

# Jeffery B Klauda

## List of Publications by Year in descending order

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148  
papers

16,033  
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50276  
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19190  
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155  
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times ranked

13699  
citing authors

#	ARTICLE	IF	CITATIONS
1	Update of the CHARMM All-Atom Additive Force Field for Lipids: Validation on Six Lipid Types. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7830-7843.	2.6	3,676
2	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 405-413.	5.3	2,567
3	CHARMM-GUI Membrane Builder toward realistic biological membrane simulations. <i>Journal of Computational Chemistry</i> , 2014, 35, 1997-2004.	3.3	1,802
4	CHARMM-GUI Membrane Builder for Mixed Bilayers and Its Application to Yeast Membranes. <i>Biophysical Journal</i> , 2009, 97, 50-58.	0.5	1,346
5	Global Distribution of Methane Hydrate in Ocean Sediment. <i>Energy &amp; Fuels</i> , 2005, 19, 459-470.	5.1	459
6	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 775-786.	5.3	388
7	An ab Initio Study on the Torsional Surface of Alkanes and Its Effect on Molecular Simulations of Alkanes and a DPPC Bilayer. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5300-5311.	2.6	303
8	A Fugacity Model for Gas Hydrate Phase Equilibria. <i>Industrial &amp; Engineering Chemistry Research</i> , 2000, 39, 3377-3386.	3.7	246
9	Simulation-Based Methods for Interpreting X-Ray Data from Lipid Bilayers. <i>Biophysical Journal</i> , 2006, 90, 2796-2807.	0.5	219
10	CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature. <i>Biophysical Journal</i> , 2014, 107, 134-145.	0.5	192
11	Update of the Cholesterol Force Field Parameters in CHARMM. <i>Journal of Physical Chemistry B</i> , 2012, 116, 203-210.	2.6	185
12	Phase behavior of clathrate hydrates: a model for single and multiple gas component hydrates. <i>Chemical Engineering Science</i> , 2003, 58, 27-41.	3.8	168
13	Molecular Dynamics and NMR Spectroscopy Studies of E. coli Lipopolysaccharide Structure and Dynamics. <i>Biophysical Journal</i> , 2013, 105, 1444-1455.	0.5	153
14	CHARMM36 United Atom Chain Model for Lipids and Surfactants. <i>Journal of Physical Chemistry B</i> , 2014, 118, 547-556.	2.6	143
15	Improving the CHARMM Force Field for Polyunsaturated Fatty Acid Chains. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9424-9431.	2.6	140
16	E. coli Outer Membrane and Interactions with OmpLA. <i>Biophysical Journal</i> , 2014, 106, 2493-2502.	0.5	128
17	CHARMMing: A New, Flexible Web Portal for CHARMM. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1920-1929.	5.4	118
18	Dynamical motions of lipids and a finite size effect in simulations of bilayers. <i>Journal of Chemical Physics</i> , 2006, 125, 144710.	3.0	117

