Douglas J Tobias

List of Publications by Year
in descending order

186	22,282	19657 61	9103 144
papers	citations	h-index	g-index

188	188	188	18425
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Constant pressure molecular dynamics algorithms. Journal of Chemical Physics, 1994, 101, 4177-4189.	3.0	4,379
2	Update of the CHARMM All-Atom Additive Force Field for Lipids: Validation on Six Lipid Types. Journal of Physical Chemistry B, 2010, 114, 7830-7843.	2.6	3,676
3	Explicit reversible integrators for extended systems dynamics. Molecular Physics, 1996, 87, 1117-1157.	1.7	1,508
4	Specific Ion Effects at the Air/Water Interface. Chemical Reviews, 2006, 106, 1259-1281.	47.7	1,200
5	Ions at the Air/Water Interface. Journal of Physical Chemistry B, 2002, 106, 6361-6373.	2.6	708
6	Molecular Structure of Salt Solutions:â€‰ A New View of the Interface with Implications for Heterogeneous Atmospheric Chemistry. Journal of Physical Chemistry B, 2001, 105, 10468-10472.	2.6	639
7	Unified Molecular Picture of the Surfaces of Aqueous Acid, Base, and Salt Solutions. Journal of Physical Chemistry B, 2005, 109, 7617-7623.	2.6	393
8	Getting Specific About Specific Ion Effects. Science, 2008, 319, 1197-1198.	12.6	296
9	The Dynamics of Protein Hydration Water: A Quantitative Comparison of Molecular Dynamics Simulations and Neutron-scattering Experiments. Biophysical Journal, 2000, 79, 3244-3257.	0.5	295
10	Interface connections of a transmembrane voltage sensor. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 15059-15064.	7.1	208
11	Watching the Low-Frequency Motions in Aqueous Salt Solutions: The Terahertz Vibrational Signatures of Hydrated Ions. Journal of the American Chemical Society, 2012, 134, 1030-1035.	13.7	201
12	Propensity of soft ions for the air/water interface. Current Opinion in Colloid and Interface Science, 2004, 9, 67-73.	7.4	200
13	Translational diffusion of hydration water correlates with functional motions in folded and intrinsically disordered proteins. Nature Communications, 2015, 6, 6490.	12.8	199
14	Airâ”Liquid Interfaces of Aqueous Solutions Containing Ammonium and Sulfate:Â Spectroscopic and Molecular Dynamics Studies. Journal of Physical Chemistry B, 2005, 109, 8861-8872.	2.6	195
15	Constant-Pressure Molecular Dynamics Investigation of Cholesterol Effects in a Dipalmitoylphosphatidylcholine Bilayer. Biophysical Journal, 1998, 75, 2147-2156.	0.5	194
16	Atomic-scale molecular dynamics simulations of lipid membranes. Current Opinion in Colloid and Interface Science, 1997, 2, 15-26.	7.4	184
17	Coincidence of Dynamical Transitions in a Soluble Protein and Its Hydration Water:â€‰ Direct Measurements by Neutron Scattering and MD Simulations. Journal of the American Chemical Society, 2008, 130, 4586-4587.	13.7	184
18	Structure and hydration of membranes embedded with voltage-sensing domains. Nature, 2009, 462, 473-479.	27.8	175

