Max L Berkowitz

List of Publications by Year in Descending Order

140 papers	25,986 citations	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	Molecular Simulations of Aqueous Electrolytes: Role of Explicit Inclusion of Charge Transfer into Force Fields. *Journal of Physical Chemistry B*, **2021**, 125, 13069-13076	3.4	2
139	Stretch-Induced Cavitation: How Critical Cavity Radius and Barrier Energy, Radius, and Energy of a Stable Cavity Depend on the Stretching Factor. *Journal of Physical Chemistry B*, **2021**, 125, 4409-4414	3.4	
138	Damage to Polystyrene Polymer Film by Shock Wave Induced Bubble Collapse. *Journal of Physical Chemistry B*, **2020**, 124, 7494-7499	3.4	4
137	Bubbles in water under stretch-induced cavitation. *Journal of Chemical Physics*, **2019**, 150, 054501	3.9	7
136	Enhanced Cavitation and Hydration Crossover of Stretched Water in the Presence of C. *Journal of Physical Chemistry Letters*, **2019**, 10, 6621-6625	6.4	
135	A comparative computational study of coarse-grained and all-atom water models in shock Hugoniot states. *Journal of Chemical Physics*, **2018**, 148, 144504	3.9	8
134	Behavior of P85 and P188 Poloxamer Molecules: Computer Simulations Using United-Atom Force-Field. *Journal of Physical Chemistry B*, **2016**, 120, 8631-41	3.4	14
133	Shock Wave-Induced Damage of a Protein by Void Collapse. *Biophysical Journal*, **2016**, 110, 147-56	2.9	19
132	Properties of Poloxamer Molecules and Poloxamer Micelles Dissolved in Water and Next to Lipid Bilayers: Results from Computer Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 5823-30	3.4	38
131	A Molecular Look at Membranes. *Current Topics in Membranes*, **2016**, 77, 1-25	2.2	3
130	Nanobubbles, cavitation, shock waves and traumatic brain injury. *Physical Chemistry Chemical Physics*, **2016**, 18, 32638-32652	3.6	21
129	Opening of the blood-brain barrier tight junction due to shock wave induced bubble collapse: a molecular dynamics simulation study. *ACS Chemical Neuroscience*, **2015**, 6, 1296-301	5.7	30
128	Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer. *Journal of Chemical Physics*, **2015**, 143, 241101	3.9	40
127	Mechanism of membrane poration by shock wave induced nanobubble collapse: a molecular dynamics study. *Journal of Physical Chemistry B*, **2015**, 119, 6225-34	3.4	48
126	Shock Wave Induced Collapse of Arrays of Nanobubbles Located Next to a Lipid Membrane: Coarse-Grained Computer Simulations. *Journal of Physical Chemistry B*, **2015**, 119, 8879-89	3.4	20
125	Shock wave interaction with a phospholipid membrane: coarse-grained computer simulations. *Journal of Chemical Physics*, **2014**, 140, 054906	3.9	33
124	Local pressure changes in lipid bilayers due to adsorption of melittin and magainin-h2 antimicrobial peptides: results from computer simulations. *Journal of Physical Chemistry B*, **2014**, 118, 12673-9	3.4	10

123	Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. *Journal of Physical Chemistry Letters*, **2014**, 5, 2711-6	6.4	39
122	Melittin creates transient pores in a lipid bilayer: results from computer simulations. *Journal of Physical Chemistry B*, **2013**, 117, 5031-42	3.4	47
121	Free energy barrier for melittin reorientation from a membrane-bound state to a transmembrane state. *Journal of Physical Chemistry B*, **2013**, 117, 13457-63	3.4	39
120	Restructuring of a model hydrophobic surface: Monte Carlo simulations using a simple coarse-grained model. *Journal of Physical Chemistry B*, **2013**, 117, 15584-90	3.4	1
119	Aqueous solutions at the interface with phospholipid bilayers. *Accounts of Chemical Research*, **2012**, 45, 74-82	24.3	88
