Douglas J Tobias

List of Publications by Citations

176 papers	18,590 citations	59 h-index	135 g-index
188 ext. papers	20,596 ext. citations	5.8 avg, IF	6.69 L-index

#	Paper	IF	Citations
176	Constant pressure molecular dynamics algorithms. *Journal of Chemical Physics*, **1994**, 101, 4177-4189	3.9	3338
175	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
174	Explicit reversible integrators for extended systems dynamics. *Molecular Physics*, **1996**, 87, 1117-1157	1.7	1296
173	Specific ion effects at the air/water interface. *Chemical Reviews*, **2006**, 106, 1259-81	68.1	1093
172	Ions at the Air/Water Interface. *Journal of Physical Chemistry B*, **2002**, 106, 6361-6373	3.4	663
171	Molecular Structure of Salt Solutions: A New View of the Interface with Implications for Heterogeneous Atmospheric Chemistry. *Journal of Physical Chemistry B*, **2001**, 105, 10468-10472	3.4	586
170	Unified molecular picture of the surfaces of aqueous acid, base, and salt solutions. *Journal of Physical Chemistry B*, **2005**, 109, 7617-23	3.4	374
169	The dynamics of protein hydration water: a quantitative comparison of molecular dynamics simulations and neutron-scattering experiments. *Biophysical Journal*, **2000**, 79, 3244-57	2.9	275
168	Chemistry. Getting specific about specific ion effects. *Science*, **2008**, 319, 1197-8	33.3	271
167	Interface connections of a transmembrane voltage sensor. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 15059-64	11.5	192
166	Propensity of soft ions for the air/water interface. *Current Opinion in Colloid and Interface Science*, **2004**, 9, 67-73	7.6	188
165	Constant-pressure molecular dynamics investigation of cholesterol effects in a dipalmitoylphosphatidylcholine bilayer. *Biophysical Journal*, **1998**, 75, 2147-56	2.9	178
164	Air-liquid interfaces of aqueous solutions containing ammonium and sulfate: spectroscopic and molecular dynamics studies. *Journal of Physical Chemistry B*, **2005**, 109, 8861-72	3.4	175
163	Atomic-scale molecular dynamics simulations of lipid membranes. *Current Opinion in Colloid and Interface Science*, **1997**, 2, 15-26	7.6	169
162	Translational diffusion of hydration water correlates with functional motions in folded and intrinsically disordered proteins. *Nature Communications*, **2015**, 6, 6490	17.4	166
161	Structure and hydration of membranes embedded with voltage-sensing domains. *Nature*, **2009**, 462, 473-9	50.4	166
160	Watching the low-frequency motions in aqueous salt solutions: the terahertz vibrational signatures of hydrated ions. *Journal of the American Chemical Society*, **2012**, 134, 1030-5	16.4	160

159	Coincidence of dynamical transitions in a soluble protein and its hydration water: direct measurements by neutron scattering and MD simulations. *Journal of the American Chemical Society*, **2008**, 130, 4586-7	16.4	156
158	Experimental validation of molecular dynamics simulations of lipid bilayers: a new approach. *Biophysical Journal*, **2005**, 88, 805-17	2.9	144
157	Explicit reversible integrators for extended systems dynamics		142
156	Surface solvation of halogen anions in water clusters: An ab initio molecular dynamics study of the Cl(H2O)6 complex. *Journal of Chemical Physics*, **2001**, 114, 7036-7044	3.9	136
155	Simulation and theory of ions at atmospherically relevant aqueous liquid-air interfaces. *Annual Review of Physical Chemistry*, **2013**, 64, 339-59	15.7	131
154	Chloride Anion on Aqueous Clusters, at the Air Water Interface, and in Liquid Water: Solvent Effects on Cl-Polarizability. *Journal of Physical Chemistry A*, **2002**, 106, 379-383	2.8	131
153	Polarizability of the nitrate anion and its solvation at the air/water interface. *Physical Chemistry Chemical Physics*, **2003**, 5, 3752	3.6	119