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19	Cholesterol Flip-Flop: Insights from Free Energy Simulation Studies. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13342-13348.	2.6	109
20	CHARMM-GUI Micelle Builder for Pure/Mixed Micelle and Protein/Micelle Complex Systems. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2171-2180.	5.4	99
21	Rotation of Lipids in Membranes: Molecular Dynamics Simulation, 31P Spin-Lattice Relaxation, and Rigid-Body Dynamics. <i>Biophysical Journal</i> , 2008, 94, 3074-3083.	0.5	94
22	Modeling Gas Hydrate Phase Equilibria in Laboratory and Natural Porous Media. <i>Industrial &amp; Engineering Chemistry Research</i> , 2001, 40, 4197-4208.	3.7	91
23	Membrane models of <i>E. coli</i> containing cyclic moieties in the aliphatic lipid chain. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012, 1818, 1205-1210.	2.6	89
24	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. <i>Biophysical Journal</i> , 2015, 109, 2012-2022.	0.5	89
25	Bilayer Properties of Lipid A from Various Gram-Negative Bacteria. <i>Biophysical Journal</i> , 2016, 111, 1750-1760.	0.5	88
26	Mesoscale inhomogeneities in aqueous solutions of small amphiphilic molecules. <i>Faraday Discussions</i> , 2013, 167, 217.	3.2	86
27	Engineering <i>Escherichia coli</i> membrane phospholipid head distribution improves tolerance and production of biorenewables. <i>Metabolic Engineering</i> , 2017, 44, 1-12.	7.0	83
28	A systematic molecular dynamics simulation study of temperature dependent bilayer structural properties. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2014, 1838, 2520-2529.	2.6	82
29	Ab Initio Intermolecular Potentials for Gas Hydrates and Their Predictions. <i>Journal of Physical Chemistry B</i> , 2002, 106, 5722-5732.	2.6	80
30	Long-Range Lennard-Jones and Electrostatic Interactions in Interfaces: Application of the Isotropic Periodic Sum Method. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4393-4400.	2.6	78
31	Developing and Testing of Lipid Force Fields with Applications to Modeling Cellular Membranes. <i>Chemical Reviews</i> , 2019, 119, 6227-6269.	47.7	72
32	Predictions of gas hydrate phase equilibria and amounts in natural sediment porous media. <i>Marine and Petroleum Geology</i> , 2003, 20, 459-470.	3.3	67
33	How Tolerant are Membrane Simulations with Mismatch in Area per Lipid between Leaflets?. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3466-3477.	5.3	64
34	CHARMM-GUI Input Generator for NAMD, Gromacs, Amber, Openmm, and CHARMM/OpenMM Simulations using the CHARMM36 Additive Force Field. <i>Biophysical Journal</i> , 2016, 110, 641a.	0.5	63
35	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 831-839.	5.4	59
36	Modeling Yeast Organelle Membranes and How Lipid Diversity Influences Bilayer Properties. <i>Biochemistry</i> , 2015, 54, 6852-6861.	2.5	58

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37	Investigation of phase transitions of saturated phosphocholine lipid bilayers via molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 1489-1501.	2.6	57
38	Probing the importance of lipid diversity in cell membranes via molecular simulation. <i>Chemistry and Physics of Lipids</i> , 2015, 192, 12-22.	3.2	56
39	Molecular dynamics simulations of cholesterol-rich membranes using a coarse-grained force field for cyclic alkanes. <i>Journal of Chemical Physics</i> , 2015, 143, 243144.	3.0	55
40	Chapter 1 Considerations for Lipid Force Field Development. <i>Current Topics in Membranes</i> , 2008, , 1-48.	0.9	54
41	Molecular Simulations of Mixed Lipid Bilayers with Sphingomyelin, Glycerophospholipids, and Cholesterol. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5197-5208.	2.6	54
42	Critical Sequence Hotspots for Binding of Novel Coronavirus to Angiotensin Converter Enzyme as Evaluated by Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10034-10047.	2.6	54
43	Adjacent Gauche Stabilization in Linear Alkanes: Implications for Polymer Models and Conformational Analysis. <i>Journal of Physical Chemistry B</i> , 2005, 109, 15684-15686.	2.6	53
44	Collective and Noncollective Models of NMR Relaxation in Lipid Vesicles and Multilayers. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5924-5929.	2.6	53
45	An extensive simulation study of lipid bilayer properties with different head groups, acyl chain lengths, and chain saturations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 3093-3104.	2.6	51
46	Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 948-958.	5.3	50
47	Lipid chain branching at the iso- and anteiso-positions in complex chlamydia membranes: A molecular dynamics study. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2011, 1808, 323-331.	2.6	49
48	Peripheral membrane proteins: Tying the knot between experiment and computation. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 1584-1593.	2.6	48
49	Influence of Cholesterol on Phospholipid Bilayer Structure and Dynamics. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11761-11772.	2.6	47
50	CHARMM36 Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Phosphatidylethanolamine, Phosphatidylglycerol, and Ether Lipids. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1581-1595.	5.3	45
51	HM-IE: Quantum Chemical Hybrid Methods for Calculating Interaction Energies. <i>Journal of Physical Chemistry A</i> , 2004, 108, 107-112.	2.5	44
52	Lipid Membranes with a Majority of Cholesterol: Applications to the Ocular Lens and Aquaporin O. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6455-6464.	2.6	44
53	CHARMMâ€œGUI <i>Nanodisc Builder</i> for modeling and simulation of various nanodisc systems. <i>Journal of Computational Chemistry</i> , 2019, 40, 893-899.	3.3	42
54	Membrane permeability of small molecules from unbiased molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2020, 153, 124107.	3.0	42

