1129-41	6.5	67
69	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, 3498-507	3.5	63
68	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, 3491-504	16.4	61
67	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, 155-63	2.9	58

66	Strong influence of periodic boundary conditions on lateral diffusion in lipid bilayer membranes. *Journal of Chemical Physics*, **2015**, 143, 243113	3.9	55
65	Bending free energy from simulation: correspondence of planar and inverse hexagonal lipid phases. *Biophysical Journal*, **2013**, 104, 2202-11	2.9	55
64	Theory of polymer-nanopore interactions refined using molecular dynamics simulations. *Journal of the American Chemical Society*, **2013**, 135, 7064-72	16.4	53
63	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, 3918-27	3.4	51
62	Chapter 1 Considerations for Lipid Force Field Development. *Current Topics in Membranes*, **2008**, 1-48	2.2	51
61	Simulations of membranes and other interfacial systems using P2(1) and Pc periodic boundary conditions. *Biophysical Journal*, **2002**, 82, 2317-25	2.9	51
60	Adjacent gauche stabilization in linear alkanes: implications for polymer models and conformational analysis. *Journal of Physical Chemistry B*, **2005**, 109, 15684-6	3.4	50
59	Brownian dynamics simulations of ion transport through the VDAC. *Biophysical Journal*, **2011**, 100, 611-619	2.9	49
58	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	16.4	49
57	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		48
56	Synexin: molecular mechanism of calcium-dependent membrane fusion and voltage-dependent calcium-channel activity. Evidence in support of the "hydrophobic bridge hypothesis" for exocytotic membrane fusion. *Annals of the New York Academy of Sciences*, **1991**, 635, 328-51	6.5	48
55	Molecular Dynamics Simulations of Neat Alkanes: The Viscosity Dependence of Rotational Relaxation. *The Journal of Physical Chemistry*, **1996**, 100, 2652-2660		47
54	Ab initio modeling of glycosyl torsions and anomeric effects in a model carbohydrate: 2-ethoxy tetrahydropyran. *Biophysical Journal*, **2007**, 93, 1-10	2.9	45
53	Collective and noncollective models of NMR relaxation in lipid vesicles and multilayers. *Journal of Physical Chemistry B*, **2008**, 112, 5924-9	3.4	44
52	Comparing simulated and experimental translation and rotation constants: range of validity for viscosity scaling. *Journal of Physical Chemistry B*, **2010**, 114, 12501-7	3.4	43
51	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, 5855-62	3.4	43
50	Simulations of Membrane-Disrupting Peptides II: AMP Piscidin 1 Favors Surface Defects over Pores. *Biophysical Journal*, **2016**, 111, 1258-1266	2.9	43
49	Structure and dynamics of helix-0 of the N-BAR domain in lipid micelles and bilayers. *Biophysical Journal*, **2008**, 95, 4315-23	2.9	40

48	Molecular modeling of lipid membrane curvature induction by a peptide: more than simply shape. *Biophysical Journal*, **2014**, 106, 1958-69	2.9	39
47	Web interface for Brownian dynamics simulation of ion transport and its applications to beta-barrel pores. *Journal of Computational Chemistry*, **2012**, 33, 331-9	3.5	38
46	Inertial effects in butane stochastic dynamics. *Journal of Chemical Physics*, **1989**, 91, 211-218	3.9	38
45	Permeability of membranes in the liquid ordered and liquid disordered phases. *Nature Communications*, **2019**, 10, 5616	17.4	37
44	Resonance raman studies of macrocyclic complexes. 2. Antiresonance and selective intensity enhancement in synthetic metal(II) porphyrin analogues. *Journal of the American Chemical Society*, **1976**, 98, 8007-14	16.4	36
43	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	16.4	35
42	Simulations of Membrane-Disrupting Peptides I: Alamethicin Pore Stability and Spontaneous Insertion. *Biophysical Journal*, **2016**, 111, 1248-1257	2.9	34
41	Gramicidin A Channel Formation Induces Local Lipid Redistribution I: Experiment and Simulation. *Biophysical Journal*, **2017**, 112, 1185-1197	2.9	31
40	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	6.4	31
39	Graph-Theoretic Analysis of Monomethyl Phosphate Clustering in Ionic Solutions. *Journal of Physical Chemistry B*, **2018**, 122, 1484-1494	3.4	31
38	Resonance raman studies of macrocyclic complexes. 1. Structural and electronic effects in synthetic metal(II) porphyrin analogues. *Journal of the American Chemical Society*, **1976**, 98, 7999-8006	16.4	31
37	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	6.4	30
36	The Curvature Induction of Surface-Bound Antimicrobial Peptides Piscidin 1 and Piscidin 3 Varies with Lipid Chain Length. *Journal of Membrane Biology*, **2015**, 248, 455-67	2.3	27
35	A dual apolipoprotein C-II mimetic-apolipoprotein C-III antagonist peptide lowers plasma triglycerides. *Science Translational Medicine*, **2020**, 12,	17.5	26
34	Discriminating the helical forms of peptides by NMR and molecular dynamics simulation. *Journal of the American Chemical Society*, **2004**, 126, 10478-84	16.4	24
33	Conformational sampling of hydrocarbon and lipid chains in an orienting potential. *Journal of Computational Chemistry*, **1994**, 15, 208-226	3.5	24
32	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	11.5	22
31	Structural properties of apolipoprotein A-I mimetic peptides that promote ABCA1-dependent cholesterol efflux. *Scientific Reports*, **2018**, 8, 2956	4.9	21