152	Interaction of Gas-Phase Ozone at 296 K with Unsaturated Self-Assembled Monolayers: A New Look at an Old System. *Journal of Physical Chemistry A*, **2004**, 108, 10473-10485	2.8	116
151	Hydroxyl radical at the air-water interface. *Journal of the American Chemical Society*, **2004**, 126, 16308-9	16.4	114
150	Molecular dynamics simulations of atmospheric oxidants at the air-water interface: solvation and accommodation of OH and O3. *Journal of Physical Chemistry B*, **2005**, 109, 15876-92	3.4	109
149	Surface Effects on Aqueous Ionic Solvation: A Molecular Dynamics Simulation Study of NaCl at the Air/Water Interface from Infinite Dilution to Saturation. *Journal of Physical Chemistry B*, **2000**, 104, 7702-7706	3.4	109
148	The Effect of an Organic Surfactant on the Liquid Vapor Interface of an Electrolyte Solution. *Journal of Physical Chemistry C*, **2007**, 111, 13497-13509	3.8	108
147	Structure and dynamics of the aqueous liquid-vapor interface: a comprehensive particle-based simulation study. *Journal of Physical Chemistry B*, **2006**, 110, 3738-46	3.4	106
146	Solvation of magnesium dication: molecular dynamics simulation and vibrational spectroscopic study of magnesium chloride in aqueous solutions. *Journal of Physical Chemistry A*, **2010**, 114, 5141-8	2.8	104
145	Hydroxide anion at the air water interface. *Chemical Physics Letters*, **2009**, 481, 2-8	2.5	103
144	Ion spatial distributions at the liquid-vapor interface of aqueous potassium fluoride solutions. *Physical Chemistry Chemical Physics*, **2008**, 10, 4778-84	3.6	98
143	Structure and vibrational spectroscopy of salt water/air interfaces: predictions from classical molecular dynamics simulations. *Journal of Physical Chemistry B*, **2005**, 109, 7934-40	3.4	96
142	Ion specificity at the peptide bond: molecular dynamics simulations of N-methylacetamide in aqueous salt solutions. *Journal of Physical Chemistry B*, **2010**, 114, 1213-20	3.4	95

141	Arginine in membranes: the connection between molecular dynamics simulations and translocon-mediated insertion experiments. *Journal of Membrane Biology*, **2011**, 239, 35-48	2.3	94
140	Spatial dependence of protein-water collective hydrogen-bond dynamics. *Physical Review Letters*, **2013**, 111, 218101	7.4	93
139	Polarizability and aqueous solvation of the sulfate dianion. *Chemical Physics Letters*, **2003**, 367, 704-710	2.5	90
138	Allosteric mechanism of water-channel gating by Ca2+-calmodulin. *Nature Structural and Molecular Biology*, **2013**, 20, 1085-92	17.6	88
137	Impact, Trapping, and Accommodation of Hydroxyl Radical and Ozone at Aqueous Salt Aerosol Surfaces. A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2003**, 107, 12690-12699	3.4	84
136	Molecular Dynamics Simulations of a Calcium Carbonate/Calcium Sulfonate Reverse Micelle *The Journal of Physical Chemistry*, **1996**, 100, 6637-6648		84
135	Molecular dynamics simulations of the solution-air interface of aqueous sodium nitrate. *Journal of Physical Chemistry A*, **2007**, 111, 3091-8	2.8	81
134	Molecular dynamics with internal coordinate constraints. *Journal of Chemical Physics*, **1988**, 89, 5115-5127	3.9	81
133	Reverse turns in blocked dipeptides are intrinsically unstable in water. *Journal of Molecular Biology*, **1990**, 216, 783-96	6.5	79
132	A voltage-sensor water pore. *Biophysical Journal*, **2006**, 91, L90-2	2.9	78
131	Toward a unified picture of the water self-ions at the air-water interface: a density functional theory perspective. *Journal of Physical Chemistry B*, **2014**, 118, 8364-72	3.4	77
130	Thermodynamics of amide hydrogen bond formation in polar and apolar solvents. *Journal of Molecular Biology*, **1989**, 209, 817-20	6.5	76
129	Re-examining the properties of the aqueous vapor-liquid interface using dispersion corrected density functional theory. *Journal of Chemical Physics*, **2011**, 135, 124712	3.9	74