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55	Membrane-Binding Mechanism of a Peripheral Membrane Protein through Microsecond Molecular Dynamics Simulations. <i>Journal of Molecular Biology</i> , 2012, 423, 847-861.	4.2	41
56	Influence of Ganglioside GM1 Concentration on Lipid Clustering and Membrane Properties and Curvature. <i>Biophysical Journal</i> , 2016, 111, 1987-1999.	0.5	41
57	Lipopolysaccharide Membrane Building and Simulation. <i>Methods in Molecular Biology</i> , 2015, 1273, 391-406.	0.9	41
58	Examination of Mixtures Containing Sphingomyelin and Cholesterol by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4833-4844.	2.6	40
59	Mesoscale Phenomena in Ternary Solutions of Tertiary Butyl Alcohol, Water, and Propylene Oxide. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5994-6006.	2.6	39
60	Semi-automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1562-1580.	5.3	39
61	Preferred Orientations of Phosphoinositides in Bilayers and Their Implications in Protein Recognition Mechanisms. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4315-4325.	2.6	38
62	Gas Hydrate Structure and Pressure Predictions Based on an Updated Fugacity-Based Model with the PSRK Equation of State. <i>Industrial &amp; Engineering Chemistry Research</i> , 2011, 50, 148-157.	3.7	36
63	Molecular Dynamics Simulations of the Cx26 Hemichannel: Insights into Voltage-Dependent Loop-Gating. <i>Biophysical Journal</i> , 2012, 102, 1341-1351.	0.5	35
64	Binding and release of cholesterol in the Osh4 protein of yeast. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 468-477.	2.6	33
65	Simulations of Pure Ceramide and Ternary Lipid Mixtures as Simple Interior Stratum Corneum Models. <i>Journal of Physical Chemistry B</i> , 2018, 122, 2757-2768.	2.6	33
66	Molecular Structure of the Long Periodicity Phase in the Stratum Corneum. <i>Journal of the American Chemical Society</i> , 2019, 141, 16930-16943.	13.7	33
67	Effect of Membrane Lipid Packing on Stable Binding of the ALPS Peptide. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1418-1429.	5.3	33
68	Monte Carlo Simulation of O <sub>2</sub> and N <sub>2</sub> Adsorption in Nanoporous Carbon (C168Schwarzite). <i>Langmuir</i> , 2003, 19, 3512-3518.	3.5	32
69	An ab Initio Study on the Effect of Carbon Surface Curvature and Ring Structure on N <sub>2</sub> (O <sub>2</sub> )@Carbon Intermolecular Potentials. <i>Journal of Physical Chemistry B</i> , 2004, 108, 9842-9851.	2.6	30
70	Sugar Binding in Lactose Permease: Anomeric State of a Disaccharide Influences Binding Structure. <i>Journal of Molecular Biology</i> , 2007, 367, 1523-1534.	4.2	30
71	Probing the Periplasmic-Open State of Lactose Permease in Response to Sugar Binding and Proton Translocation. <i>Journal of Molecular Biology</i> , 2010, 404, 506-521.	4.2	30
72	Microsecond-timescale simulations suggest 5-HT <sub>2A</sub> -mediated preactivation of the 5-HT <sub>3A</sub> serotonin receptor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 405-414.	7.1	29

