Jeffery B Klauda

List of Publications by Year in Descending Order

131 papers	10,732 citations	41 h-index	103 g-index
155 ext. papers	13,758 ext. citations	3.7 avg, IF	6.43 L-index

#	Paper	IF	Citations
131	GraphVAMPNet, using graph neural networks and variational approach to Markov processes for dynamical modeling of biomolecules.. *Journal of Chemical Physics*, **2022**, 156, 184103	3.9	2
130	Symmetric and Asymmetric Models for the Plasma Membrane: A Simulation Study. *Journal of Physical Chemistry B*, **2021**, 125, 11418-11431	3.4	0
129	Variational embedding of protein folding simulations using Gaussian mixture variational autoencoders. *Journal of Chemical Physics*, **2021**, 155, 194108	3.9	3
128	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
127	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	4.2	1
126	Impact of PIP2 Lipids, Force Field Parameters, and Mutational Analysis on the Binding of the Osh4R Domain. *Journal of Physical Chemistry B*, **2021**, 125, 5296-5308	3.4	
125	Considerations of Recent All-Atom Lipid Force Field Development. *Journal of Physical Chemistry B*, **2021**, 125, 5676-5682	3.4	1
124	Estimating localization of various statins within a POPC bilayer. *Chemistry and Physics of Lipids*, **2021**, 236, 105074	3.7	3
123	Simulations of Diabetic and Non-Diabetic Peripheral Nerve Myelin Lipid Bilayers. *Journal of Physical Chemistry B*, **2021**, 125, 6201-6213	3.4	0
122	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
121	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
120	Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2. *Biophysical Journal*, **2021**, 120, 2902-2913	2.9	9
119	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. *Journal of Chemical Information and Modeling*, **2021**, 61, 831-839	6.1	10
118	Interfacial properties of aqueous solutions of butanol isomers and cyclohexane. *Fluid Phase Equilibria*, **2020**, 513, 112551	2.5	1
117	Update of the CHARMM36 United Atom Chain Model for Hydrocarbons and Phospholipids. *Journal of Physical Chemistry B*, **2020**, 124, 6797-6812	3.4	6
116	Rapid, quantitative therapeutic screening for Alzheimer's enzymes enabled by optimal signal transduction with transistors. *Analyst, The*, **2020**, 145, 2925-2936	5	2
115	Critical Sequence Hot-spots for Binding of nCOV-2019 to ACE2 as Evaluated by Molecular Simulations **2020**,		3

114	Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2 **2020**,		4
113	How Do Ethanolamine Plasmalogens Contribute to Order and Structure of Neurological Membranes?. *Journal of Physical Chemistry B*, **2020**, 124, 828-839	3.4	10
112	Microsecond-timescale simulations suggest 5-HT-mediated preactivation of the 5-HT serotonin receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 405-414	11.5	14
111	Molecular dynamics simulations of ethanol permeation through single and double-lipid bilayers. *Journal of Chemical Physics*, **2020**, 153, 125101	3.9	7
110	Critical Sequence Hotspots for Binding of Novel Coronavirus to Angiotensin Converter Enzyme as Evaluated by Molecular Simulations. *Journal of Physical Chemistry B*, **2020**, 124, 10034-10047	3.4	39
109	Membrane permeability of small molecules from unbiased molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 153, 124107	3.9	15
108	CHARMM-GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. *Journal of Computational Chemistry*, **2019**, 40, 893-899	3.5	27
107	Isothermal Titration Calorimetry of Be with Phosphatidylserine Models Guides All-Atom Force-Field Development for Lipid-Ion Interactions. *Journal of Physical Chemistry B*, **2019**, 123, 1554-1565	3.4	1
106	Reproducible Performance Improvements to Monolayer MoS Transistors through Exposed Material Forming Gas Annealing. *ACS Applied Materials & Interfaces*, **2019**, 11, 16683-16692	9.5	13
105	Physical Properties of Bacterial Outer Membrane Models: Neutron Reflectometry & Molecular Simulation. *Biophysical Journal*, **2019**, 116, 1095-1104	2.9	16
104	Mannobiose-Grafting Shifts PEI Charge and Biphasic Dependence on pH. *Macromolecular Chemistry and Physics*, **2019**, 220, 1800423	2.6	6
103	Structure and Permeability of Ceramide Bilayers and Multilayers. *Journal of Physical Chemistry B*, **2019**, 123, 2525-2535	3.4	11
102	Setting Up All-Atom Molecular Dynamics Simulations to Study the Interactions of Peripheral Membrane Proteins with Model Lipid Bilayers. *Methods in Molecular Biology*, **2019**, 1949, 325-339	1.4	4
101	Quantum capacitance-limited MoS biosensors enable remote label-free enzyme measurements. *Nanoscale*, **2019**, 11, 15622-15632	7.7	10
100	Probing the pH Effects on Sugar Binding to a Polysaccharide Lyase. *Journal of Physical Chemistry B*, **2019**, 123, 7123-7136	3.4	3
99	Molecular Structure of the Long Periodicity Phase in the Stratum Corneum. *Journal of the American Chemical Society*, **2019**, 141, 16930-16943	16.4	20
98	Developing and Testing of Lipid Force Fields with Applications to Modeling Cellular Membranes. *Chemical Reviews*, **2019**, 119, 6227-6269	68.1	48
97	Modeling Lipid Membranes **2019**, 741-759		