128	Insertion of short transmembrane helices by the Sec61 translocon. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 11588-93	11.5	72
127	Calculation of free energy surfaces using the methods of thermodynamic perturbation theory. *Chemical Physics Letters*, **1987**, 142, 472-476	2.5	69
126	Hydration water mobility is enhanced around tau amyloid fibers. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 6365-70	11.5	68
125	Does Nitric Acid Dissociate at the Aqueous Solution Surface?. *Journal of Physical Chemistry C*, **2011**, 115, 21183-21190	3.8	64
124	Uptake and Collision Dynamics of Gas Phase Ozone at Unsaturated Organic Interfaces. *Journal of Physical Chemistry A*, **2004**, 108, 5806-5814	2.8	63

123	Environmental Dependence of the Dynamics of Protein Hydration Water. *Journal of the American Chemical Society*, **1999**, 121, 9740-9741	16.4	61
122	Reaction paths and free energy profiles for conformational transitions: An internal coordinate approach. *Journal of Chemical Physics*, **1991**, 95, 7612-7625	3.9	61
121	Electrochemical Surface Potential Due to Classical Point Charge Models Drives Anion Adsorption to the Air-Water Interface. *Journal of Physical Chemistry Letters*, **2012**, 3, 1565-70	6.4	60
120	Acyl-chain methyl distributions of liquid-ordered and -disordered membranes. *Biophysical Journal*, **2011**, 100, 1455-62	2.9	60
119	Molecular dynamics investigation of the surface/bulk equilibrium in an ethanol□water solution. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 559-563		60
118	Water wires in atomistic models of the Hv1 proton channel. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 286-93	3.8	58
117	Molecular biophysics of Orai store-operated Ca2+ channels. *Biophysical Journal*, **2015**, 108, 237-46	2.9	57
116	The thermodynamics of solvophobic effects: A molecular-dynamics study of n-butane in carbon tetrachloride and water. *Journal of Chemical Physics*, **1990**, 92, 2582-2592	3.9	56
115	Separating instability from aggregation propensity in □-crystallin variants. *Biophysical Journal*, **2011**, 100, 498-506	2.9	55
114	Relation between surface tension and ion adsorption at the air-water interface: a molecular dynamics simulation study. *Journal of Physical Chemistry A*, **2009**, 113, 7286-93	2.8	53
113	Effects of solvent damping on side chain and backbone contributions to the protein boson peak. *Journal of Chemical Physics*, **2001**, 115, 1607-1612	3.9	53
112	Ambient Pressure X-ray Photoelectron Spectroscopy and Molecular Dynamics Simulation Studies of Liquid/Vapor Interfaces of Aqueous NaCl, RbCl, and RbBr Solutions. *Journal of Physical Chemistry C*, **2012**, 116, 4545-4555	3.8	52
111	Accommodation coefficients for water vapor at the air/water interface. *Chemical Physics Letters*, **2004**, 393, 249-255	2.5	52
110	Experimental and theoretical characterization of adsorbed water on self-assembled monolayers: understanding the interaction of water with atmospherically relevant surfaces. *Journal of Physical Chemistry A*, **2009**, 113, 2060-9	2.8	51
109	Enhanced surface photochemistry in chloride-nitrate ion mixtures. *Physical Chemistry Chemical Physics*, **2008**, 10, 5668-77	3.6	51
108	Surface organization of aqueous MgCl2 and application to atmospheric marine aerosol chemistry. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 6616-21	11.5	50
107	The low-temperature inflection observed in neutron scattering measurements of proteins is due to methyl rotation: direct evidence using isotope labeling and molecular dynamics simulations. *Journal of the American Chemical Society*, **2010**, 132, 4990-1	16.4	50
106	Amplitudes and Frequencies of Protein Dynamics: Analysis of Discrepancies between Neutron Scattering and Molecular Dynamics Simulations. *Journal of the American Chemical Society*, **2000**, 122, 10450-10451	16.4	50