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73	Parameterization of the CHARMM All-Atom Force Field for Ether Lipids and Model Linear Ethers. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6744-6754.	2.6	28
74	Biophysical Changes of Lipid Membranes in the Presence of Ethanol at Varying Concentrations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 13134-13141.	2.6	27
75	Physical Properties of Bacterial Outer Membrane Models: Neutron Reflectometry & Molecular Simulation. <i>Biophysical Journal</i> , 2019, 116, 1095-1104.	0.5	27
76	Orientation of Fluorescent Lipid Analogue BODIPY-PC to Probe Lipid Membrane Properties: Insights from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6157-6165.	2.6	26
77	Molecular Dynamics Simulations of Ceramide and Ceramide-Phosphatidylcholine Bilayers. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10091-10104.	2.6	26
78	Dual Action of Hydrotropes at the Water/Oil Interface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16423-16431.	3.1	24
79	How Do Ethanolamine Plasmalogens Contribute to Order and Structure of Neurological Membranes?. <i>Journal of Physical Chemistry B</i> , 2020, 124, 828-839.	2.6	23
80	Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2. <i>Biophysical Journal</i> , 2021, 120, 2902-2913.	0.5	22
81	Lipid-Linked Oligosaccharides in Membranes Sample Conformations That Facilitate Binding to Oligosaccharyltransferase. <i>Biophysical Journal</i> , 2014, 107, 1885-1895.	0.5	21
82	Reproducible Performance Improvements to Monolayer MoS <sub>2</sub> Transistors through Exposed Material Forming Gas Annealing. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 16683-16692.	8.0	21
83	Simulations of simple linoleic acid-containing lipid membranes and models for the soybean plasma membranes. <i>Journal of Chemical Physics</i> , 2017, 146, 215103.	3.0	20
84	Structure and Permeability of Ceramide Bilayers and Multilayers. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2525-2535.	2.6	19
85	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. <i>Biophysical Journal</i> , 2015, 109, 2090-2100.	0.5	18
86	Models for the <i>Stratum Corneum</i> Lipid Matrix: Effects of Ceramide Concentration, Ceramide Hydroxylation, and Free Fatty Acid Protonation. <i>Journal of Physical Chemistry B</i> , 2018, 122, 11996-12008.	2.6	18
87	Preferred Binding Mechanism of Osh4 <sup>Δ</sup> ™s Amphipathic Lipid-Packing Sensor Motif, Insights from Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9713-9723.	2.6	18
88	Molecular dynamics simulations of ethanol permeation through single and double-lipid bilayers. <i>Journal of Chemical Physics</i> , 2020, 153, 125101.	3.0	18
89	GraphVAMPNet, using graph neural networks and variational approach to Markov processes for dynamical modeling of biomolecules. <i>Journal of Chemical Physics</i> , 2022, 156, 184103.	3.0	18
90	Perspective: Computational modeling of accurate cellular membranes with molecular resolution. <i>Journal of Chemical Physics</i> , 2018, 149, 220901.	3.0	17

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91	Hierarchical Modeling O <sub>2</sub> and N <sub>2</sub> Adsorption in C168 Schwarzite: From Quantum Mechanics to Molecular Simulation. <i>Journal of Physical Chemistry B</i> , 2004, 108, 9852-9860.	2.6	16
92	Simulations of simple Bovine and Homo sapiens outer cortex ocular lens membrane models with a majority concentration of cholesterol. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 2134-2144.	2.6	16
93	Update of the CHARMM36 United Atom Chain Model for Hydrocarbons and Phospholipids. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6797-6812.	2.6	16
94	Influence of Ester-Modified Lipids on Bilayer Structure. <i>Langmuir</i> , 2013, 29, 14196-14203.	3.5	15
95	Hierarchical Modeling N <sub>2</sub> Adsorption on the Surface of and within a C <sub>60</sub> Crystal: From Quantum Mechanics to Molecular Simulation. <i>Journal of Physical Chemistry B</i> , 2005, 109, 4731-4737.	2.6	13
96	Quantum capacitance-limited MoS <sub>2</sub> biosensors enable remote label-free enzyme measurements. <i>Nanoscale</i> , 2019, 11, 15622-15632.	5.6	13
97	STAnalyzer: A web-based user interface for simulation trajectory analysis. <i>Journal of Computational Chemistry</i> , 2014, 35, 957-963.	3.3	12
98	Water Orientation at Ceramide/Water Interfaces Studied by Heterodyne-Detected Vibrational Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23692-23697.	3.1	12
99	CHARMM Force Field Parameters for Nitroalkanes and Nitroarenes. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 107-115.	5.3	11
100	Variational embedding of protein folding simulations using Gaussian mixture variational autoencoders. <i>Journal of Chemical Physics</i> , 2021, 155, 194108.	3.0	11
101	Two sterols, two bilayers: insights on membrane structure from molecular dynamics. <i>Molecular Simulation</i> , 2017, 43, 1179-1188.	2.0	10
102	The Role of Lipid Interactions in Simulations of the $\beta$ -Hemolysin Ion-Channel-Forming Toxin. <i>Biophysical Journal</i> , 2018, 115, 1720-1730.	0.5	10
103	Location and Conformational Ensemble of Menaquinone and Menaquinol, and Protein-Lipid Modulations in Archaeal Membranes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4714-4725.	2.6	10
104	Molecular dynamics simulations of palmitoyloleoylphosphatidylglycerol bilayers. <i>Molecular Simulation</i> , 2015, 41, 948-954.	2.0	9
105	Mannobiose-Grafting Shifts PEI Charge and Biphasic Dependence on pH. <i>Macromolecular Chemistry and Physics</i> , 2019, 220, 1800423.	2.2	9
106	Setting Up All-Atom Molecular Dynamics Simulations to Study the Interactions of Peripheral Membrane Proteins with Model Lipid Bilayers. <i>Methods in Molecular Biology</i> , 2019, 1949, 325-339.	0.9	8
107	Considerations of Recent All-Atom Lipid Force Field Development. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5676-5682.	2.6	8
108	Modeling <i>Pseudomonas aeruginosa</i> inner plasma membrane in planktonic and biofilm modes. <i>Journal of Chemical Physics</i> , 2018, 149, 215102.	3.0	7



