

# Max L Berkowitz

## List of Publications by Citations

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140  
papers

25,986  
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62  
h-index

145  
g-index

145  
ext. papers

28,628  
ext. citations

4.3  
avg, IF

6.77  
L-index

#	Paper	IF	Citations
140	A smooth particle mesh Ewald method. <i>Journal of Chemical Physics</i> , <b>1995</b> , 103, 8577-8593	3.9	14532
139	Ewald summation for systems with slab geometry. <i>Journal of Chemical Physics</i> , <b>1999</b> , 111, 3155-3162	3.9	978
138	Molecular hardness and softness, local hardness and softness, hardness and softness kernels, and relations among these quantities. <i>Journal of Chemical Physics</i> , <b>1988</b> , 88, 2554-2557	3.9	354
137	Many-body effects in molecular dynamics simulations of Na+(H <sub>2</sub> O) <sub>n</sub> and Cl(H <sub>2</sub> O) <sub>n</sub> clusters. <i>Journal of Chemical Physics</i> , <b>1991</b> , 95, 1954-1963	3.9	300
136	Molecular Dynamics Simulation of Sodium Dodecyl Sulfate Micelle in Water: Micellar Structural Characteristics and Counterion Distribution. <i>Journal of Physical Chemistry B</i> , <b>2002</b> , 106, 3788-3793	3.4	293
135	Local structural order and molecular associations in water-DMSO mixtures. Molecular dynamics study. <i>Journal of the American Chemical Society</i> , <b>1992</b> , 114, 7889-7896	16.4	276
134	On the concept of local hardness in chemistry. <i>Journal of the American Chemical Society</i> , <b>1985</b> , 107, 6811-6814	16.4	270
133	Structure of dipalmitoylphosphatidylcholine/cholesterol bilayer at low and high cholesterol concentrations: molecular dynamics simulation. <i>Biophysical Journal</i> , <b>1999</b> , 77, 2075-89	2.9	252
132	Aqueous solutions next to phospholipid membrane surfaces: insights from simulations. <i>Chemical Reviews</i> , <b>2006</b> , 106, 1527-39	68.1	218
131	Molecular dynamics simulation of a dipalmitoylphosphatidylcholine bilayer with NaCl. <i>Biophysical Journal</i> , <b>2003</b> , 84, 3743-50	2.9	205
130	Transcription of ground-state density-functional theory into a local thermodynamics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1984</b> , 81, 8028-31	11.5	198
129	Simulation of Sodium Dodecyl Sulfate at the WaterVapor and WaterCarbon Tetrachloride Interfaces at Low Surface Coverage. <i>Journal of Physical Chemistry B</i> , <b>1997</b> , 101, 3793-3799	3.4	191
128	A classical fluid-like approach to the density-functional formalism of many-electron systems. <i>Journal of Chemical Physics</i> , <b>1985</b> , 83, 2976-2983	3.9	175
127	Structure and dynamics of water at the Pt(111) interface: Molecular dynamics study. <i>Journal of Chemical Physics</i> , <b>1991</b> , 94, 2110-2117	3.9	171
126	Molecular dynamics with stochastic boundary conditions. <i>Chemical Physics Letters</i> , <b>1982</b> , 90, 215-217	2.5	167
125	Dielectric constant of water at high electric fields: Molecular dynamics study. <i>Journal of Chemical Physics</i> , <b>1999</b> , 110, 7935-7942	3.9	164
124	Molecular Dynamics Simulations of Sodium Dodecyl Sulfate Micelle in Water: The Behavior of Water. <i>Journal of Physical Chemistry B</i> , <b>2002</b> , 106, 10902-10907	3.4	161