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19	Experimental Validation of Molecular Dynamics Simulations of Lipid Bilayers: A New Approach. Biophysical Journal, 2005, 88, 805-817.	0.5	161
20	Simulation and Theory of Ions at Atmospherically Relevant Aqueous Liquid-Air Interfaces. Annual Review of Physical Chemistry, 2013, 64, 339-359.	10.8	151
21	Surface solvation of halogen anions in water clusters: An ab initio molecular dynamics study of the Clâ¯(H2O)6 complex. Journal of Chemical Physics, 2001, 114, 7036-7044.	3.0	148
22	Explicit reversible integrators for extended systems dynamics. Molecular Physics, 1996, 87, 1117-1157.	1.7	148
23	Chloride Anion on Aqueous Clusters, at the Airâ¯Water Interface, and in Liquid Water:Â Solvent Effects on Cl-Polarizability. Journal of Physical Chemistry A, 2002, 106, 379-383.	2.5	134
24	Polarizability of the nitrate anion and its solvation at the air/water interface. Physical Chemistry Chemical Physics, 2003, 5, 3752.	2.8	129
25	Hydroxyl Radical at the Airâ¯Water Interface. Journal of the American Chemical Society, 2004, 126, 16308-16309.	13.7	128
26	Interaction of Gas-Phase Ozone at 296 K with Unsaturated Self-Assembled Monolayers:Â A New Look at an Old System. Journal of Physical Chemistry A, 2004, 108, 10473-10485.	2.5	123
27	Molecular Dynamics Simulations of Atmospheric Oxidants at the Airâ¯Water Interface:Â Solvation and Accommodation of OH and O3. Journal of Physical Chemistry B, 2005, 109, 15876-15892.	2.6	121
28	Solvation of Magnesium Dication: Molecular Dynamics Simulation and Vibrational Spectroscopic Study of Magnesium Chloride in Aqueous Solutions. Journal of Physical Chemistry A, 2010, 114, 5141-5148.	2.5	119
29	Hydroxide anion at the airâ€“water interface. Chemical Physics Letters, 2009, 481, 2-8.	2.6	118
30	Surface Effects on Aqueous Ionic Solvation:Â 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.	2.6	117
31	Structure and Dynamics of the Aqueous Liquidâ¯Vapor Interface:Â A Comprehensive Particle-Based Simulation StudyâŠ¥. Journal of Physical Chemistry B, 2006, 110, 3738-3746.	2.6	115
32	The Effect of an Organic Surfactant on the Liquidâ¯Vapor Interface of an Electrolyte Solution. Journal of Physical Chemistry C, 2007, 111, 13497-13509.	3.1	115
33	Spatial Dependence of Protein-Water Collective Hydrogen-Bond Dynamics. Physical Review Letters, 2013, 111, 218101.	7.8	111
34	Ion Specificity at the Peptide Bond: Molecular Dynamics Simulations of N-Methylacetamide in Aqueous Salt Solutions. Journal of Physical Chemistry B, 2010, 114, 1213-1220.	2.6	107
35	Arginine in Membranes: The Connection Between Molecular Dynamics Simulations and Translocon-Mediated Insertion Experiments. Journal of Membrane Biology, 2011, 239, 35-48.	2.1	104
36	Structure and Vibrational Spectroscopy of Salt Water/Air Interfaces:Â Predictions from Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2005, 109, 7934-7940.	2.6	103

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37	Ion spatial distributions at the liquidâ€“vapor interface of aqueous potassium fluoride solutions. Physical Chemistry Chemical Physics, 2008, 10, 4778.	2.8	103
38	Introduction:â€‰ Structure and Chemistry at Aqueous Interfaces. Chemical Reviews, 2006, 106, 1137-1139.	47.7	102
39	Allosteric mechanism of water-channel gating by Ca2+â€“calmodulin. Nature Structural and Molecular Biology, 2013, 20, 1085-1092.	8.2	102
40	Polarizability and aqueous solvation of the sulfate dianion. Chemical Physics Letters, 2003, 367, 704-710.	2.6	98
41	Molecular Dynamics Simulations of a Calcium Carbonate/Calcium Sulfonate Reverse Micelleâ€. The Journal of Physical Chemistry, 1996, 100, 6637-6648.	2.9	94
42	Molecular Dynamics Simulations of the Solutionâ^'Air Interface of Aqueous Sodium Nitrate. Journal of Physical Chemistry A, 2007, 111, 3091-3098.	2.5	91
43	Molecular dynamics with internal coordinate constraints. Journal of Chemical Physics, 1988, 89, 5115-5127.	3.0	90
44	Thermodynamics of amide hydrogen bond formation in polar and apolar solvents. Journal of Molecular Biology, 1989, 209, 817-820.	4.2	90
45	Toward a Unified Picture of the Water Self-Ions at the Airâ€“Water Interface: A Density Functional Theory Perspective. Journal of Physical Chemistry B, 2014, 118, 8364-8372.	2.6	90
46	A Voltage-Sensor Water Pore. Biophysical Journal, 2006, 91, L90-L92.	0.5	89
47	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.	2.6	88
48	Reverse turns in blocked dipeptides are intrinsically unstable in water. Journal of Molecular Biology, 1990, 216, 783-796.	4.2	84
49	Re-examining the properties of the aqueous vaporâ€“liquid interface using dispersion corrected density functional theory. Journal of Chemical Physics, 2011, 135, 124712.	3.0	82
50	Hydration water mobility is enhanced around tau amyloid fibers. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 6365-6370.	7.1	79
51	Calculation of free energy surfaces using the methods of thermodynamic perturbation theory. Chemical Physics Letters, 1987, 142, 472-476.	2.6	76
52	Insertion of short transmembrane helices by the Sec61 translocon. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11588-11593.	7.1	76
53	Does Nitric Acid Dissociate at the Aqueous Solution Surface?. Journal of Physical Chemistry C, 2011, 115, 21183-21190.	3.1	73
54	Acyl-Chain Methyl Distributions of Liquid-Ordered and -Disordered Membranes. Biophysical Journal, 2011, 100, 1455-1462.	0.5	70