118	Binding and reorientation of melittin in a POPC bilayer: computer simulations. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 2975-81	3.8	51
117	Resolving the structure of a model hydrophobic surface: DODAB monolayers on mica. *RSC Advances* , **2012**, 2, 4181	3.7	9
116	Molecular dynamics simulation study of the water-mediated interaction between zwitterionic and charged surfaces. *Journal of Chemical Physics*, **2012**, 136, 024501	3.9	9
115	Difference between magainin-2 and melittin assemblies in phosphatidylcholine bilayers: results from coarse-grained simulations. *Journal of Physical Chemistry B*, **2012**, 116, 3021-30	3.4	67
114	Role of water in atomic resolution AFM in solutions. *Physical Chemistry Chemical Physics*, **2011**, 13, 12584-94	3.4	51
113	Influence of the arrangement and secondary structure of melittin peptides on the formation and stability of toroidal pores. *Biochimica Et Biophysica Acta - Biomembranes*, **2011**, 1808, 2258-66	3.8	32
112	Restructuring of hydrophobic surfaces created by surfactant adsorption to mica surfaces. *Langmuir*, **2011**, 27, 11737-41	4	19
111	Molecular dynamics simulation study of interaction between model rough hydrophobic surfaces. *Journal of Physical Chemistry A*, **2011**, 115, 6059-67	2.8	10
110	Thermodynamic and hydrogen-bonding analyses of the interaction between model lipid bilayers. *Journal of Physical Chemistry B*, **2010**, 114, 3013-9	3.4	19
109	Fluctuations in number of water molecules confined between nanoparticles. *Journal of Physical Chemistry B*, **2010**, 114, 13410-4	3.4	29
108	Mechanism of interaction of monovalent ions with phosphatidylcholine lipid membranes. *Journal of Physical Chemistry B*, **2010**, 114, 9504-9	3.4	81
107	A molecular dynamics study of the early stages of amyloid-beta(1-42) oligomerization: the role of lipid membranes. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2533-45	4.2	48
106	Effects of alkali cations and halide anions on the DOPC lipid membrane. *Journal of Physical Chemistry A*, **2009**, 113, 7235-43	2.8	133

105	Origin of the hydration force: water-mediated interaction between two hydrophilic plates. *Journal of Physical Chemistry B*, **2009**, 113, 13222-8	3.4	46
104	Orientational dynamics of water in phospholipid bilayers with different hydration levels. *Journal of Physical Chemistry B*, **2009**, 113, 7676-80	3.4	54
103	Structure of the amyloid-beta (1-42) monomer absorbed to model phospholipid bilayers: a molecular dynamics study. *Journal of Physical Chemistry B*, **2009**, 113, 14480-6	3.4	70
102	Detailed molecular dynamics simulations of model biological membranes containing cholesterol. *Biochimica Et Biophysica Acta - Biomembranes*, **2009**, 1788, 86-96	3.8	131
101	Interaction between amyloid-beta (1-42) peptide and phospholipid bilayers: a molecular dynamics study. *Biophysical Journal*, **2009**, 96, 785-97	2.9	98
100	Molecular model of a cell plasma membrane with an asymmetric multicomponent composition: water permeation and ion effects. *Biophysical Journal*, **2009**, 96, 4493-501	2.9	63
99	Chapter 9 On the Nature of Lipid Rafts: Insights from Molecularly Detailed Simulations of Model Biological Membranes Containing Mixtures of Cholesterol and Phospholipids. *Current Topics in Membranes*, **2008**, 257-279	2.2	1
98	Hydronium and hydroxide at the interface between water and hydrophobic media. *Physical Chemistry Chemical Physics*, **2008**, 10, 4975-80	3.6	65
97	Energetics of cholesterol transfer between lipid bilayers. *Journal of Physical Chemistry B*, **2008**, 112, 3807-11	3.4	56