123	Molecular dynamics simulation of a membrane/water interface: the ordering of water and its relation to the hydration force. <i>Langmuir</i> , <b>1993</b> , 9, 3122-3131	4	156
122	Structures of $\text{Cl}(\text{H}_2\text{O})_n$ and $\text{F}(\text{H}_2\text{O})_n$ ( $n=2,3,\dots,15$ ) clusters. Molecular dynamics computer simulations. <i>Journal of Chemical Physics</i> , <b>1994</b> , 100, 3085-3093	3.9	146
121	The dielectric constant of SPC/E water. <i>Chemical Physics Letters</i> , <b>1989</b> , 155, 173-176	2.5	145
120	Mixed bilayer containing dipalmitoylphosphatidylcholine and dipalmitoylphosphatidylserine: lipid complexation, ion binding, and electrostatics. <i>Biophysical Journal</i> , <b>2003</b> , 85, 3120-31	2.9	140
119	Effect of the treatment of long-range forces on the dynamics of ions in aqueous solutions. <i>Journal of Chemical Physics</i> , <b>1995</b> , 102, 450-456	3.9	139
118	Molecular dynamics simulation of dipalmitoylphosphatidylserine bilayer with $\text{Na}^+$ counterions. <i>Biophysical Journal</i> , <b>2002</b> , 82, 1818-27	2.9	138
117	United atom force field for phospholipid membranes: Constant pressure molecular dynamics simulation of dipalmitoylphosphatidicholine/water system. <i>Journal of Computational Chemistry</i> , <b>1999</b> , 20, 531-545	3.5	136
116	Electric-field induced restructuring of water at a platinum-water interface: A molecular dynamics computer simulation. <i>Physical Review Letters</i> , <b>1995</b> , 74, 3193-3196	7.4	135
115	Effects of alkali cations and halide anions on the DOPC lipid membrane. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 7235-43	2.8	133
114	Detailed molecular dynamics simulations of model biological membranes containing cholesterol. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , <b>2009</b> , 1788, 86-96	3.8	131
113	Complexation of phosphatidylcholine lipids with cholesterol. <i>Biophysical Journal</i> , <b>2004</b> , 86, 1345-56	2.9	130
112	Sodium chloride ion pair interaction in water: computer simulation. <i>Chemical Physics Letters</i> , <b>1984</b> , 105, 577-580	2.5	129
111	Density functional approach to frontier controlled reactions. <i>Journal of the American Chemical Society</i> , <b>1987</b> , 109, 4823-4825	16.4	122
110	Molecular dynamics simulation of the structure of dimyristoylphosphatidylcholine bilayers with cholesterol, ergosterol, and lanosterol. <i>Biophysical Journal</i> , <b>2001</b> , 80, 1649-58	2.9	120
109	Computer Simulations of Sodium Dodecyl Sulfate at Liquid/Liquid and Liquid/Vapor Interfaces. <i>Journal of Physical Chemistry B</i> , <b>2000</b> , 104, 5302-5308	3.4	113
108	Computer simulation study of the interface width of the liquid/liquid interface. <i>Physical Review Letters</i> , <b>2001</b> , 87, 176101	7.4	112
107	Structure and dynamics of $\text{Cl}(\text{H}_2\text{O})_{20}$ clusters: The effect of the polarizability and the charge of the ion. <i>Journal of Chemical Physics</i> , <b>1992</b> , 96, 8288-8294	3.9	112
106	Dynamical properties of phospholipid bilayers from computer simulation. <i>Biophysical Journal</i> , <b>1999</b> , 76, 2081-9	2.9	111