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55	Enhanced surface photochemistry in chlorideâ€“nitrate ion mixtures. Physical Chemistry Chemical Physics, 2008, 10, 5668.	2.8	69
56	Uptake and Collision Dynamics of Gas Phase Ozone at Unsaturated Organic Interfaces. Journal of Physical Chemistry A, 2004, 108, 5806-5814.	2.5	68
57	Water wires in atomistic models of the Hv1 proton channel. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 286-293.	2.6	67
58	Electrochemical Surface Potential Due to Classical Point Charge Models Drives Anion Adsorption to the Airâ€“Water Interface. Journal of Physical Chemistry Letters, 2012, 3, 1565-1570.	4.6	67
59	Molecular dynamics investigation of the surface/bulk equilibrium in an ethanolâ€“water solution. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 559-563.	1.7	64
60	Relation between Surface Tension and Ion Adsorption at the Airâ^'Water Interface: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry A, 2009, 113, 7286-7293.	2.5	64
61	Separating Instability from Aggregation Propensity in Î³S-Crystallin Variants. Biophysical Journal, 2011, 100, 498-506.	0.5	64
62	Molecular Biophysics of Orai Store-Operated Ca2+ Channels. Biophysical Journal, 2015, 108, 237-246.	0.5	64
63	Reaction paths and free energy profiles for conformational transitions: An internal coordinate approach. Journal of Chemical Physics, 1991, 95, 7612-7625.	3.0	63
64	Environmental Dependence of the Dynamics of Protein Hydration Water. Journal of the American Chemical Society, 1999, 121, 9740-9741.	13.7	63
65	The thermodynamics of solvophobic effects: A molecularâ€dynamics study of nâ€butane in carbon tetrachloride and water. Journal of Chemical Physics, 1990, 92, 2582-2592.	3.0	62
66	On the Coupling between the Collective Dynamics of Proteins and Their Hydration Water. Journal of Physical Chemistry Letters, 2014, 5, 1181-1186.	4.6	59
67	Accommodation coefficients for water vapor at the air/water interface. Chemical Physics Letters, 2004, 393, 249-255.	2.6	58
68	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.	3.1	58
69	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, 2060-2069.	2.5	56
70	Surface organization of aqueous MgCl ₂ and application to atmospheric marine aerosol chemistry. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 6616-6621.	7.1	56
71	Effects of solvent damping on side chain and backbone contributions to the protein boson peak. Journal of Chemical Physics, 2001, 115, 1607-1612.	3.0	54
72	Nitrate Ion Photolysis in Thin Water Films in the Presence of Bromide Ions. Journal of Physical Chemistry A, 2011, 115, 5810-5821.	2.5	54