96	Effect of Membrane Lipid Packing on Stable Binding of the ALPS Peptide. *Journal of Chemical Theory and Computation*, **2019**, 15, 1418-1429	6.4	14
95	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. *Journal of Chemical Theory and Computation*, **2019**, 15, 775-786	6.4	152
94	Simulations of Pure Ceramide and Ternary Lipid Mixtures as Simple Interior Stratum Corneum Models. *Journal of Physical Chemistry B*, **2018**, 122, 2757-2768	3.4	21
93	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
92	Investigation of phase transitions of saturated phosphocholine lipid bilayers via molecular dynamics simulations. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 1489-1501	3.8	37
91	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
90	Aggregation of modified hexabenzocoronenes as models for early stage asphaltene self-assembly. *Molecular Simulation*, **2018**, 44, 992-1003	2	2
89	Simulations of simple Bovine and Homo sapiens outer cortex ocular lens membrane models with a majority concentration of cholesterol. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 2134-2144	3.8	13
88	Engineering the Microbial Cell Membrane To Improve Bioproduction. *ACS Symposium Series*, **2018**, 25-39	0.4	2
87	Modeling inner plasma membrane in planktonic and biofilm modes. *Journal of Chemical Physics*, **2018**, 149, 215102	3.9	4
86	Perspective: Computational modeling of accurate cellular membranes with molecular resolution. *Journal of Chemical Physics*, **2018**, 149, 220901	3.9	9
85	Models for the Stratum Corneum Lipid Matrix: Effects of Ceramide Concentration, Ceramide Hydroxylation, and Free Fatty Acid Protonation. *Journal of Physical Chemistry B*, **2018**, 122, 11996-12008	3.4	11
84	The Role of Lipid Interactions in Simulations of the Hemolysin Ion-Channel-Forming Toxin. *Biophysical Journal*, **2018**, 115, 1720-1730	2.9	7
83	Preferred Binding Mechanism of Osh4 Amphipathic Lipid-Packing Sensor Motif, Insights from Molecular Dynamics. *Journal of Physical Chemistry B*, **2018**, 122, 9713-9723	3.4	11
82	Structural Events in a Bacterial Uniporter Leading to Translocation of Glucose to the Cytosol. *Journal of Molecular Biology*, **2018**, 430, 3337-3352	6.5	7
81	Examination of Mixtures Containing Sphingomyelin and Cholesterol by Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 4833-4844	3.4	33
80	Molecular Simulations of Mixed Lipid Bilayers with Sphingomyelin, Glycerophospholipids, and Cholesterol. *Journal of Physical Chemistry B*, **2017**, 121, 5197-5208	3.4	37
79	Simulations of simple linoleic acid-containing lipid membranes and models for the soybean plasma membranes. *Journal of Chemical Physics*, **2017**, 146, 215103	3.9	13