105	Structure and dynamics of water at the interface with phospholipid bilayers. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 224702	3.9	110
104	The Origin of the Hydration Interaction of Lipid Bilayers from MD Simulation of Dipalmitoylphosphatidylcholine Membranes in Gel and Liquid Crystalline Phases. <i>Langmuir</i> , <b>1995</b> , 11, 4519-4531	4	110
103	Solvation structure of a sodium chloride ion pair in water. <i>Journal of the American Chemical Society</i> , <b>1986</b> , 108, 1755-1761	16.4	102
102	Dynamics of ion solvation in a Stockmayer fluid. <i>Journal of Chemical Physics</i> , <b>1992</b> , 96, 3092-3101	3.9	100
101	Diffusion-controlled reactions: A variational formula for the optimum reaction coordinate. <i>Journal of Chemical Physics</i> , <b>1983</b> , 79, 5563-5565	3.9	100
100	Interaction between amyloid-beta (1-42) peptide and phospholipid bilayers: a molecular dynamics study. <i>Biophysical Journal</i> , <b>2009</b> , 96, 785-97	2.9	98
99	A molecular dynamics study of the structure and dynamics of water between dilaurylphosphatidylethanolamine bilayers. <i>Langmuir</i> , <b>1992</b> , 8, 233-240	4	97
98	Stabilization energies of Cl <sup>-</sup> Br <sup>-</sup> and I <sup>-</sup> ions in water clusters. <i>Journal of Chemical Physics</i> , <b>1993</b> , 99, 4222-4224	3.9	96
97	The solvation of Cl <sup>-</sup> Br <sup>-</sup> and I <sup>-</sup> in acetonitrile clusters: Photoelectron spectroscopy and molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>1996</b> , 105, 2675-2685	3.9	95
96	Water structure and dynamics in phosphate fluorosurfactant based reverse micelle: A computer simulation study. <i>Journal of Chemical Physics</i> , <b>2003</b> , 118, 1937-1944	3.9	90
95	Aqueous solutions at the interface with phospholipid bilayers. <i>Accounts of Chemical Research</i> , <b>2012</b> , 45, 74-82	24.3	88
94	An algorithm to describe molecular scale rugged surfaces and its application to the study of a water/lipid bilayer interface. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 2199-2205	3.9	85
93	Chemical Potential Equalization Principle: Direct Approach from Density Functional Theory. <i>Journal of Physical Chemistry A</i> , <b>1997</b> , 101, 5687-5691	2.8	84
92	Mechanism of interaction of monovalent ions with phosphatidylcholine lipid membranes. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 9504-9	3.4	81
91	Liquid-vapor interface of TIP4P water: comparison between a polarizable and a nonpolarizable model. <i>Chemical Physics Letters</i> , <b>1991</b> , 176, 61-66	2.5	77
90	Molecular dynamics simulation of DPPC bilayer in DMSO. <i>Biophysical Journal</i> , <b>1999</b> , 76, 2472-8	2.9	76
89	The limiting ionic conductivity of Na <sup>+</sup> and Cl <sup>-</sup> ions in aqueous solutions: Molecular dynamics simulation. <i>Journal of Chemical Physics</i> , <b>1987</b> , 86, 376-382	3.9	75
88	Structure of Phosphate Fluorosurfactant Based Reverse Micelles in Supercritical Carbon Dioxide. <i>Langmuir</i> , <b>2002</b> , 18, 7371-7376	4	73

87	Structure of the amyloid-beta (1-42) monomer absorbed to model phospholipid bilayers: a molecular dynamics study. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 14480-6	3.4	70
86	Role of Water in the Hydration Force Acting between Lipid Bilayers. <i>Langmuir</i> , <b>1996</b> , 12, 2625-2629	4	69
85	Difference between magainin-2 and melittin assemblies in phosphatidylcholine bilayers: results from coarse-grained simulations. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 3021-30	3.4	67
84	Hydronium and hydroxide at the interface between water and hydrophobic media. <i>Physical Chemistry Chemical Physics</i> , <b>2008</b> , 10, 4975-80	3.6	65
83	The implementation of slab geometry for membrane-channel molecular dynamics simulations. <i>Biophysical Journal</i> , <b>2003</b> , 85, 97-107	2.9	64
82	Molecular model of a cell plasma membrane with an asymmetric multicomponent composition: water permeation and ion effects. <i>Biophysical Journal</i> , <b>2009</b> , 96, 4493-501	2.9	63
81	Enthalpies of formation and stabilization energies of Br $\square$ (H $_2$ O) $_n$ ( $n=1,2, \square 15$ ) clusters. Comparisons between molecular dynamics computer simulations and experiment. <i>Chemical Physics Letters</i> , <b>1994</b> , 218, 377-382	2.5	63
80	Molecular dynamics simulation of dipalmitoylphosphatidylcholine membrane with cholesterol sulfate. <i>Biophysical Journal</i> , <b>2000</b> , 78, 1672-80	2.9	62
79	Generalized Langevin dynamics simulations with arbitrary time-dependent memory kernels. <i>Journal of Chemical Physics</i> , <b>1983</b> , 78, 3256-3261	3.9	62
78	Cube to cage transitions in (H $_2$ O) $_n$ ( $n=12, 16, \text{ and } 20$ ). <i>Journal of Chemical Physics</i> , <b>1996</b> , 105, 3715-3721	3.9	61
77	Structure and dynamics of high-pressure TIP4P water. <i>Journal of Chemical Physics</i> , <b>1987</b> , 87, 6682-6686	3.9	58
76	Theory of vibrational relaxation in solids: The competition between local phonon and roton receiving modes. <i>Chemical Physics</i> , <b>1979</b> , 37, 369-388	2.3	58
75	Molecular dynamics simulations of bilayers containing mixtures of sphingomyelin with cholesterol and phosphatidylcholine with cholesterol. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 12888-97	3.4	57
74	Molecular dynamics simulations of tips2 water restricted by a spherical hydrophobic boundary. <i>Chemical Physics Letters</i> , <b>1985</b> , 113, 278-282	2.5	57
73	Energetics of cholesterol transfer between lipid bilayers. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 3803-11	3.4	56
72	A molecular dynamics study of the effect of temperature on the structure and dynamics of water between Pt walls. <i>Chemical Physics Letters</i> , <b>1989</b> , 162, 32-38	2.5	56
71	Structure and Dynamics of Water in the Presence of Charged Surfactant Monolayers at the Water-CCl $_4$ Interface. A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , <b>1997</b> , 101, 10775-10780	3.4	55
70	Molecular Dynamics Simulation Studies of Polyether and Perfluoropolyether Surfactant Based Reverse Micelles in Supercritical Carbon Dioxide. <i>Journal of Physical Chemistry B</i> , <b>2003</b> , 107, 12906-12916	3.4	55