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73	The impact of clothing on ozone and squalene ozonolysis products in indoor environments. Communications Chemistry, 2019, 2, .	4.5	54
74	Self-Induced Docking Site of a Deeply Embedded Peripheral Membrane Protein. Biophysical Journal, 2007, 92, 517-524.	0.5	53
75	Proton-Coupled Dynamics in Lactose Permease. Structure, 2012, 20, 1893-1904.	3.3	53
76	Amplitudes and Frequencies of Protein Dynamics:Â Analysis of Discrepancies between Neutron Scattering and Molecular Dynamics Simulations. Journal of the American Chemical Society, 2000, 122, 10450-10451.	13.7	52
77	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, 4990-4991.	13.7	52
78	A molecular picture of surface interactions of organic compounds on prevalent indoor surfaces: limonene adsorption on SiO₂. Chemical Science, 2019, 10, 2906-2914.	7.4	52
79	Terahertz absorption of dilute aqueous solutions. Journal of Chemical Physics, 2012, 137, 235103.	3.0	51
80	Orientation and Structure of Acetonitrile in Water at the Liquidâ€“Vapor Interface: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2016, 120, 17555-17563.	3.1	50
81	Molecular Dynamics Simulations of Supported Phospholipid/Alkanethiol Bilayers on a Gold(111) Surface. Biophysical Journal, 1999, 77, 964-972.	0.5	49
82	Investigation of Finite System-Size Effects in Molecular Dynamics Simulations of Lipid Bilayers. Journal of Physical Chemistry B, 2006, 110, 24157-24164.	2.6	48
83	Thermodynamics of iodide adsorption at the instantaneous air-water interface. Journal of Chemical Physics, 2013, 138, 114709.	3.0	48
84	Structure of Large Nitrateâ^'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, 12805-12814.	2.5	47
85	Dynamics of SecY Translocons with Translocation-Defective Mutations. Structure, 2010, 18, 847-857.	3.3	47
86	Dissociation of Strong Acid Revisited: X-ray Photoelectron Spectroscopy and Molecular Dynamics Simulations of HNO₃ in Water. Journal of Physical Chemistry B, 2011, 115, 9445-9451.	2.6	46
87	Stability of a model Î²-sheet in water. Journal of Molecular Biology, 1992, 227, 1244-1252.	4.2	43
88	Methyl Group Dynamics as a Probe of the Protein Dynamical Transition. Journal of the American Chemical Society, 2004, 126, 15928-15929.	13.7	43
89	Inertial Suppression of Protein Dynamics in a Binary Glycerolâ^'Trehalose Glass. Journal of Physical Chemistry B, 2006, 110, 22953-22956.	2.6	42
90	Hygroscopic Growth and Deliquescence of NaCl Nanoparticles Mixed with Surfactant SDS. Journal of Physical Chemistry B, 2010, 114, 2435-2449.	2.6	42

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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, 12037-12049.	2.6	41
92	Anomalous behavior of water inside the SecY translocon. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 9016-9021.	7.1	41
93	Vector and parallel algorithms for the molecular dynamics simulation of macromolecules on shared-memory computers. Journal of Computational Chemistry, 1991, 12, 1270-1277.	3.3	40
94	Microscopic Wetting of Mixed Self-assembled Monolayers: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2009, 113, 4161-4169.	2.6	40
95	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.	3.1	40
96	Molecular dynamics investigation of an ethanol-water solution. Physica A: Statistical Mechanics and Its Applications, 1996, 231, 117-122.	2.6	38
97	Molecular Dynamics Simulations of a Pulmonary Surfactant Protein B Peptide in a Lipid Monolayer. Biophysical Journal, 2003, 84, 2169-2180.	0.5	36
98	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.	3.5	36
99	Coupling of Retinal, Protein, and Water Dynamics in Squid Rhodopsin. Biophysical Journal, 2010, 99, 2200-2207.	0.5	35
100	Specific cation effects at aqueous solutionâ˜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.	7.1	34
101	Down-State Model of the Voltage-Sensing Domain of a Potassium Channel. Biophysical Journal, 2010, 98, 2857-2866.	0.5	33
102	Spectral Signatures of the Pentagonal Water Cluster in Bacteriorhodopsin. ChemPhysChem, 2008, 9, 2703-2707.	2.1	32
103	Hydration dynamics of purple membranes. Faraday Discussions, 2009, 141, 99-116.	3.2	31
104	Quantitative interpretation of molecular dynamics simulations for X-ray photoelectron spectroscopy of aqueous solutions. Journal of Chemical Physics, 2016, 144, 154704.	3.0	31
105	Thermal Fluctuations of the Unusually Symmetric and Stable Superoxide Tetrahydrate Complex:Â An ab Initio Molecular Dynamics Study. Journal of Physical Chemistry A, 2002, 106, 10969-10976.	2.5	30
106	Interleaflet mixing and coupling in liquid-disordered phospholipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 354-362.	2.6	29
107	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.	7.1	29
108	Conformational flexibility in free energy simulations. Chemical Physics Letters, 1989, 156, 256-260.	2.6	28