96	Molecular dynamics simulations of bilayers containing mixtures of sphingomyelin with cholesterol and phosphatidylcholine with cholesterol. *Journal of Physical Chemistry B*, **2007**, 111, 12888-97	3.4	57
95	Molecular dynamics simulations of SOPS and sphingomyelin bilayers containing cholesterol. *Biophysical Journal*, **2007**, 92, 1284-95	2.9	38
94	The behavior of reorientational correlation functions of water at the water-lipid bilayer interface. *Journal of Chemical Physics*, **2006**, 125, 094713	3.9	36
93	Hydration force between model hydrophilic surfaces: computer simulations. *Journal of Chemical Physics*, **2006**, 124, 101101	3.9	47
92	Aqueous solutions next to phospholipid membrane surfaces: insights from simulations. *Chemical Reviews*, **2006**, 106, 1527-39	68.1	218
91	The effect of water structure and surface charge correlations on the hydration force acting between model hydrophilic surfaces. *Molecular Physics*, **2006**, 104, 3607-3617	1.7	9
90	The effect of the rigidity of perfluoropolyether surfactant on its behavior at the water/supercritical carbon dioxide interface. *Journal of Physical Chemistry B*, **2005**, 109, 21725-31	3.4	14
89	Structure and dynamics of water at the interface with phospholipid bilayers. *Journal of Chemical Physics*, **2005**, 123, 224702	3.9	110
88	Computer Simulation Studies of Water States in Perfluoro Polyether Reverse Micelles: Effects of Changing the Counterion *Journal of Physical Chemistry A*, **2004**, 108, 9768-9776	2.8	49

87	Exterior site occupancy infers chloride-induced proton gating in a prokaryotic homolog of the ClC chloride channel. *Biophysical Journal*, **2004**, 87, 1686-96	2.9	51
86	Molecular dynamics simulation of a reverse micelle self assembly in supercritical CO2. *Journal of the American Chemical Society*, **2004**, 126, 10254-5	16.4	41
85	Complexation of phosphatidylcholine lipids with cholesterol. *Biophysical Journal*, **2004**, 86, 1345-56	2.9	130
84	Molecular Dynamics Simulation Studies of Polyether and Perfluoropolyether Surfactant Based Reverse Micelles in Supercritical Carbon Dioxide. *Journal of Physical Chemistry B*, **2003**, 107, 12906-12916	3.4	55
83	Water structure and dynamics in phosphate fluorosurfactant based reverse micelle: A computer simulation study. *Journal of Chemical Physics*, **2003**, 118, 1937-1944	3.9	90
82	The implementation of slab geometry for membrane-channel molecular dynamics simulations. *Biophysical Journal*, **2003**, 85, 97-107	2.9	64
81	Mixed bilayer containing dipalmitoylphosphatidylcholine and dipalmitoylphosphatidylserine: lipid complexation, ion binding, and electrostatics. *Biophysical Journal*, **2003**, 85, 3120-31	2.9	140
80	Molecular dynamics simulation of a dipalmitoylphosphatidylcholine bilayer with NaCl. *Biophysical Journal*, **2003**, 84, 3743-50	2.9	205
79	An algorithm to describe molecular scale rugged surfaces and its application to the study of a water/lipid bilayer interface. *Journal of Chemical Physics*, **2003**, 119, 2199-2205	3.9	85
78	Monte Carlo simulation of homopolymer chains. I. Second virial coefficient. *Journal of Chemical Physics*, **2003**, 118, 4721-4732	3.9	26
77	Molecular Dynamics Simulations of Sodium Dodecyl Sulfate Micelle in Water: The Behavior of Water. *Journal of Physical Chemistry B*, **2002**, 106, 10902-10907	3.4	161
76	Structure of Phosphate Fluorosurfactant Based Reverse Micelles in Supercritical Carbon Dioxide. *Langmuir*, **2002**, 18, 7371-7376	4	73
75	Molecular Dynamics Simulation of Sodium Dodecyl Sulfate Micelle in Water: Micellar Structural Characteristics and Counterion Distribution. *Journal of Physical Chemistry B*, **2002**, 106, 3788-3793	3.4	293
74	Molecular dynamics simulation of dipalmitoylphosphatidylserine bilayer with Na+ counterions. *Biophysical Journal*, **2002**, 82, 1818-27	2.9	138