69	Computer simulation of a water/membrane interface. <i>Langmuir</i> , <b>1991</b> , 7, 1042-1044	4	55
68	Oriental dynamics of water in phospholipid bilayers with different hydration levels. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 7676-80	3-4	54
67	Photodetachment spectra of Cl(H <sub>2</sub> O) <sub>n</sub> clusters. Predictions and comparisons. <i>Chemical Physics Letters</i> , <b>1997</b> , 264, 31-38	2.5	54
66	Molecular Dynamics Study of Water next to Electrified Ag(111) Surfaces. <i>Langmuir</i> , <b>1996</b> , 12, 3747-3752	4	54
65	Binding and reorientation of melittin in a POPC bilayer: computer simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , <b>2012</b> , 1818, 2975-81	3.8	51
64	Role of water in atomic resolution AFM in solutions. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 12584-94	3.94	51
63	Exterior site occupancy infers chloride-induced proton gating in a prokaryotic homolog of the ClC chloride channel. <i>Biophysical Journal</i> , <b>2004</b> , 87, 1686-96	2.9	51
62	The structure of water at platinum/water interfaces Molecular dynamics computer simulations. <i>Surface Science</i> , <b>1995</b> , 335, 401-415	1.8	51
61	Exponential approximation for the density matrix and the Wigner distribution. <i>Chemical Physics Letters</i> , <b>1986</b> , 129, 486-488	2.5	51
60	Comparison of the structure and dynamics of water at the Pt(111) and Pt(100) interfaces: molecular dynamics study. <i>Chemical Physics Letters</i> , <b>1991</b> , 177, 426-432	2.5	50
59	Role of Rotational and Translational Local Modes in Vibrational Relaxation in Solids: A Study of NH and ND in Solid Ar. <i>Physical Review Letters</i> , <b>1977</b> , 39, 1000-1004	7.4	50
58	Computer Simulation Studies of Water States in Perfluoro Polyether Reverse Micelles: Effects of Changing the Counterion. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 9768-9776	2.8	49
57	Vibrational relaxation of molecules in solids: The role of rotational and of translational local modes. <i>Chemical Physics Letters</i> , <b>1977</b> , 49, 260-264	2.5	49
56	Mechanism of membrane poration by shock wave induced nanobubble collapse: a molecular dynamics study. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 6225-34	3.4	48
55	A molecular dynamics study of the early stages of amyloid-beta(1-42) oligomerization: the role of lipid membranes. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2010</b> , 78, 2533-45	4.2	48
54	Melittin creates transient pores in a lipid bilayer: results from computer simulations. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 5031-42	3.4	47
53	Hydration force between model hydrophilic surfaces: computer simulations. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 101101	3.9	47
52	Origin of the hydration force: water-mediated interaction between two hydrophilic plates. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 13222-8	3.4	46

