Max L Berkowitz

List of Publications by Year
in descending order

139 papers	30,898 citations	17405 63 h-index	10708 138 g-index
145 all docs	145 docs citations	145 times ranked	25354 citing authors

#	Article	IF	Citations
1	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.	1.2	0
2	Molecular Simulations of Aqueous Electrolytes: Role of Explicit Inclusion of Charge Transfer into Force Fields. Journal of Physical Chemistry B, 2021, 125, 13069-13076.	1.2	6
3	Damage to Polystyrene Polymer Film by Shock Wave Induced Bubble Collapse. Journal of Physical Chemistry B, 2020, 124, 7494-7499.	1.2	9
4	Enhanced Cavitation and Hydration Crossover of Stretched Water in the Presence of C₆₀. Journal of Physical Chemistry Letters, 2019, 10, 6621-6625.	2.1	1
5	Bubbles in water under stretch-induced cavitation. Journal of Chemical Physics, 2019, 150, 054501.	1.2	10
6	A comparative computational study of coarse-grained and all-atom water models in shock Hugoniot states. Journal of Chemical Physics, 2018, 148, 144504.	1.2	9
7	Nanobubbles, cavitation, shock waves and traumatic brain injury. Physical Chemistry Chemical Physics, 2016, 18, 32638-32652.	1.3	37
8	Behavior of P85 and P188 Poloxamer Molecules: Computer Simulations Using United-Atom Force-Field. Journal of Physical Chemistry B, 2016, 120, 8631-8641.	1.2	14
9	Shock Wave-Induced Damage of a Protein by Void Collapse. Biophysical Journal, 2016, 110, 147-156.	0.2	22
10	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, 5823-5830.	1.2	45
11	A Molecular Look at Membranes. Current Topics in Membranes, 2016, 77, 1-25.	0.5	3
12	Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer. Journal of Chemical Physics, 2015, 143, 241101.	1.2	53
13	Mechanism of Membrane Poration by Shock Wave Induced Nanobubble Collapse: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 6225-6234.	1.2	67
14	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, 8879-8889.	1.2	28
15	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, 1296-1301.	1.7	40
16	Shock wave interaction with a phospholipid membrane: Coarse-grained computer simulations. Journal of Chemical Physics, 2014, 140, 054906.	1.2	40
17	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, 12673-12679.	1.2	11
18	Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. Journal of Physical Chemistry Letters, 2014, 5, 2711-2716.	2.1	46

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19	Melittin Creates Transient Pores in a Lipid Bilayer: Results from Computer Simulations. Journal of Physical Chemistry B, 2013, 117, 5031-5042.	1.2	58
20	Free Energy Barrier for Melittin Reorientation from a Membrane-Bound State to a Transmembrane State. Journal of Physical Chemistry B, 2013, 117, 13457-13463.	1.2	45
21	Restructuring of a Model Hydrophobic Surface: Monte Carlo Simulations Using a Simple Coarse-Grained Model. Journal of Physical Chemistry B, 2013, 117, 15584-15590.	1.2	1
22	Aqueous Solutions at the Interface with Phospholipid Bilayers. Accounts of Chemical Research, 2012, 45, 74-82.	7.6	100
23	Binding and reorientation of melittin in a POPC bilayer: Computer simulations. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 2975-2981.	1.4	56
24	Resolving the structure of a model hydrophobic surface: DODAB monolayers on mica. RSC Advances, 2012, 2, 4181.	1.7	10
25	Molecular dynamics simulation study of the water-mediated interaction between zwitterionic and charged surfaces. Journal of Chemical Physics, 2012, 136, 024501.	1.2	10
26	Difference between Magainin-2 and Melittin Assemblies in Phosphatidylcholine Bilayers: Results from Coarse-Grained Simulations. Journal of Physical Chemistry B, 2012, 116, 3021-3030.	1.2	81
27	Molecular Dynamics Simulation Study of Interaction between Model Rough Hydrophobic Surfaces. Journal of Physical Chemistry A, 2011, 115, 6059-6067.	1.1	13
28	Role of water in atomic resolution AFM in solutions. Physical Chemistry Chemical Physics, 2011, 13, 12584.	1.3	54
29	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, 2258-2266.	1.4	36
30	Restructuring of Hydrophobic Surfaces Created by Surfactant Adsorption to Mica Surfaces. Langmuir, 2011, 27, 11737-11741.	1.6	22
31	A molecular dynamics study of the early stages of amyloidâ€Î²(1â€“42) oligomerization: The role of lipid membranes. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2533-2545.	1.5	52
32	Thermodynamic and Hydrogen-Bonding Analyses of the Interaction between Model Lipid Bilayers. Journal of Physical Chemistry B, 2010, 114, 3013-3019.	1.2	20
33	Fluctuations in Number of Water Molecules Confined between Nanoparticles. Journal of Physical Chemistry B, 2010, 114, 13410-13414.	1.2	30
34	Mechanism of Interaction of Monovalent Ions with Phosphatidylcholine Lipid Membranes. Journal of Physical Chemistry B, 2010, 114, 9504-9509.	1.2	89
35	Effects of Alkali Cations and Halide Anions on the DOPC Lipid Membrane. Journal of Physical Chemistry A, 2009, 113, 7235-7243.	1.1	144
36	Origin of the Hydration Force: Water-Mediated Interaction between Two Hydrophilic Plates. Journal of Physical Chemistry B, 2009, 113, 13222-13228.	1.2	47