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109	Hydration Dynamics in a Partially Denatured Ensemble of the Globular Protein Human Î±-Lactalbumin Investigated with Molecular Dynamics Simulations. Biophysical Journal, 2008, 95, 5257-5267.	0.5	28
110	Assembly and stability of Î±-helical membrane proteins. Soft Matter, 2012, 8, 7742.	2.7	28
111	Microscopic Origin of Gating Current Fluctuations in a Potassium Channel Voltage Sensor. Biophysical Journal, 2012, 102, L44-L46.	0.5	28
112	Specific Anion Effects on Na⁺ Adsorption at the Aqueous Solutionâ€“Air Interface: MD Simulations, SESSA Calculations, and Photoelectron Spectroscopy Experiments. Journal of Physical Chemistry B, 2018, 122, 910-918.	2.6	28
113	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.	2.6	28
114	Nitrate ion photochemistry at interfaces: a new mechanism for oxidation of Î±-pinene. Physical Chemistry Chemical Physics, 2008, 10, 3063.	2.8	27
115	What Is the Driving Force behind the Adsorption of Hydrophobic Molecules on Hydrophilic Surfaces?. Journal of Physical Chemistry Letters, 2019, 10, 468-473.	4.6	27
116	Effect of Magnesium Cation on the Interfacial Properties of Aqueous Salt Solutions. Journal of Physical Chemistry A, 2010, 114, 8359-8368.	2.5	26
117	Calmodulin Gates Aquaporin 0 Permeability through a Positively Charged Cytoplasmic Loop. Journal of Biological Chemistry, 2017, 292, 185-195.	3.4	26
118	Solvent-Shared Ion Pairs at the Airâ€“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.	2.5	26
119	Two transmembrane dimers of the bovine papillomavirus E5 oncoprotein clamp the PDGF Î² receptor in an active dimeric conformation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E7262-E7271.	7.1	26
120	Experimental and Simulation Studies of Aquaporin 0 Water Permeability and Regulation. Chemical Reviews, 2019, 119, 6015-6039.	47.7	25
121	Electronic Polarization and Hydration of the Dimethyl phosphate Anion:Â An ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2001, 105, 5827-5832.	2.6	23
122	The role of proteinâ€“solvent hydrogen bond dynamics in the structural relaxation of a protein in glycerol versus water. European Biophysics Journal, 2008, 37, 701-709.	2.2	23
123	Ab Initio Molecular Dynamics Study of the Solvated OHCl^{â¯} Complex: Implications for the Atmospheric Oxidation of Chloride Anion to Molecular Chlorine. Journal of Physical Chemistry A, 2008, 112, 4644-4650.	2.5	22
124	Structural Plasticity in the Topology of the Membrane-Interacting Domain of HIV-1 gp41. Biophysical Journal, 2014, 106, 610-620.	0.5	22
125	Transmembrane helices containing a charged arginine are thermodynamically stable. European Biophysics Journal, 2017, 46, 627-637.	2.2	21
126	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.	2.8	20

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127	Increased hydrophobic surface exposure in the cataract-related G18V variant of human Î³S-crystallin. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 325-332.	2.4	20
128	Dynamics of the Internal Water Molecules in Squid Rhodopsin. Biophysical Journal, 2009, 96, 2572-2576.	0.5	19
129	Structural Dynamics of the S4 Voltage-Sensor Helix in Lipid Bilayers Lacking Phosphate Groups. Journal of Physical Chemistry B, 2011, 115, 8732-8738.	2.6	18
130	Interaction of Water Vapor with the Surfaces of Imidazolium-Based Ionic Liquid Nanoparticles and Thin Films. Journal of Physical Chemistry B, 2012, 116, 11255-11265.	2.6	18
131	A Transporter Converted into a Sensor, a Phototaxis Signaling Mutant of Bacteriorhodopsin at 3.0ÂÃ.... Journal of Molecular Biology, 2012, 415, 455-463.	4.2	18
132	Coupling between the voltage-sensing and pore domains in a voltage-gated potassium channel. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 1726-1736.	2.6	18
133	Voltage Sensing in Membranes: From Macroscopic Currents to Molecular Motions. Journal of Membrane Biology, 2015, 248, 419-430.	2.1	18
134	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.	2.1	18
135	Characterization of sub-nanosecond dynamics of the molten globule state of Î±-lactalbumin using quasielastic neutron scattering and molecular dynamics simulations. Chemical Physics, 2003, 292, 435-443.	1.9	17
136	Diffraction-Based Density Restraints for Membrane and Membrane-Peptide Molecular Dynamics Simulations. Biophysical Journal, 2006, 91, 3617-3629.	0.5	17
137	Direct Evidence of Conformational Changes Associated with Voltage Gating in a Voltage Sensor Protein by Time-Resolved X-ray/Neutron Interferometry. Langmuir, 2014, 30, 4784-4796.	3.5	16
138	Molecular Mechanism of Aggregation of the Cataract-Related Î³D-Crystallin W42R Variant from Multiscale Atomistic Simulations. Biochemistry, 2019, 58, 3691-3699.	2.5	16
139	Cooperativity and allostery in aquaporin 0 regulation by Ca2+. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 988-996.	2.6	16
140	Impact of Adsorbed Water on the Interaction of Limonene with Hydroxylated SiO2: Implications of Ï€-Hydrogen Bonding for Surfaces in Humid Environments. Journal of Physical Chemistry A, 2020, 124, 10592-10599.	2.5	16
141	Molecular Dynamics Simulations of a Powder Model of the Intrinsically Disordered Protein Tau. Journal of Physical Chemistry B, 2015, 119, 12580-12589.	2.6	15
142	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, 12941-12944.	2.6	14
143	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, 4770-4778.	2.6	14
144	Structural Relaxation Processes and Collective Dynamics of Water in Biomolecular Environments. Journal of Physical Chemistry B, 2019, 123, 480-486.	2.6	14