30	Molecular dynamics simulations of water wires in a lipid bilayer and water/octane model systems. *Journal of Chemical Physics*, **2002**, 116, 2663-2664	3.9	20
29	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. *Journal of Chemical Theory and Computation*, **2019**, 15, 3854-3867	6.4	19
28	Parameterization of the CHARMM All-Atom Force Field for Ether Lipids and Model Linear Ethers. *Journal of Physical Chemistry B*, **2018**, 122, 6744-6754	3.4	18
27	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	6.4	16
26	Assessing smectic liquid-crystal continuum models for elastic bilayer deformations. *Chemistry and Physics of Lipids*, **2013**, 169, 19-26	3.7	16
25	The tension of a curved surface from simulation. *Journal of Chemical Physics*, **2012**, 137, 234101	3.9	16
24	Gramicidin A Channel Formation Induces Local Lipid Redistribution II: A 3D Continuum Elastic Model. *Biophysical Journal*, **2017**, 112, 1198-1213	2.9	15
23	Membrane permeability of small molecules from unbiased molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 153, 124107	3.9	15
22	Molecular dynamics simulations of lipid nanodiscs. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 2094-2107	3.8	14
21	A Comparision of Methods for Computing Transition Rates from Molecular Dynamics Simulation. *Molecular Simulation*, **1994**, 13, 25-38	2	14
20	Langevin dynamics of a linear rotor in a Maier Saupe potential: Kramers turnover of the flipping rate. *Journal of Chemical Physics*, **1992**, 97, 5098-5100	3.9	14
19	Anisotropic bead models for molecular hydrodynamics. *Journal of Chemical Physics*, **1989**, 90, 5729-5734	3.9	13
18	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	3.4	12
17	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	6.4	11
16	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	3.8	11
15	Surface Shear Viscosity and Interleaflet Friction from Nonequilibrium Simulations of Lipid Bilayers. *Journal of Chemical Theory and Computation*, **2019**, 15, 6471-6481	6.4	9
14	Revisiting Volumes of Lipid Components in Bilayers. *Journal of Physical Chemistry B*, **2019**, 123, 2697-2709	3.4	9
13	Molecular dynamics simulation of methyl group relaxation in water. *Journal of Chemical Physics*, **1991**, 94, 4097-4098	3.9	9

12	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	6.4	8
11	Characterization of Specific Ion Effects on PI(4,5)P Clustering: Molecular Dynamics Simulations and Graph-Theoretic Analysis. *Journal of Physical Chemistry B*, **2020**, 124, 1183-1196	3.4	7
10	Mannobiose-Grafting Shifts PEI Charge and Biphasic Dependence on pH. *Macromolecular Chemistry and Physics*, **2019**, 220, 1800423	2.6	6
9	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	0	6
8	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	6.4	6
7	Incorporation of □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	3.4	4
6	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	6.4	4
5	Location and Conformational Ensemble of Menaquinone and Menaquinol, and Protein-Lipid Modulations in Archaeal Membranes. *Journal of Physical Chemistry B*, **2021**, 125, 4714-4725	3.4	3
4	Quantitative Characterization of Protein-Lipid Interactions by Free Energy Simulation between Binary Bilayers. *Journal of Chemical Theory and Computation*, **2019**, 15, 6491-6503	6.4	2
3	Developing initial conditions for simulations of asymmetric membranes: a practical recommendation. *Biophysical Journal*, **2021**, 120, 5041-5059	2.9	2
2	PLD2-PI(4,5)P2 interactions in fluid phase membranes: Structural modeling and molecular dynamics simulations. *PLoS ONE*, **2020**, 15, e0236201	3.7	2
1	Development of CHARMM Additive Potential Energy Parameters for □Methyl Amino Acids. *Journal of Physical Chemistry B*, **2021**, 125, 11687-11696	3.4	