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37	Orientational Dynamics of Water in Phospholipid Bilayers with Different Hydration Levels. Journal of Physical Chemistry B, 2009, 113, 7676-7680.	1.2	57
38	Structure of the Amyloid-Î² (1â˜'42) Monomer Absorbed To Model Phospholipid Bilayers: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2009, 113, 14480-14486.	1.2	75
39	Detailed molecular dynamics simulations of model biological membranes containing cholesterol. Biochimica Et Biophysica Acta - Biomembranes, 2009, 1788, 86-96.	1.4	149
40	Interaction Between Amyloid-Î² (1â€"42) Peptide and Phospholipid Bilayers: A Molecular Dynamics Study. Biophysical Journal, 2009, 96, 785-797.	0.2	108
41	Molecular Model of a Cell Plasma Membrane With an Asymmetric Multicomponent Composition: Water Permeation and Ion Effects. Biophysical Journal, 2009, 96, 4493-4501.	0.2	75
42	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.	0.5	1
43	Hydronium and hydroxide at the interface between water and hydrophobic media. Physical Chemistry Chemical Physics, 2008, 10, 4975.	1.3	68
44	Energetics of Cholesterol Transfer between Lipid Bilayers. Journal of Physical Chemistry B, 2008, 112, 3807-3811.	1.2	62
45	Molecular Dynamics Simulations of Bilayers Containing Mixtures of Sphingomyelin with Cholesterol and Phosphatidylcholine with Cholesterol. Journal of Physical Chemistry B, 2007, 111, 12888-12897.	1.2	57
46	Molecular Dynamics Simulations of SOPS and Sphingomyelin Bilayers Containing Cholesterol. Biophysical Journal, 2007, 92, 1284-1295.	0.2	47
47	Aqueous Solutions next to Phospholipid Membrane Surfaces:â€‰ Insights from Simulations. Chemical Reviews, 2006, 106, 1527-1539.	23.0	238
48	The effect of water structure and surface charge correlations on the hydration force acting between model hydrophilic surfaces. Molecular Physics, 2006, 104, 3607-3617.	0.8	9
49	The behavior of reorientational correlation functions of water at the water-lipid bilayer interface. Journal of Chemical Physics, 2006, 125, 094713.	1.2	42
50	Hydration force between model hydrophilic surfaces: Computer simulations. Journal of Chemical Physics, 2006, 124, 101101.	1.2	50
51	Structure and dynamics of water at the interface with phospholipid bilayers. Journal of Chemical Physics, 2005, 123, 224702.	1.2	122
52	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, 21725-21731.	1.2	14
53	Computer Simulation Studies of Water States in Perfluoro Polyether Reverse Micelles:Â Effects of Changing the Counterionâ€. Journal of Physical Chemistry A, 2004, 108, 9768-9776.	1.1	49
54	Exterior Site Occupancy Infers Chloride-Induced Proton Gating in a Prokaryotic Homolog of the ClC Chloride Channel. Biophysical Journal, 2004, 87, 1686-1696.	0.2	54