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109	Structural Events in a Bacterial Uniporter Leading to Translocation of Glucose to the Cytosol. Journal of Molecular Biology, 2018, 430, 3337-3352.	4.2	7
110	Probing the pH Effects on Sugar Binding to a Polysaccharide Lyase. Journal of Physical Chemistry B, 2019, 123, 7123-7136.	2.6	7
111	Estimating localization of various statins within a POPC bilayer. Chemistry and Physics of Lipids, 2021, 236, 105074.	3.2	7
112	All-Atom Modeling of Complex Cellular Membranes. Langmuir, 2022, 38, 3-17.	3.5	6
113	Sterol Binding and Membrane Lipid Attachment to the Osh4 Protein of Yeast. Journal of Physical Chemistry B, 2010, 114, 13562-13573.	2.6	5
114	Interplay of Specific Trans- and Juxtamembrane Interfaces in Plexin A3 Dimerization and Signal Transduction. Biochemistry, 2016, 55, 4928-4938.	2.5	5
115	Modeling structural transitions from the periplasmic-open state of lactose permease and interpretations of spin label experiments. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1541-1552.	2.6	5
116	A replica exchange umbrella sampling (REUS) approach to predict host-guest binding free energies in SAMPL8 challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 667-677.	2.9	5
117	A Comparative Study of Nitrogen Physisorption on Different C70Crystal Structures Using an Ab Initio Based Potential. Journal of Physical Chemistry B, 2005, 109, 17267-17273.	2.6	4
118	Interfacial properties of aqueous solutions of butanol isomers and cyclohexane. Fluid Phase Equilibria, 2020, 513, 112551.	2.5	4
119	Rapid, quantitative therapeutic screening for Alzheimer's enzymes enabled by optimal signal transduction with transistors. Analyst, The, 2020, 145, 2925-2936.	3.5	4
120	Simulations of Diabetic and Non-Diabetic Peripheral Nerve Myelin Lipid Bilayers. Journal of Physical Chemistry B, 2021, 125, 6201-6213.	2.6	4
121	Symmetric and Asymmetric Models for the <i>Arabidopsis thaliana</i> Plasma Membrane: A Simulation Study. Journal of Physical Chemistry B, 2021, 125, 11418-11431.	2.6	4
122	Modeling the membrane binding mechanism of a lipid transport protein Osh4 to single membranes. Biophysical Journal, 2022, 121, 1560-1575.	0.5	4
123	Leaflet Asymmetry Modeling in the Lipid Composition of <i>Escherichia coli</i> Cytoplasmic Membranes. Journal of Physical Chemistry B, 2022, 126, 184-196.	2.6	4
124	Probing the Ripple Phase of Lipid Bilayers using Molecular Simulations. Biophysical Journal, 2016, 110, 86a.	0.5	2
125	Engineering the Microbial Cell Membrane To Improve Bioproduction. ACS Symposium Series, 2018, , 25-39.	0.5	2
126	Aggregation of modified hexabenzocoronenes as models for early stage asphaltene self-assembly. Molecular Simulation, 2018, 44, 992-1003.	2.0	2