78	Molecular Dynamics Simulations of Ceramide and Ceramide-Phosphatidylcholine Bilayers. *Journal of Physical Chemistry B*, **2017**, 121, 10091-10104	3.4	18
77	Engineering Escherichia coli membrane phospholipid head distribution improves tolerance and production of biorenewables. *Metabolic Engineering*, **2017**, 44, 1-12	9.7	61
76	Two sterols, two bilayers: insights on membrane structure from molecular dynamics. *Molecular Simulation*, **2017**, 43, 1179-1188	2	8
75	Dual Action of Hydrotropes at the Water/Oil Interface. *Journal of Physical Chemistry C*, **2017**, 121, 16423-16431	3.8	17
74	An extensive simulation study of lipid bilayer properties with different head groups, acyl chain lengths, and chain saturations. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 3093-3104	3.8	32
73	Influence of Cholesterol on Phospholipid Bilayer Structure and Dynamics. *Journal of Physical Chemistry B*, **2016**, 120, 11761-11772	3.4	36
72	Bilayer Properties of Lipid A from Various Gram-Negative Bacteria. *Biophysical Journal*, **2016**, 111, 1750-1760	2.9	60
71	Influence of Ganglioside GM1 Concentration on Lipid Clustering and Membrane Properties and Curvature. *Biophysical Journal*, **2016**, 111, 1987-1999	2.9	29
70	Modeling structural transitions from the periplasmic-open state of lactose permease and interpretations of spin label experiments. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1541-52	3.8	4
69	Probing the Ripple Phase of Lipid Bilayers using Molecular Simulations. *Biophysical Journal*, **2016**, 110, 86a	2.9	2
68	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. *Journal of Chemical Theory and Computation*, **2016**, 12, 405-13	6.4	1303
67	The simultaneous mass and energy evaporation (SM2E) model. *Journal of Occupational and Environmental Hygiene*, **2016**, 13, 243-53	2.9	1
66	Peripheral membrane proteins: Tying the knot between experiment and computation. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1584-93	3.8	32
65	Modeling Lipid Membranes **2016**, 1-19		
64	CHARMM-GUI Input Generator for NAMD, Gromacs, Amber, Openmm, and CHARMM/OpenMM Simulations using the CHARMM36 Additive Force Field. *Biophysical Journal*, **2016**, 110, 641a	2.9	21
63	Effects of Spin-Labels on Membrane Burial Depth of MARCKS-ED Residues. *Biophysical Journal*, **2016**, 111, 1600-1603	2.9	
62	Water Orientation at Ceramide/Water Interfaces Studied by Heterodyne-Detected Vibrational Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulation. *Journal of Physical Chemistry C*, **2016**, 120, 23692-23697	3.8	11
61	Interplay of Specific Trans- and Juxtamembrane Interfaces in Plexin A3 Dimerization and Signal Transduction. *Biochemistry*, **2016**, 55, 4928-38	3.2	3