73	Effects of oxygenated sterol on phospholipid bilayer properties: a molecular dynamics simulation. *Chemistry and Physics of Lipids*, **2001**, 112, 31-9	3.7	36
72	Molecular dynamics simulation of the structure of dimyristoylphosphatidylcholine bilayers with cholesterol, ergosterol, and lanosterol. *Biophysical Journal*, **2001**, 80, 1649-58	2.9	120
71	Computer simulation study of the interface width of the liquid/liquid interface. *Physical Review Letters*, **2001**, 87, 176101	7.4	112
70	Effects of the polarizability and water density constraint on the structure of water near charged surfaces: Molecular dynamics simulations. *Journal of Chemical Physics*, **2000**, 112, 10491-10495	3.9	28

69	Molecular dynamics simulation of dipalmitoylphosphatidylcholine membrane with cholesterol sulfate. *Biophysical Journal*, **2000**, 78, 1672-80	2.9	62
68	Computer Simulations of Sodium Dodecyl Sulfate at Liquid/Liquid and Liquid/Vapor Interfaces. *Journal of Physical Chemistry B*, **2000**, 104, 5302-5308	3.4	113
67	Dielectric constant of water at high electric fields: Molecular dynamics study. *Journal of Chemical Physics*, **1999**, 110, 7935-7942	3.9	164
66	Molecular dynamics simulation of fluorination effects on a phospholipid bilayer. *Journal of Chemical Physics*, **1999**, 111, 9864-9870	3.9	43
65	Aqueous solution near charged Ag(111) surfaces: comparison between a computer simulation and experiment. *Chemical Physics Letters*, **1999**, 301, 81-86	2.5	31
64	United atom force field for phospholipid membranes: Constant pressure molecular dynamics simulation of dipalmitoylphosphatidicholine/water system. *Journal of Computational Chemistry*, **1999**, 20, 531-545	3.5	136
63	Ewald summation for systems with slab geometry. *Journal of Chemical Physics*, **1999**, 111, 3155-3162	3.9	978
62	Structure of dipalmitoylphosphatidylcholine/cholesterol bilayer at low and high cholesterol concentrations: molecular dynamics simulation. *Biophysical Journal*, **1999**, 77, 2075-89	2.9	252
61	Dynamical properties of phospholipid bilayers from computer simulation. *Biophysical Journal*, **1999**, 76, 2081-9	2.9	111
60	Molecular dynamics simulation of DPPC bilayer in DMSO. *Biophysical Journal*, **1999**, 76, 2472-8	2.9	76
59	Molecular and Atomic Dipole Moments in Heteronuclear and Homonuclear Diatomics. Density Functional Approach. *Journal of Physical Chemistry A*, **1998**, 102, 4808-4812	2.8	8
58	Molecular polarizability and atomic properties: Density functional approach. *Journal of Chemical Physics*, **1998**, 109, 10142-10147	3.9	6
57	Structure and Dynamics of Water in the Presence of Charged Surfactant Monolayers at the Water□CCl4 Interface. A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **1997**, 101, 10775-10780	3.4	55
56	Chemical Potential Equalization Principle: Direct Approach from Density Functional Theory. *Journal of Physical Chemistry A*, **1997**, 101, 5687-5691	2.8	84
55	Simulation of Sodium Dodecyl Sulfate at the Water□Vapor and Water□Carbon Tetrachloride Interfaces at Low Surface Coverage. *Journal of Physical Chemistry B*, **1997**, 101, 3793-3799	3.4	191
54	Photodetachment spectra of Cl□(H2O)n clusters. Predictions and comparisons. *Chemical Physics Letters*, **1997**, 264, 31-38	2.5	54
53	Thermally Induced Structural Changes in F-(H2O)11 and Cl-(H2O)11 Clusters: Molecular Dynamics Computer Simulations. *The Journal of Physical Chemistry*, **1996**, 100, 1350-1356		38
52	Role of Water in the Hydration Force Acting between Lipid Bilayers. *Langmuir*, **1996**, 12, 2625-2629	4	69