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55	Molecular Dynamics Simulation of a Reverse Micelle Self Assembly in Supercritical CO2. Journal of the American Chemical Society, 2004, 126, 10254-10255.	6.6	44
56	Complexation of Phosphatidylcholine Lipids with Cholesterol. Biophysical Journal, 2004, 86, 1345-1356.	0.2	143
57	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.	1.2	58
58	Water structure and dynamics in phosphate fluorosurfactant based reverse micelle: A computer simulation study. Journal of Chemical Physics, 2003, 118, 1937-1944.	1.2	91
59	The Implementation of Slab Geometry for Membrane-Channel Molecular Dynamics Simulations. Biophysical Journal, 2003, 85, 97-107.	0.2	76
60	Mixed Bilayer Containing Dipalmitoylphosphatidylcholine and Dipalmitoylphosphatidylserine: Lipid Complexation, Ion Binding, and Electrostatics. Biophysical Journal, 2003, 85, 3120-3131.	0.2	148
61	Molecular Dynamics Simulation of a Dipalmitoylphosphatidylcholine Bilayer with NaCl. Biophysical Journal, 2003, 84, 3743-3750.	0.2	226
62	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.	1.2	90
63	Monte Carlo simulation of homopolymer chains. I. Second virial coefficient. Journal of Chemical Physics, 2003, 118, 4721-4732.	1.2	30
64	Molecular Dynamics Simulations of Sodium Dodecyl Sulfate Micelle in Water:â€‰ The Behavior of Water. Journal of Physical Chemistry B, 2002, 106, 10902-10907.	1.2	173
65	Structure of Phosphate Fluorosurfactant Based Reverse Micelles in Supercritical Carbon Dioxide. Langmuir, 2002, 18, 7371-7376.	1.6	78
66	Molecular Dynamics Simulation of Sodium Dodecyl Sulfate Micelle in Water:Â Micellar Structural Characteristics and Counterion Distribution. Journal of Physical Chemistry B, 2002, 106, 3788-3793.	1.2	334
67	Molecular Dynamics Simulation of Dipalmitoylphosphatidylserine Bilayer with Na+ Counterions. Biophysical Journal, 2002, 82, 1818-1827.	0.2	145
68	Molecular Dynamics Simulation of the Structure of Dimyristoylphosphatidylcholine Bilayers with Cholesterol, Ergosterol, and Lanosterol. Biophysical Journal, 2001, 80, 1649-1658.	0.2	129
69	Computer Simulation Study of the Interface Width of the Liquid/Liquid Interface. Physical Review Letters, 2001, 87, 176101.	2.9	128
70	Effects of oxygenated sterol on phospholipid bilayer properties: a molecular dynamics simulation. Chemistry and Physics of Lipids, 2001, 112, 31-39.	1.5	39
71	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.	1.2	33
72	Molecular Dynamics Simulation of Dipalmitoylphosphatidylcholine Membrane with Cholesterol Sulfate. Biophysical Journal, 2000, 78, 1672-1680.	0.2	62