105	Self-induced docking site of a deeply embedded peripheral membrane protein. *Biophysical Journal*, **2007**, 92, 517-24	2.9	49
104	On the Coupling between the Collective Dynamics of Proteins and Their Hydration Water. *Journal of Physical Chemistry Letters*, **2014**, 5, 1181-6	6.4	47
103	Investigation of finite system-size effects in molecular dynamics simulations of lipid bilayers. *Journal of Physical Chemistry B*, **2006**, 110, 24157-64	3.4	47
102	Proton-coupled dynamics in lactose permease. *Structure*, **2012**, 20, 1893-904	5.2	46
101	Molecular dynamics simulations of supported phospholipid/alkanethiol bilayers on a gold(111) surface. *Biophysical Journal*, **1999**, 77, 964-72	2.9	45
100	Terahertz absorption of dilute aqueous solutions. *Journal of Chemical Physics*, **2012**, 137, 235103	3.9	44
99	Nitrate ion photolysis in thin water films in the presence of bromide ions. *Journal of Physical Chemistry A*, **2011**, 115, 5810-21	2.8	44
98	Structure of large nitrate-water clusters at ambient temperatures: simulations with effective fragment potentials and force fields with implications for atmospheric chemistry. *Journal of Physical Chemistry A*, **2009**, 113, 12805-14	2.8	44
97	Thermodynamics of iodide adsorption at the instantaneous air-water interface. *Journal of Chemical Physics*, **2013**, 138, 114709	3.9	43
96	Dissociation of strong acid revisited: X-ray photoelectron spectroscopy and molecular dynamics simulations of HNO3 in water. *Journal of Physical Chemistry B*, **2011**, 115, 9445-51	3.4	42
95	Inertial suppression of protein dynamics in a binary glycerol-trehalose glass. *Journal of Physical Chemistry B*, **2006**, 110, 22953-6	3.4	42
94	Methyl group dynamics as a probe of the protein dynamical transition. *Journal of the American Chemical Society*, **2004**, 126, 15928-9	16.4	42
93	Orientation and Structure of Acetonitrile in Water at the Liquid□Vapor Interface: A Molecular Dynamics Simulation Study. *Journal of Physical Chemistry C*, **2016**, 120, 17555-17563	3.8	42
92	Dynamics of SecY translocons with translocation-defective mutations. *Structure*, **2010**, 18, 847-57	5.2	41
91	Sensitivity of 2D IR spectra to peptide helicity: a concerted experimental and simulation study of an octapeptide. *Journal of Physical Chemistry B*, **2009**, 113, 12037-49	3.4	39
90	Stability of a model beta-sheet in water. *Journal of Molecular Biology*, **1992**, 227, 1244-52	6.5	39
89	The impact of clothing on ozone and squalene ozonolysis products in indoor environments. *Communications Chemistry*, **2019**, 2,	6.3	38
88	Microscopic wetting of mixed self-assembled monolayers: a molecular dynamics study. *Journal of Physical Chemistry B*, **2009**, 113, 4161-9	3.4	37

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86	Vector and parallel algorithms for the molecular dynamics simulation of macromolecules on shared-memory computers. *Journal of Computational Chemistry*, **1991**, 12, 1270-1277	3.5	36
85	Molecular dynamics simulations of a pulmonary surfactant protein B peptide in a lipid monolayer. *Biophysical Journal*, **2003**, 84, 2169-80	2.9	35
84	Anomalous behavior of water inside the SecY translocon. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 9016-21	11.5	34
83	Investigation of Interfacial and Bulk Dissociation of HBr, HCl, and HNO3 Using Density Functional Theory-Based Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2014**, 118, 29412-29420	3.8	33
82	A molecular picture of surface interactions of organic compounds on prevalent indoor surfaces: limonene adsorption on SiO. *Chemical Science*, **2019**, 10, 2906-2914	9.4	32
81	Coupling of retinal, protein, and water dynamics in squid rhodopsin. *Biophysical Journal*, **2010**, 99, 2200-7	2.9	31