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127	A reengineered common chain cytokine augments CD8+ T cell–dependent immunotherapy. JCI Insight, 2022, 7, .	5.0	2
128	Computational Study of the Allosteric Effects of p5 on CDK5–p25 Hyperactivity as Alternative Inhibitory Mechanisms in Neurodegeneration. Journal of Physical Chemistry B, 2022, 126, 5033-5044.	2.6	2
129	Developing CHARMM-Compatible Lipid Parameters for Ceramides and United Atom Chains. Biophysical Journal, 2013, 104, 591a.	0.5	1
130	The simultaneous mass and energy evaporation (SM2E) model. Journal of Occupational and Environmental Hygiene, 2016, 13, 243-253.	1.0	1
131	Simulation of Linoleoyl-Containing Pure Lipid Bilayer and Soybean Plasma Membranes. Biophysical Journal, 2017, 112, 82a.	0.5	1
132	Isothermal Titration Calorimetry of Be <sup>2+</sup> with Phosphatidylserine Models Guides All-Atom Force-Field Development for Lipid–Ion Interactions. Journal of Physical Chemistry B, 2019, 123, 1554-1565.	2.6	1
133	Modifying the CHARMM36 Lipid Force Field for LJ-PME Simulations. Biophysical Journal, 2020, 118, 87a.	0.5	1
134	Impact of PIP2 Lipids, Force Field Parameters, and Mutational Analysis on the Binding of the Osh4 <sup>TM</sup> s Î± <sub>6</sub> –Î± <sub>7</sub> Domain. Journal of Physical Chemistry B, 2021, 125, 5296-5308.	2.6	1
135	Binding of A Natural Sterol to the Osh4 Protein of Yeast and Membrane Attachment. Biophysical Journal, 2010, 98, 241a.	0.5	0
136	A Modified Lipid Force Field for Charmm: Development and Application to Single-Celled Organism Membranes. Biophysical Journal, 2010, 98, 282a.	0.5	0
137	Molecular Dynamics Simulations on the Periplasmic-Open State Lactose Permease. Biophysical Journal, 2015, 108, 466a.	0.5	0
138	Effects of Spin-Labels on Membrane Burial Depth of MARCKS-ED Residues. Biophysical Journal, 2016, 111, 1600-1603.	0.5	0
139	Analyzing the Effects of Lipid Type on the Î±-Hemolysin Nanopore and Å5HT3 Receptor Structure and Gating using Molecular Dynamics Simulations. Biophysical Journal, 2017, 112, 275a-276a.	0.5	0
140	CHARMM-GUI Lecture Series on Molecular Modeling and Simulation. Biophysical Journal, 2018, 114, 184a.	0.5	0
141	Probing Plexin A3 Dimerization and the Importance of the Near Membrane Extracellular Residues. Biophysical Journal, 2018, 114, 423a.	0.5	0
142	Label-Free Enzyme Activity Measurements with Quantum-Limited Biosensors. Biophysical Journal, 2019, 116, 146a.	0.5	0
143	Modeling Lipid Membranes. , 2019, , 741-759.		0
144	Update of the CHARMM36 United Atom Chain Model for Lipids. Biophysical Journal, 2020, 118, 88a.	0.5	0

#	ARTICLE	IF	CITATIONS
145	Investigation of Allosteric Inhibition Mechanisms by the Peptide p5 on the Alzheimer's Disease (AD) Pathological Complex cdk5-p25 through Molecular Dynamics Simulations. Biophysical Journal, 2020, 118, 206a.	0.5	0
146	Virtual Issue on Docking. Journal of Physical Chemistry B, 2021, 125, 5455-5457.	2.6	0
147	Modeling Lipid Membranes. , 2016, , 1-19.		0
148	Experimental investigation of the mechanism of lipid-binding of the ALPS-like motif of Osh4 protein. Biophysical Journal, 2022, 121, 221a-222a.	0.5	0