51	Molecular Dynamics Study of Water next to Electrified Ag(111) Surfaces. *Langmuir*, **1996**, 12, 3747-3752	4	54
50	The solvation of Cl⁻, Br⁻, and I⁻ in acetonitrile clusters: Photoelectron spectroscopy and molecular dynamics simulations. *Journal of Chemical Physics*, **1996**, 105, 2675-2685	3.9	95
49	Cube to cage transitions in (H2O)n (n=12, 16, and 20). *Journal of Chemical Physics*, **1996**, 105, 3715-3721	3.9	61
48	Electric-field induced restructuring of water at a platinum-water interface: A molecular dynamics computer simulation. *Physical Review Letters*, **1995**, 74, 3193-3196	7.4	135
47	Effect of the treatment of long-range forces on the dynamics of ions in aqueous solutions. *Journal of Chemical Physics*, **1995**, 102, 450-456	3.9	139
46	The structure of water at platinum/water interfaces Molecular dynamics computer simulations. *Surface Science*, **1995**, 335, 401-415	1.8	51
45	A smooth particle mesh Ewald method. *Journal of Chemical Physics*, **1995**, 103, 8577-8593	3.9	14532
44	The Origin of the Hydration Interaction of Lipid Bilayers from MD Simulation of Dipalmitoylphosphatidylcholine Membranes in Gel and Liquid Crystalline Phases. *Langmuir*, **1995**, 11, 4519-4531	4	110
43	Interaction Forces between Membrane Surfaces. *Advances in Chemistry Series*, **1994**, 3-25		2
42	Structures of Cl⁻(H2O)n and F⁻(H2O)n (n=2,3,...,15) clusters. Molecular dynamics computer simulations. *Journal of Chemical Physics*, **1994**, 100, 3085-3093	3.9	146
41	Enthalpies of formation and stabilization energies of Br⁻(H2O)n (n=1,2, ⁻15) clusters. Comparisons between molecular dynamics computer simulations and experiment. *Chemical Physics Letters*, **1994**, 218, 377-382	2.5	63
40	Effect of ion⁻electrode contact on the energetics of the heterogeneous electron transfer. *Chemical Physics Letters*, **1994**, 227, 561-566	2.5	34
39	Molecular dynamics simulation of a membrane/water interface: the ordering of water and its relation to the hydration force. *Langmuir*, **1993**, 9, 3122-3131	4	156
38	Free energy profiles for lithium(1+) and iodide ions approaching the platinum(100) surface: a molecular dynamics study. *The Journal of Physical Chemistry*, **1993**, 97, 13803-13806		30
37	Mobility of stretched water. *Journal of Chemical Physics*, **1993**, 98, 9859-9862	3.9	24
36	Stabilization energies of Cl⁻, Br⁻, and I⁻ ions in water clusters. *Journal of Chemical Physics*, **1993**, 99, 4222-4224	3.9	96
35	Ion solvation in water clusters. *Zeitschrift F⁻ Physik D-Atoms Molecules and Clusters*, **1993**, 26, 166-168		22
34	Solvation Dynamics in a Stockmayer Fluid **1993**, 461-483		

33	Structure and dynamics of Cl(H2O)20 clusters: The effect of the polarizability and the charge of the ion. *Journal of Chemical Physics*, **1992**, 96, 8288-8294	3.9	112
32	Dynamics of ion solvation in a Stockmayer fluid. *Journal of Chemical Physics*, **1992**, 96, 3092-3101	3.9	100
31	Ultrafast solvation dynamics in a Stockmayer fluid. *Journal of Chemical Physics*, **1992**, 97, 5253-5254	3.9	35
30	Local structural order and molecular associations in water-DMSO mixtures. Molecular dynamics study. *Journal of the American Chemical Society*, **1992**, 114, 7889-7896	16.4	276
29	A molecular dynamics study of the structure and dynamics of water between dilauroylphosphatidylethanolamine bilayers. *Langmuir*, **1992**, 8, 233-240	4	97
28	Comparison of the structure and dynamics of water at the Pt(111) and Pt(100) interfaces: molecular dynamics study. *Chemical Physics Letters*, **1991**, 177, 426-432	2.5	50
27	Liquid–vapor interface of TIP4P water: comparison between a polarizable and a nonpolarizable model. *Chemical Physics Letters*, **1991**, 176, 61-66	2.5	77