80	Hygroscopic growth and deliquescence of NaCl nanoparticles mixed with surfactant SDS. *Journal of Physical Chemistry B*, **2010**, 114, 2435-49	3.4	31
79	Spectral signatures of the pentagonal water cluster in bacteriorhodopsin. *ChemPhysChem*, **2008**, 9, 2703-7	3.2	31
78	Specific cation effects at aqueous solution-vapor interfaces: Surfactant-like behavior of Li revealed by experiments and simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 13363-13368	11.5	29
77	Down-state model of the voltage-sensing domain of a potassium channel. *Biophysical Journal*, **2010**, 98, 2857-66	2.9	29
76	Quantitative interpretation of molecular dynamics simulations for X-ray photoelectron spectroscopy of aqueous solutions. *Journal of Chemical Physics*, **2016**, 144, 154704	3.9	29
75	Hydration dynamics of purple membranes. *Faraday Discussions*, **2009**, 141, 99-116; discussion 175-207	3.6	28
74	Thermal Fluctuations of the Unusually Symmetric and Stable Superoxide Tetrahydrate Complex: An ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry A*, **2002**, 106, 10969-10976	2.8	27
73	Conformational flexibility in free energy simulations. *Chemical Physics Letters*, **1989**, 156, 256-260	2.5	26
72	Hydration dynamics in a partially denatured ensemble of the globular protein human alpha-lactalbumin investigated with molecular dynamics simulations. *Biophysical Journal*, **2008**, 95, 5257-67	2.9	25
71	Assembly and Stability of Helical Membrane Proteins. *Soft Matter*, **2012**, 8, 7742-7752	3.6	24
70	Nitrate ion photochemistry at interfaces: a new mechanism for oxidation of alpha-pinene. *Physical Chemistry Chemical Physics*, **2008**, 10, 3063-71	3.6	24

69	Interleaflet mixing and coupling in liquid-disordered phospholipid bilayers. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 354-62	3.8	23
68	Modelling consortium for chemistry of indoor environments (MOCCIE): integrating chemical processes from molecular to room scales. *Environmental Sciences: Processes and Impacts*, **2019**, 21, 1240-1254	4.3	22
67	Solvent-Shared Ion Pairs at the Air-Solution Interface of Magnesium Chloride and Sulfate Solutions Revealed by Sum Frequency Spectroscopy and Molecular Dynamics Simulations. *Journal of Physical Chemistry A*, **2017**, 121, 6450-6459	2.8	21
66	Microscopic origin of gating current fluctuations in a potassium channel voltage sensor. *Biophysical Journal*, **2012**, 102, L44-6	2.9	21
65	Effect of magnesium cation on the interfacial properties of aqueous salt solutions. *Journal of Physical Chemistry A*, **2010**, 114, 8359-68	2.8	21
64	Ab initio molecular dynamics study of the solvated OHCl- complex: implications for the atmospheric oxidation of chloride anion to molecular chlorine. *Journal of Physical Chemistry A*, **2008**, 112, 4644-50	2.8	21
63	Electronic Polarization and Hydration of the Dimethyl phosphate Anion:□An ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2001**, 105, 5827-5832	3.4	21
62	Calmodulin Gates Aquaporin 0 Permeability through a Positively Charged Cytoplasmic Loop. *Journal of Biological Chemistry*, **2017**, 292, 185-195	5.4	20
61	Specific Anion Effects on Na Adsorption at the Aqueous Solution-Air Interface: MD Simulations, SESSA Calculations, and Photoelectron Spectroscopy Experiments. *Journal of Physical Chemistry B*, **2018**, 122, 910-918	3.4	20
60	Structural plasticity in the topology of the membrane-interacting domain of HIV-1 gp41. *Biophysical Journal*, **2014**, 106, 610-20	2.9	20
59	The role of protein-solvent hydrogen bond dynamics in the structural relaxation of a protein in glycerol versus water. *European Biophysics Journal*, **2008**, 37, 701-9	1.9	19
58	A transporter converted into a sensor, a phototaxis signaling mutant of bacteriorhodopsin at 3.0□ *Journal of Molecular Biology*, **2012**, 415, 455-63	6.5	18
