Philippe H HÃ¼nenberger

List of Publications by Year
in descending order

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126 papers	10,951 citations	41344 49 h-index	32842 100 g-index
128 all docs	128 docs citations	128 times ranked	9300 citing authors

#	Article	IF	Citations
1	Simultaneous parametrization of torsional and thirdâ€neighbor interaction terms in forceâ€field development: The LLSâ€SC algorithm. Journal of Computational Chemistry, 2022, , .	3.3	1
2	RestraintMaker: a graph-based approach to select distance restraints in free-energy calculations with dual topology. Journal of Computer-Aided Molecular Design, 2022, 36, 175-192.	2.9	5
3	Replica-Exchange Enveloping Distribution Sampling Using Generalized AMBER Force-Field Topologies: Application to Relative Hydration Free-Energy Calculations for Large Sets of Molecules. Journal of Chemical Information and Modeling, 2022, 62, 3043-3056.	5.4	5
4	The Role of Surface Chemistry in the Orientational Behavior of Water at an Interface. Journal of Physical Chemistry B, 2022, 126, 4697-4710.	2.6	3
5	Evaluation of nine condensed-phase force fields of the GROMOS, CHARMM, OPLS, AMBER, and OpenFF families against experimental cross-solvation free energies. Physical Chemistry Chemical Physics, 2021, 23, 13055-13074.	2.8	9
6	Systematic optimization of a fragment-based force field against experimental pure-liquid properties considering large compound families: application to oxygen and nitrogen compounds. Physical Chemistry Chemical Physics, 2021, 23, 17774-17793.	2.8	9
7	Solvent-scaling as an alternative to coarse-graining in adaptive-resolution simulations: The adaptive solvent-scaling (AdSoS) scheme. Journal of Chemical Physics, 2021, 155, 094107.	3.0	2
8	Efficient Alchemical Intermediate States in Free Energy Calculations Using Î»-Enveloping Distribution Sampling. Journal of Chemical Theory and Computation, 2021, 17, 5805-5815.	5.3	8
9	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bioâ€Molecular Systems: Overview and Perspective on Issues. ChemPhysChem, 2021, 22, 264-282.	2.1	12
10	Reaction-field electrostatics in molecular dynamics simulations: development of a conservative scheme compatible with an atomic cutoff. Physical Chemistry Chemical Physics, 2020, 22, 26419-26437.	2.8	16
11	Systematic Optimization of a Fragment-Based Force Field against Experimental Pure-Liquid Properties Considering Large Compound Families: Application to Saturated Haloalkanes. Journal of Chemical Theory and Computation, 2020, 16, 7525-7555.	5.3	21
12	An Alternative to Conventional Î»-Intermediate States in Alchemical Free Energy Calculations: Î»-Enveloping Distribution Sampling. Journal of Chemical Information and Modeling, 2020, 60, 5407-5423.	5.4	18
13	Evaluating Classical Force Fields against Experimental Cross-Solvation Free Energies. Journal of Chemical Theory and Computation, 2020, 16, 7556-7580.	5.3	28
14	The Conveyor Belt Umbrella Sampling (CBUS) Scheme: Principle and Application to the Calculation of the Absolute Binding Free Energies of Alkali Cations to Crown Ethers. Journal of Chemical Theory and Computation, 2020, 16, 2474-2493.	5.3	1
15	Interfacial solvation can explain attraction between like-charged objects in aqueous solution. Journal of Chemical Physics, 2020, 152, 104713.	3.0	17
16	Overcoming Orthogonal Barriers in Alchemical Free Energy Calculations: On the Relative Merits of Î»-Variations, Î»-Extrapolations, and Biasing. Journal of Chemical Theory and Computation, 2020, 16, 1630-1645.	5.3	20
17	Influence of the Treatment of Nonbonded Interactions on the Thermodynamic and Transport Properties of Pure Liquids Calculated Using the 2016H66 Force Field. Journal of Chemical Theory and Computation, 2019, 15, 1806-1826.	5.3	28
18	<scp>Vase</scp>â€<scp>Kite</scp> Equilibrium of Resorcin[4]arene Cavitands Investigated Using Molecular Dynamics Simulations with Ballâ€andâ€Stick Local Elevation Umbrella Sampling. Helvetica Chimica Acta, 2019, 102, e1900060.	1.6	3