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145	HIFs: New arginine mimic inhibitors of the Hv1 channel with improved VSDâ€“ligand interactions. Journal of General Physiology, 2021, 153, .	1.9	14
146	Multiphase Ozonolysis of Oleic Acid-Based Lipids: Quantitation of Major Products and Kinetic Multilayer Modeling. Environmental Science & Technology, 2022, 56, 7716-7728.	10.0	14
147	A Simple Protocol for Identification of Helical and Mobile Residues in Membrane Proteins. Journal of Molecular Biology, 1995, 253, 391-395.	4.2	13
148	Interactions of Cl^{â^'} and OH Radical in Aqueous Solution. Journal of Physical Chemistry A, 2009, 113, 8823-8825.	2.5	13
149	Molecular Orientation at the Squalene/Air Interface from Sum Frequency Generation Spectroscopy and Atomistic Modeling. Journal of Physical Chemistry B, 2021, 125, 3932-3941.	2.6	13
150	â€œBind and Crawlâ€•Association Mechanism of Leishmania major Peroxidase and Cytochrome c Revealed by Brownian and Molecular Dynamics Simulations. Biochemistry, 2015, 54, 7272-7282.	2.5	12
151	Multi-Conformation Monte Carlo: A Method for Introducing Flexibility in Efficient Simulations of Many-Protein Systems. Journal of Physical Chemistry B, 2016, 120, 8115-8126.	2.6	12
152	Interactions of Tyrosine in Leu-Enkephalin at a Membraneâ^'Water Interface: An Ultrafast Two-Dimensional Infrared Study Combined with Density Functional Calculations and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 1180-1190.	2.6	11
153	Molecular Arrangement of a Mixture of Organosulfur Surfactants at the Aqueous Solutionâ€“Vapor Interface Studied by Photoelectron Intensity and Angular Distribution Measurements and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2019, 123, 8160-8170.	3.1	11
154	Molecular Dynamics Simulations of Aqueous Pullulan Oligomers. Biomacromolecules, 2005, 6, 1239-1251.	5.4	10
155	Adsorption of constitutional isomers of cyclic monoterpenes on hydroxylated silica surfaces. Journal of Chemical Physics, 2021, 154, 124703.	3.0	10
156	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.	2.6	9
157	Heterogeneous Interactions of Prevalent Indoor Oxygenated Organic Compounds on Hydroxylated SiO2 Surfaces. Environmental Science & Technology, 2021, 55, 6623-6630.	10.0	9
158	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.	3.1	8
159	Electrostatic interactions and hydrogen bond dynamics in chloride pumping by halorhodopsin. Biochimica Et Biophysica Acta - Bioenergetics, 2014, 1837, 1964-1972.	1.0	8
160	Insights on small molecule binding to the Hv1 proton channel from free energy calculations with molecular dynamics simulations. Scientific Reports, 2020, 10, 13587.	3.3	8
161	A novel Hv1 inhibitor reveals a new mechanism of inhibition of a voltage-sensing domain. Journal of General Physiology, 2021, 153, .	1.9	8
162	Human Î±B-crystallin discriminates between aggregation-prone and function-preserving variants of a client protein. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129502.	2.4	7

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163	Diffusivelike Motions in a Solvent-Free Protein-Polymer Hybrid. Physical Review Letters, 2021, 126, 088102.	7.8	7
164	Interactions of gaseous HNO₃and water with individual and mixed alkyl self-assembled monolayers at room temperature. Physical Chemistry Chemical Physics, 2014, 16, 2358-2367.	2.8	6
165	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.	2.6	6
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