57	Increased hydrophobic surface exposure in the cataract-related G18V variant of human □-crystallin. *Biochimica Et Biophysica Acta - General Subjects*, **2016**, 1860, 325-32	4	17
56	Coupling between the voltage-sensing and pore domains in a voltage-gated potassium channel. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 1726-36	3.8	17
55	Dynamics of the internal water molecules in squid rhodopsin. *Biophysical Journal*, **2009**, 96, 2572-6	2.9	17
54	Multiscale Modeling of Human Skin Oil-Induced Indoor Air Chemistry: Combining Kinetic Models and Molecular Dynamics. *Journal of Physical Chemistry B*, **2020**, 124, 3836-3843	3.4	17
53	What Is the Driving Force behind the Adsorption of Hydrophobic Molecules on Hydrophilic Surfaces?. *Journal of Physical Chemistry Letters*, **2019**, 10, 468-473	6.4	17
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51	Diffraction-based density restraints for membrane and membrane-peptide molecular dynamics simulations. *Biophysical Journal*, **2006**, 91, 3617-29	2.9	16
50	Characterization of sub-nanosecond dynamics of the molten globule state of □actalbumin using quasielastic neutron scattering and molecular dynamics simulations. *Chemical Physics*, **2003**, 292, 435-443	2.3	16
49	Transmembrane helices containing a charged arginine are thermodynamically stable. *European Biophysics Journal*, **2017**, 46, 627-637	1.9	15
48	Direct evidence of conformational changes associated with voltage gating in a voltage sensor protein by time-resolved X-ray/neutron interferometry. *Langmuir*, **2014**, 30, 4784-96	4	15
47	Structural dynamics of the S4 voltage-sensor helix in lipid bilayers lacking phosphate groups. *Journal of Physical Chemistry B*, **2011**, 115, 8732-8	3.4	15
46	Experimental and Simulation Studies of Aquaporin 0 Water Permeability and Regulation. *Chemical Reviews*, **2019**, 119, 6015-6039	68.1	14
45	Refining Protein Penetration into the Lipid Bilayer Using Fluorescence Quenching and Molecular Dynamics Simulations: The Case of Diphtheria Toxin Translocation Domain. *Journal of Membrane Biology*, **2018**, 251, 379-391	2.3	14
44	Production of gas phase NO2 and halogens from the photolysis of thin water films containing nitrate, chloride and bromide ions at room temperature. *Physical Chemistry Chemical Physics*, **2013**, 15, 17636-46	3.6	14
43	Molecular Dynamics Simulations of a Powder Model of the Intrinsically Disordered Protein Tau. *Journal of Physical Chemistry B*, **2015**, 119, 12580-9	3.4	13
42	Validation of depth-dependent fluorescence quenching in membranes by molecular dynamics simulation of tryptophan octyl ester in POPC bilayer. *Journal of Physical Chemistry B*, **2013**, 117, 4770-8	3.4	13
41	Two transmembrane dimers of the bovine papillomavirus E5 oncoprotein clamp the PDGF □ receptor in an active dimeric conformation. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E7262-E7271	11.5	13
40	Direct comparisons of experimental and calculated neutron structure factors of pure solvents as a method for force field validation. *Journal of Physical Chemistry B*, **2007**, 111, 12941-4	3.4	13
39	Voltage-dependent structural models of the human Hv1 proton channel from long-timescale molecular dynamics simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 13490-13498	11.5	12
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36	Interactions of Cl- and OH radical in aqueous solution. *Journal of Physical Chemistry A*, **2009**, 113, 8823-5	2.8	11
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33	Molecular dynamics simulations of aqueous pullulan oligomers. *Biomacromolecules*, **2005**, 6, 1239-51	6.9	10
32	Molecular Mechanism of Aggregation of the Cataract-Related D-Crystallin W42R Variant from Multiscale Atomistic Simulations. *Biochemistry*, **2019**, 58, 3691-3699	3.2	9
31	"Bind and Crawl" Association Mechanism of Leishmania major Peroxidase and Cytochrome c Revealed by Brownian and Molecular Dynamics Simulations. *Biochemistry*, **2015**, 54, 7272-82	3.2	9