60	Biophysical Changes of Lipid Membranes in the Presence of Ethanol at Varying Concentrations. *Journal of Physical Chemistry B*, **2015**, 119, 13134-41	3.4	21
59	Modeling Yeast Organelle Membranes and How Lipid Diversity Influences Bilayer Properties. *Biochemistry*, **2015**, 54, 6852-61	3.2	42
58	Probing the importance of lipid diversity in cell membranes via molecular simulation. *Chemistry and Physics of Lipids*, **2015**, 192, 12-22	3.7	43
57	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. *Biophysical Journal*, **2015**, 109, 2012-22	2.9	60
56	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. *Biophysical Journal*, **2015**, 109, 2090-100	2.9	14
55	Molecular dynamics simulations of palmitoyloleoylphosphatidylglycerol bilayers. *Molecular Simulation*, **2015**, 41, 948-954	2	8
54	Molecular dynamics simulations of cholesterol-rich membranes using a coarse-grained force field for cyclic alkanes. *Journal of Chemical Physics*, **2015**, 143, 243144	3.9	44
53	How Tolerant are Membrane Simulations with Mismatch in Area per Lipid between Leaflets?. *Journal of Chemical Theory and Computation*, **2015**, 11, 3466-77	6.4	44
52	Lipopolysaccharide membrane building and simulation. *Methods in Molecular Biology*, **2015**, 1273, 391-406	1.4	31
51	ST-analyzer: a web-based user interface for simulation trajectory analysis. *Journal of Computational Chemistry*, **2014**, 35, 957-63	3.5	11
50	Lipid-linked oligosaccharides in membranes sample conformations that facilitate binding to oligosaccharyltransferase. *Biophysical Journal*, **2014**, 107, 1885-1895	2.9	17
49	CHARMM-GUI Membrane Builder toward realistic biological membrane simulations. *Journal of Computational Chemistry*, **2014**, 35, 1997-2004	3.5	1004
48	Preferred orientations of phosphoinositides in bilayers and their implications in protein recognition mechanisms. *Journal of Physical Chemistry B*, **2014**, 118, 4315-25	3.4	21
47	A systematic molecular dynamics simulation study of temperature dependent bilayer structural properties. *Biochimica Et Biophysica Acta - Biomembranes*, **2014**, 1838, 2520-9	3.8	63
46	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
45	CHARMM36 united atom chain model for lipids and surfactants. *Journal of Physical Chemistry B*, **2014**, 118, 547-56	3.4	99
44	Mesoscale phenomena in ternary solutions of tertiary butyl alcohol, water, and propylene oxide. *Journal of Physical Chemistry B*, **2014**, 118, 5994-6006	3.4	32
43	E. coli outer membrane and interactions with OmpLA. *Biophysical Journal*, **2014**, 106, 2493-502	2.9	97

42	Mesoscale inhomogeneities in aqueous solutions of small amphiphilic molecules. *Faraday Discussions*, **2013**, 167, 217-38	3.6	69
41	Molecular dynamics and NMR spectroscopy studies of E. coli lipopolysaccharide structure and dynamics. *Biophysical Journal*, **2013**, 105, 1444-55	2.9	125
40	CHARMM-GUI micelle builder for pure/mixed micelle and protein/micelle complex systems. *Journal of Chemical Information and Modeling*, **2013**, 53, 2171-80	6.1	61
39	Influence of ester-modified lipids on bilayer structure. *Langmuir*, **2013**, 29, 14196-203	4	14
38	Molecular dynamics simulations of the Cx26 hemichannel: insights into voltage-dependent loop-gating. *Biophysical Journal*, **2012**, 102, 1341-51	2.9	32
37	Membrane models of E. coli containing cyclic moieties in the aliphatic lipid chain. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 1205-10	3.8	72
36	Improving the CHARMM force field for polyunsaturated fatty acid chains. *Journal of Physical Chemistry B*, **2012**, 116, 9424-31	3.4	102
35	Membrane-binding mechanism of a peripheral membrane protein through microsecond molecular dynamics simulations. *Journal of Molecular Biology*, **2012**, 423, 847-61	6.5	32
34	Update of the cholesterol force field parameters in CHARMM. *Journal of Physical Chemistry B*, **2012**, 116, 203-10	3.4	147
33	Lipid membranes with a majority of cholesterol: applications to the ocular lens and aquaporin 0. *Journal of Physical Chemistry B*, **2011**, 115, 6455-64	3.4	38
32	Orientation of fluorescent lipid analogue BODIPY-PC to probe lipid membrane properties: insights from molecular dynamics simulations. *Journal of Physical Chemistry B*, **2011**, 115, 6157-65	3.4	24
31	Gas Hydrate Structure and Pressure Predictions Based on an Updated Fugacity-Based Model with the PSRK Equation of State. *Industrial & Engineering Chemistry Research*, **2011**, 50, 148-157	3.9	32
30	Lipid chain branching at the iso- and anteiso-positions in complex Chlamydia membranes: a molecular dynamics study. *Biochimica Et Biophysica Acta - Biomembranes*, **2011**, 1808, 323-31	3.8	41
29	Cholesterol flip-flop: insights from free energy simulation studies. *Journal of Physical Chemistry B*, **2010**, 114, 13342-8	3.4	97
28	Sterol binding and membrane lipid attachment to the Osh4 protein of yeast. *Journal of Physical Chemistry B*, **2010**, 114, 13562-73	3.4	4
27	Probing the periplasmic-open state of lactose permease in response to sugar binding and proton translocation. *Journal of Molecular Biology*, **2010**, 404, 506-21	6.5	28
26	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
25	Binding and release of cholesterol in the Osh4 protein of yeast. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 468-77	4.2	29