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73	Computer Simulations of Sodium Dodecyl Sulfate at Liquid/Liquid and Liquid/Vapor Interfaces. Journal of Physical Chemistry B, 2000, 104, 5302-5308.	1.2	118
74	Dielectric constant of water at high electric fields: Molecular dynamics study. Journal of Chemical Physics, 1999, 110, 7935-7942.	1.2	183
75	Molecular dynamics simulation of fluorination effects on a phospholipid bilayer. Journal of Chemical Physics, 1999, 111, 9864-9870.	1.2	47
76	Aqueous solution near charged Ag(111) surfaces: comparison between a computer simulation and experiment. Chemical Physics Letters, 1999, 301, 81-86.	1.2	36
77	United atom force field for phospholipid membranes: Constant pressure molecular dynamics simulation of dipalmitoylphosphatidicholine/water system. Journal of Computational Chemistry, 1999, 20, 531-545.	1.5	136
78	Ewald summation for systems with slab geometry. Journal of Chemical Physics, 1999, 111, 3155-3162.	1.2	1,157
79	Structure of Dipalmitoylphosphatidylcholine/Cholesterol Bilayer at Low and High Cholesterol Concentrations: Molecular Dynamics Simulation. Biophysical Journal, 1999, 77, 2075-2089.	0.2	271
80	Dynamical Properties of Phospholipid Bilayers from Computer Simulation. Biophysical Journal, 1999, 76, 2081-2089.	0.2	120
81	Molecular Dynamics Simulation of DPPC Bilayer in DMSO. Biophysical Journal, 1999, 76, 2472-2478.	0.2	79
82	Molecular and Atomic Dipole Moments in Heteronuclear and Homonuclear Diatomics. Density Functional Approach. Journal of Physical Chemistry A, 1998, 102, 4808-4812.	1.1	9
83	Molecular polarizability and atomic properties: Density functional approach. Journal of Chemical Physics, 1998, 109, 10142-10147.	1.2	8
84	Structure and Dynamics of Water in the Presence of Charged Surfactant Monolayers at the Waterâ^'CCl4 Interface. A Molecular Dynamics Study. Journal of Physical Chemistry B, 1997, 101, 10775-10780.	1.2	59
85	Chemical Potential Equalization Principle:Â Direct Approach from Density Functional Theory. Journal of Physical Chemistry A, 1997, 101, 5687-5691.	1.1	93
86	Simulation of Sodium Dodecyl Sulfate at the Waterâ^'Vapor and Waterâ^'Carbon Tetrachloride Interfaces at Low Surface Coverage. Journal of Physical Chemistry B, 1997, 101, 3793-3799.	1.2	201
87	Photodetachment spectra of Clâ^'(H2O)n clusters. Predictions and comparisons. Chemical Physics Letters, 1997, 264, 31-38.	1.2	54
88	Role of Water in the Hydration Force Acting between Lipid Bilayers. Langmuir, 1996, 12, 2625-2629.	1.6	71
89	Molecular Dynamics Study of Water next to Electrified Ag(111) Surfaces. Langmuir, 1996, 12, 3747-3752.	1.6	55
90	The solvation of Clâ^', Brâ^', and Iâ^' in acetonitrile clusters: Photoelectron spectroscopy and molecular dynamics simulations. Journal of Chemical Physics, 1996, 105, 2675-2685.	1.2	103

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91	Cube to cage transitions in (H2O)n (n=12, 16, and 20). Journal of Chemical Physics, 1996, 105, 3715-3721.	1.2	63
92	Thermally Induced Structural Changes in F-(H2O)11and Cl-(H2O)11Clusters:Â Molecular Dynamics Computer Simulations. The Journal of Physical Chemistry, 1996, 100, 1350-1356.	2.9	39
93	Electric-Field Induced Restructuring of Water at a Platinum-Water Interface: A Molecular Dynamics Computer Simulation. Physical Review Letters, 1995, 74, 3193-3196.	2.9	149
94	Effect of the treatment of longâ€range forces on the dynamics of ions in aqueous solutions. Journal of Chemical Physics, 1995, 102, 450-456.	1.2	148
95	The structure of water at platinum/water interfaces Molecular dynamics computer simulations. Surface Science, 1995, 335, 401-415.	0.8	54
96	A smooth particle mesh Ewald method. Journal of Chemical Physics, 1995, 103, 8577-8593.	1.2	18,266
97	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.	1.6	117
98	Interaction Forces between Membrane Surfaces. Advances in Chemistry Series, 1994, , 3-25.	0.6	3
99	Structures of Clâ¯(H2O)n and Fâ¯(H2O)n (n=2,3,...,15) clusters. Molecular dynamics computer simulations. Journal of Chemical Physics, 1994, 100, 3085-3093.	1.2	154
100	Enthalpies of formation and stabilization energies of Brâ¯ (H2O)n (n=1,2, â€¦, 15) clusters. Comparisons between molecular dynamics computer simulations and experiment. Chemical Physics Letters, 1994, 218, 377-382.	1.2	65
101	Effect of ionâ€"electrode contact on the energetics of the heterogeneous electron transfer. Chemical Physics Letters, 1994, 227, 561-566.	1.2	35
102	Ion solvation in water clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 166-168.	1.0	22
103	Molecular dynamics simulation of a membrane/water interface: the ordering of water and its relation to the hydration force. Langmuir, 1993, 9, 3122-3131.	1.6	172
104	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.	2.9	33
105	Mobility of stretched water. Journal of Chemical Physics, 1993, 98, 9859-9862.	1.2	25
106	Stabilization energies of Clâ¯, Brâ¯, and Iâ¯ ions in water clusters. Journal of Chemical Physics, 1993, 99, 4222-4224.	1.2	100
107	Solvation Dynamics in a Stockmayer Fluid. , 1993, , 461-483.		0
108	Structure and dynamics of Clâ¯(H2O)20 clusters: The effect of the polarizability and the charge of the ion. Journal of Chemical Physics, 1992, 96, 8288-8294.	1.2	118