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29	D2O Water Interaction with Textured Carboxylic Acid-Terminated Monolayer Surfaces Characterized by Temperature-Programmed Desorption and Molecular Dynamics. *Journal of Physical Chemistry C*, **2010**, 114, 1570-1579	3.8	8
28	Multi-Conformation Monte Carlo: A Method for Introducing Flexibility in Efficient Simulations of Many-Protein Systems. *Journal of Physical Chemistry B*, **2016**, 120, 8115-26	3.4	8
27	Atomistic Modeling of Ion Conduction through the Voltage-Sensing Domain of the Shaker K Ion Channel. *Journal of Physical Chemistry B*, **2017**, 121, 3804-3812	3.4	7
26	Molecular Orientation at the Squalene/Air Interface from Sum Frequency Generation Spectroscopy and Atomistic Modeling. *Journal of Physical Chemistry B*, **2021**, 125, 3932-3941	3.4	7
25	Specific ion interactions with aromatic rings in aqueous solutions: Comparison of molecular dynamics simulations with a thermodynamic solute partitioning model and Raman spectroscopy. *Chemical Physics Letters*, **2015**, 638, 1-8	2.5	6
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22	Cooperativity and allostery in aquaporin 0 regulation by Ca. *Biochimica Et Biophysica Acta - Biomembranes*, **2019**, 1861, 988-996	3.8	5
21	Impact of Adsorbed Water on the Interaction of Limonene with Hydroxylated SiO: Implications of Hydrogen Bonding for Surfaces in Humid Environments. *Journal of Physical Chemistry A*, **2020**, 124, 10592-10599	2.8	5
20	Human B-crystallin discriminates between aggregation-prone and function-preserving variants of a client protein. *Biochimica Et Biophysica Acta - General Subjects*, **2020**, 1864, 129502	4	5
19	Gating energetics of a voltage-dependent K channel pore domain. *Journal of Computational Chemistry*, **2017**, 38, 1472-1478	3.5	4
18	A comment on "pH and the surface tension of water" (J. K. Beattie, A. M. Djerdjev, A. Gray-Weale, N. Kallay, J. Lützenkirchen, T. Preočanin, A. Selmani, J. Colloid Interface Sci. 422 (2014) 54.). *Journal of Colloid and Interface Science*, **2015**, 448, 593	9.3	4
17	Molecular Arrangement of a Mixture of Organosulfur Surfactants at the Aqueous Solution/Vapor Interface Studied by Photoelectron Intensity and Angular Distribution Measurements and Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2019**, 123, 8160-8170	3.8	4
16	Diffusivelike Motions in a Solvent-Free Protein-Polymer Hybrid. *Physical Review Letters*, **2021**, 126, 088102	7.4	4

15	Voltage-Dependent Profile Structures of a Kv-Channel via Time-Resolved Neutron Interferometry. *Biophysical Journal*, **2019**, 117, 751-766	2.9	2
14	Molecular Dynamics Investigation of the Lamellar Liquid-Crystal D-Phase in the Octylammonium Chloride/Water System. *Molecular Simulation*, **1996**, 16, 219-228	2	2
13	Protein Hydration Water. *Springer Series in Cluster Physics*, **2003**, 213-225		2
12	Insights on small molecule binding to the Hv1 proton channel from free energy calculations with molecular dynamics simulations. *Scientific Reports*, **2020**, 10, 13587	4.9	2
11	Heterogeneous Interactions of Prevalent Indoor Oxygenated Organic Compounds on Hydroxylated SiO Surfaces. *Environmental Science & Technology*, **2021**, 55, 6623-6630	10.3	2
10	HIFs: New arginine mimic inhibitors of the Hv1 channel with improved VSD-ligand interactions. *Journal of General Physiology*, **2021**, 153,	3.4	2
9	A novel Hv1 inhibitor reveals a new mechanism of inhibition of a voltage-sensing domain. *Journal of General Physiology*, **2021**, 153,	3.4	2
8	Role of Conformational Flexibility in Monte Carlo Simulations of Many-Protein Systems. *Journal of Chemical Theory and Computation*, **2019**, 15, 1399-1408	6.4	2
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