26	Structure and dynamics of water at the Pt(111) interface: Molecular dynamics study. *Journal of Chemical Physics*, **1991**, 94, 2110-2117	3.9	171
25	Computer simulation of a water/membrane interface. *Langmuir*, **1991**, 7, 1042-1044	4	55
24	Many-body effects in molecular dynamics simulations of Na+(H2O)n and Cl(H2O)n clusters. *Journal of Chemical Physics*, **1991**, 95, 1954-1963	3.9	300
23	A molecular dynamics study of the effect of temperature on the structure and dynamics of water between Pt walls. *Chemical Physics Letters*, **1989**, 162, 32-38	2.5	56
22	The dielectric constant of SPC/E water. *Chemical Physics Letters*, **1989**, 155, 173-176	2.5	145
21	Molecular hardness and softness, local hardness and softness, hardness and softness kernels, and relations among these quantities. *Journal of Chemical Physics*, **1988**, 88, 2554-2557	3.9	354
20	Temperature dependence of conductance of the Li+, Cs+, and Cl− ions in water: Molecular dynamics simulation. *Journal of Chemical Physics*, **1988**, 88, 7104-7110	3.9	32
19	Density functional approach to frontier controlled reactions. *Journal of the American Chemical Society*, **1987**, 109, 4823-4825	16.4	122
18	Structure and dynamics of high-pressure TIP4P water. *Journal of Chemical Physics*, **1987**, 87, 6682-6686	3.9	58
17	The limiting ionic conductivity of Na+ and Cl− ions in aqueous solutions: Molecular dynamics simulation. *Journal of Chemical Physics*, **1987**, 86, 376-382	3.9	75
16	Exponential approximation for the density matrix and the Wigner distribution. *Chemical Physics Letters*, **1986**, 129, 486-488	2.5	51

15	Solvation structure of a sodium chloride ion pair in water. *Journal of the American Chemical Society*, **1986**, 108, 1755-1761	16.4	102
14	Molecular dynamics simulations of tips2 water restricted by a spherical hydrophobic boundary. *Chemical Physics Letters*, **1985**, 113, 278-282	2.5	57
13	A classical fluid-like approach to the density-functional formalism of many-electron systems. *Journal of Chemical Physics*, **1985**, 83, 2976-2983	3.9	175
12	On the concept of local hardness in chemistry. *Journal of the American Chemical Society*, **1985**, 107, 6811-6814	16.4	270
11	Sodium chloride ion pair interaction in water: computer simulation. *Chemical Physics Letters*, **1984**, 105, 577-580	2.5	129
10	Transcription of ground-state density-functional theory into a local thermodynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **1984**, 81, 8028-31	11.5	198
9	Generalized Langevin dynamics simulations with arbitrary time-dependent memory kernels. *Journal of Chemical Physics*, **1983**, 78, 3256-3261	3.9	62
8	Diffusion-controlled reactions: A variational formula for the optimum reaction coordinate. *Journal of Chemical Physics*, **1983**, 79, 5563-5565	3.9	100
7	Molecular dynamics with stochastic boundary conditions. *Chemical Physics Letters*, **1982**, 90, 215-217	2.5	167
6	Memory kernels from molecular dynamics. *Journal of Chemical Physics*, **1981**, 75, 2462-2463	3.9	31
5	Theory of vibrational relaxation in solids: The competition between local phonon and roton receiving modes. *Chemical Physics*, **1979**, 37, 369-388	2.3	58
4	Role of Rotational and Translational Local Modes in Vibrational Relaxation in Solids: A Study of NH and ND in Solid Ar. *Physical Review Letters*, **1977**, 39, 1000-1004	7.4	50
3	Vibrational relaxation of molecules in solids: The role of rotational and of translational local modes. *Chemical Physics Letters*, **1977**, 49, 260-264	2.5	49
2	A smooth particle mesh Ewald method		1
1	Molecular Detailed Simulations of Lipid Bilayers. *Reviews in Computational Chemistry*,253-286		5