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109	Dynamics of ion solvation in a Stockmayer fluid. Journal of Chemical Physics, 1992, 96, 3092-3101.	1.2	104
110	Ultrafast solvation dynamics in a Stockmayer fluid. Journal of Chemical Physics, 1992, 97, 5253-5254.	1.2	35
111	Local structural order and molecular associations in water-DMSO mixtures. Molecular dynamics study. Journal of the American Chemical Society, 1992, 114, 7889-7896.	6.6	298
112	A molecular dynamics study of the structure and dynamics of water between dilauroylphosphatidylethanolamine bilayers. Langmuir, 1992, 8, 233-240.	1.6	106
113	Structure and dynamics of water at the Pt(111) interface: Molecular dynamics study. Journal of Chemical Physics, 1991, 94, 2110-2117.	1.2	179
114	Computer simulation of a water/membrane interface. Langmuir, 1991, 7, 1042-1044.	1.6	58
115	Manyâ€body effects in molecular dynamics simulations of Na+(H2O)n and Clâ^'(H2O)n clusters. Journal of Chemical Physics, 1991, 95, 1954-1963.	1.2	322
116	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.	1.2	55
117	Liquidâ€"vapor interface of TIP4P water: comparison between a polarizable and a nonpolarizable model. Chemical Physics Letters, 1991, 176, 61-66.	1.2	79
118	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.	1.2	58
119	The dielectric constant of SPC/E water. Chemical Physics Letters, 1989, 155, 173-176.	1.2	164
120	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.	1.2	397
121	Temperature dependence of conductance of the Li+, Cs+, and Clâ^'ions in water: Molecular dynamics simulation. Journal of Chemical Physics, 1988, 88, 7104-7110.	1.2	33
122	Density functional approach to frontier controlled reactions. Journal of the American Chemical Society, 1987, 109, 4823-4825.	6.6	144
123	Structure and dynamics of highâ€pressure TIP4P water. Journal of Chemical Physics, 1987, 87, 6682-6686.	1.2	58
124	The limiting ionic conductivity of Na+and Clâ^'ions in aqueous solutions: Molecular dynamics simulation. Journal of Chemical Physics, 1987, 86, 376-382.	1.2	88
125	Solvation structure of a sodium chloride ion pair in water. Journal of the American Chemical Society, 1986, 108, 1755-1761.	6.6	108
126	Exponential approximation for the density matrix and the Wigner's distribution. Chemical Physics Letters, 1986, 129, 486-488.	1.2	58

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127	Molecular dynamics simulations of tips2 water restricted by a spherical hydrophobic boundary. Chemical Physics Letters, 1985, 113, 278-282.	1.2	65
128	A classical fluidâ€like approach to the densityâ€functional formalism of manyâ€electron systems. Journal of Chemical Physics, 1985, 83, 2976-2983.	1.2	191
129	On the concept of local hardness in chemistry. Journal of the American Chemical Society, 1985, 107, 6811-6814.	6.6	307
130	Sodium chloride ion pair interaction in water: computer simulation. Chemical Physics Letters, 1984, 105, 577-580.	1.2	135
131	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, 8028-8031.	3.3	232
132	Generalized Langevin dynamics simulations with arbitrary timeâ€dependent memory kernels. Journal of Chemical Physics, 1983, 78, 3256-3261.	1.2	71
133	Diffusionâ€controlled reactions: A variational formula for the optimum reaction coordinate. Journal of Chemical Physics, 1983, 79, 5563-5565.	1.2	108
134	Molecular dynamics with stochastic boundary conditions. Chemical Physics Letters, 1982, 90, 215-217.	1.2	185
135	Memory kernels from molecular dynamics. Journal of Chemical Physics, 1981, 75, 2462-2463.	1.2	40
136	Theory of vibrational relaxation in solids: The competition between local phonon and roton receiving modes. Chemical Physics, 1979, 37, 369-388.	0.9	62
137	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.	2.9	54
138	Vibrational relaxation of molecules in solids: The role of rotational and of translational local modes. Chemical Physics Letters, 1977, 49, 260-264.	1.2	54
139	A smooth particle mesh Ewald method. , 0, .		1