51	Molecular dynamics simulation of fluorination effects on a phospholipid bilayer. <i>Journal of Chemical Physics</i> , <b>1999</b> , 111, 9864-9870	3.9	43
50	Molecular dynamics simulation of a reverse micelle self assembly in supercritical CO <sub>2</sub> . <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 10254-5	16.4	41
49	Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 241101	3.9	40
48	Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 2711-6	6.4	39
47	Free energy barrier for melittin reorientation from a membrane-bound state to a transmembrane state. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 13457-63	3.4	39
46	Properties of Poloxamer Molecules and Poloxamer Micelles Dissolved in Water and Next to Lipid Bilayers: Results from Computer Simulations. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 5823-30	3.4	38
45	Thermally Induced Structural Changes in F-(H <sub>2</sub> O) <sub>11</sub> and Cl-(H <sub>2</sub> O) <sub>11</sub> Clusters: Molecular Dynamics Computer Simulations. <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 1350-1356		38
44	Molecular dynamics simulations of SOPS and sphingomyelin bilayers containing cholesterol. <i>Biophysical Journal</i> , <b>2007</b> , 92, 1284-95	2.9	38
43	The behavior of reorientational correlation functions of water at the water-lipid bilayer interface. <i>Journal of Chemical Physics</i> , <b>2006</b> , 125, 094713	3.9	36
42	Effects of oxygenated sterol on phospholipid bilayer properties: a molecular dynamics simulation. <i>Chemistry and Physics of Lipids</i> , <b>2001</b> , 112, 31-9	3.7	36
41	Ultrafast solvation dynamics in a Stockmayer fluid. <i>Journal of Chemical Physics</i> , <b>1992</b> , 97, 5253-5254	3.9	35
40	Effect of ion electrode contact on the energetics of the heterogeneous electron transfer. <i>Chemical Physics Letters</i> , <b>1994</b> , 227, 561-566	2.5	34
39	Shock wave interaction with a phospholipid membrane: coarse-grained computer simulations. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 054906	3.9	33
38	Influence of the arrangement and secondary structure of melittin peptides on the formation and stability of toroidal pores. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , <b>2011</b> , 1808, 2258-66	3.8	32
37	Temperature dependence of conductance of the Li <sup>+</sup> , Cs <sup>+</sup> , and Cl <sup>-</sup> ions in water: Molecular dynamics simulation. <i>Journal of Chemical Physics</i> , <b>1988</b> , 88, 7104-7110	3.9	32
36	Aqueous solution near charged Ag(111) surfaces: comparison between a computer simulation and experiment. <i>Chemical Physics Letters</i> , <b>1999</b> , 301, 81-86	2.5	31
35	Memory kernels from molecular dynamics. <i>Journal of Chemical Physics</i> , <b>1981</b> , 75, 2462-2463	3.9	31
34	Opening of the blood-brain barrier tight junction due to shock wave induced bubble collapse: a molecular dynamics simulation study. <i>ACS Chemical Neuroscience</i> , <b>2015</b> , 6, 1296-301	5.7	30