24	CHARMM-GUI Membrane Builder for mixed bilayers and its application to yeast membranes. *Biophysical Journal*, **2009**, 97, 50-8	2.9	891
23	Chapter 1 Considerations for Lipid Force Field Development. *Current Topics in Membranes*, **2008**, 1-48	2.2	51
22	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
21	Collective and noncollective models of NMR relaxation in lipid vesicles and multilayers. *Journal of Physical Chemistry B*, **2008**, 112, 5924-9	3.4	44
20	CHARMMing: a new, flexible web portal for CHARMM. *Journal of Chemical Information and Modeling* , **2008**, 48, 1920-9	6.1	105
19	CHARMM Force Field Parameters for Nitroalkanes and Nitroarenes. *Journal of Chemical Theory and Computation*, **2008**, 4, 107-15	6.4	10
18	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
17	Sugar binding in lactose permease: anomeric state of a disaccharide influences binding structure. *Journal of Molecular Biology*, **2007**, 367, 1523-34	6.5	30
16	Dynamical motions of lipids and a finite size effect in simulations of bilayers. *Journal of Chemical Physics*, **2006**, 125, 144710	3.9	106
15	Simulation-based methods for interpreting x-ray data from lipid bilayers. *Biophysical Journal*, **2006**, 90, 2796-807	2.9	188
14	Hierarchical modeling N2 adsorption on the surface of and within a C60 crystal: from quantum mechanics to molecular simulation. *Journal of Physical Chemistry B*, **2005**, 109, 4731-7	3.4	13
13	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
12	A comparative study of nitrogen physisorption on different C70 crystal structures using an ab initio based potential. *Journal of Physical Chemistry B*, **2005**, 109, 17267-73	3.4	4
11	Global Distribution of Methane Hydrate in Ocean Sediment. *Energy & Fuels*, **2005**, 19, 459-470	4.1	374
10	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
9	HM-IE: Quantum Chemical Hybrid Methods for Calculating Interaction Energies. *Journal of Physical Chemistry A*, **2004**, 108, 107-112	2.8	43
8	Hierarchical Modeling O2 and N2 Adsorption in C168 Schwarzite: From Quantum Mechanics to Molecular Simulation. *Journal of Physical Chemistry B*, **2004**, 108, 9852-9860	3.4	14
7	An ab Initio Study on the Effect of Carbon Surface Curvature and Ring Structure on N2(O2)Carbon Intermolecular Potentials. *Journal of Physical Chemistry B*, **2004**, 108, 9842-9851	3.4	29

6	Phase behavior of clathrate hydrates: a model for single and multiple gas component hydrates. *Chemical Engineering Science*, **2003**, 58, 27-41	4.4	147
5	Monte Carlo Simulation of O2 and N2 Adsorption in Nanoporous Carbon (C168 Schwarzite). *Langmuir*, **2003**, 19, 3512-3518	4	30
4	Predictions of gas hydrate phase equilibria and amounts in natural sediment porous media. *Marine and Petroleum Geology*, **2003**, 20, 459-470	4.7	57
3	Ab Initio Intermolecular Potentials for Gas Hydrates and Their Predictions. *Journal of Physical Chemistry B*, **2002**, 106, 5722-5732	3.4	73
2	Modeling Gas Hydrate Phase Equilibria in Laboratory and Natural Porous Media. *Industrial & Engineering Chemistry Research*, **2001**, 40, 4197-4208	3.9	73
1	A Fugacity Model for Gas Hydrate Phase Equilibria. *Industrial & Engineering Chemistry Research*, **2000**, 39, 3377-3386	3.9	208