33	Free energy profiles for lithium(1+) and iodide ions approaching the platinum(100) surface: a molecular dynamics study. <i>The Journal of Physical Chemistry</i> , <b>1993</b> , 97, 13803-13806		30
32	Fluctuations in number of water molecules confined between nanoparticles. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 13410-4	3.4	29
31	Effects of the polarizability and water density constraint on the structure of water near charged surfaces: Molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>2000</b> , 112, 10491-10495	3.9	28
30	Monte Carlo simulation of homopolymer chains. I. Second virial coefficient. <i>Journal of Chemical Physics</i> , <b>2003</b> , 118, 4721-4732	3.9	26
29	Mobility of stretched water. <i>Journal of Chemical Physics</i> , <b>1993</b> , 98, 9859-9862	3.9	24
28	Ion solvation in water clusters. <i>Zeitschrift für Physik D-Atoms Molecules and Clusters</i> , <b>1993</b> , 26, 166-168		22
27	Nanobubbles, cavitation, shock waves and traumatic brain injury. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 32638-32652	3.6	21
26	Shock Wave Induced Collapse of Arrays of Nanobubbles Located Next to a Lipid Membrane: Coarse-Grained Computer Simulations. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 8879-89	3.4	20
25	Shock Wave-Induced Damage of a Protein by Void Collapse. <i>Biophysical Journal</i> , <b>2016</b> , 110, 147-56	2.9	19
24	Restructuring of hydrophobic surfaces created by surfactant adsorption to mica surfaces. <i>Langmuir</i> , <b>2011</b> , 27, 11737-41	4	19
23	Thermodynamic and hydrogen-bonding analyses of the interaction between model lipid bilayers. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 3013-9	3.4	19
22	Behavior of P85 and P188 Poloxamer Molecules: Computer Simulations Using United-Atom Force-Field. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 8631-41	3.4	14
21	The effect of the rigidity of perfluoropolyether surfactant on its behavior at the water/supercritical carbon dioxide interface. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 21725-31	3.4	14
20	Local pressure changes in lipid bilayers due to adsorption of melittin and magainin-h2 antimicrobial peptides: results from computer simulations. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 12673-9	3.4	10
19	Molecular dynamics simulation study of interaction between model rough hydrophobic surfaces. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 6059-67	2.8	10
18	Resolving the structure of a model hydrophobic surface: DODAB monolayers on mica. <i>RSC Advances</i> , <b>2012</b> , 2, 4181	3.7	9
17	Molecular dynamics simulation study of the water-mediated interaction between zwitterionic and charged surfaces. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 024501	3.9	9
16	The effect of water structure and surface charge correlations on the hydration force acting between model hydrophilic surfaces. <i>Molecular Physics</i> , <b>2006</b> , 104, 3607-3617	1.7	9



15	A comparative computational study of coarse-grained and all-atom water models in shock Hugoniot states. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 144504	3.9	8
14	Molecular and Atomic Dipole Moments in Heteronuclear and Homonuclear Diatomics. Density Functional Approach. <i>Journal of Physical Chemistry A</i> , <b>1998</b> , 102, 4808-4812	2.8	8
13	Bubbles in water under stretch-induced cavitation. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 054501	3.9	7
12	Molecular polarizability and atomic properties: Density functional approach. <i>Journal of Chemical Physics</i> , <b>1998</b> , 109, 10142-10147	3.9	6
11	Molecular Detailed Simulations of Lipid Bilayers. <i>Reviews in Computational Chemistry</i> , 253-286		5
10	Damage to Polystyrene Polymer Film by Shock Wave Induced Bubble Collapse. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 7494-7499	3.4	4
9	A Molecular Look at Membranes. <i>Current Topics in Membranes</i> , <b>2016</b> , 77, 1-25	2.2	3
8	Interaction Forces between Membrane Surfaces. <i>Advances in Chemistry Series</i> , <b>1994</b> , 3-25		2
7	Molecular Simulations of Aqueous Electrolytes: Role of Explicit Inclusion of Charge Transfer into Force Fields. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 13069-13076	3.4	2
6	Restructuring of a model hydrophobic surface: Monte Carlo simulations using a simple coarse-grained model. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 15584-90	3.4	1
5	Chapter 9 On the Nature of Lipid Rafts: Insights from Molecularly Detailed Simulations of Model Biological Membranes Containing Mixtures of Cholesterol and Phospholipids. <i>Current Topics in Membranes</i> , <b>2008</b> , 257-279	2.2	1
4	A smooth particle mesh Ewald method		1
3	Enhanced Cavitation and Hydration Crossover of Stretched Water in the Presence of C. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 6621-6625	6.4	
2	Solvation Dynamics in a Stockmayer Fluid <b>1993</b> , 461-483		
1	Stretch-Induced Cavitation: How Critical Cavity Radius and Barrier Energy, Radius, and Energy of a Stable Cavity Depend on the Stretching Factor. <i>Journal of Physical Chemistry B</i> , <b>2021</b> , 125, 4409-4414	3.4	