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19	Alchemical Free-Energy Calculations by Multiple-Replica Î»-Dynamics: The Conveyor Belt Thermodynamic Integration Scheme. Journal of Chemical Theory and Computation, 2019, 15, 2392-2419.	5.3	17
20	Absolute proton hydration free energy, surface potential of water, and redox potential of the hydrogen electrode from first principles: QM/MM MD free-energy simulations of sodium and potassium hydration. Journal of Chemical Physics, 2018, 148, 222814.	3.0	71
21	Single-Ion Thermodynamics from First Principles: Calculation of the Absolute Hydration Free Energy and Single-Electrode Potential of Aqueous Li⁺ Using ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 6443-6459.	5.3	18
22	Simulating Bilayers of Nonionic Surfactants with the GROMOS-Compatible 2016H66 Force Field. Langmuir, 2017, 33, 10225-10238.	3.5	12
23	Solventâ€Modulated Influence of Intramolecular Hydrogenâ€Bonding on the Conformational Properties of the Hydroxymethyl Group in Glucose and Galactose: A Molecular Dynamics Simulation Study. Helvetica Chimica Acta, 2017, 100, e1600158.	1.6	11
24	Revision of the GROMOS 56A6_{CARBO} force field: Improving the description of ringâ€conformational equilibria in hexopyranoseâ€based carbohydrates chains. Journal of Computational Chemistry, 2016, 37, 354-365.	3.3	77
25	Origin of Asymmetric Solvation Effects for Ions in Water and Organic Solvents Investigated Using Molecular Dynamics Simulations: The Swain Acityâ€“Basity Scale Revisited. Journal of Physical Chemistry B, 2016, 120, 8485-8517.	2.6	39
26	A GROMOS-Compatible Force Field for Small Organic Molecules in the Condensed Phase: The 2016H66 Parameter Set. Journal of Chemical Theory and Computation, 2016, 12, 3825-3850.	5.3	118
27	Orthogonal sampling in free-energy calculations of residue mutations in a tripeptide: TI versusÎ»-LEUS. Journal of Computational Chemistry, 2015, 36, 1686-1697.	3.3	14
28	Phase-transition properties of glycerolâ€“dipalmitate lipid bilayers investigated using molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2015, 59, 136-147.	2.4	2
29	Flexible Boundaries for Multiresolution Solvation: An Algorithm for Spatial Multiscaling in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 5447-5463.	5.3	12
30	Multistate Î»-Local-Elevation Umbrella-Sampling (MS-Î»-LEUS): Method and Application to the Complexation of Cations by Crown Ethers. Journal of Chemical Theory and Computation, 2015, 11, 2575-2588.	5.3	14
31	On the ambiguity of conformational states: A B&S-LEUS simulation study of the helical conformations of decaalanine in water. Journal of Chemical Physics, 2015, 142, 165102.	3.0	4
32	Long-timescale motions in glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2015, 55, 48-64.	2.4	6
33	Effect of methanol on the phase-transition properties of glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulations: In quest of the biphasic effect. Journal of Molecular Graphics and Modelling, 2015, 55, 85-104.	2.4	8
34	Effect of the cosolutes trehalose and methanol on the equilibrium and phase-transition properties of glycerol-monopalmitate lipid bilayers investigated using molecular dynamics simulations. European Biophysics Journal, 2014, 43, 517-544.	2.2	10
35	Local Elevation Umbrella Sampling Applied to the Calculation of Alchemical Free-Energy Changes via Î»-Dynamics: The Î»-LEUS Scheme. Journal of Chemical Theory and Computation, 2014, 10, 3006-3022.	5.3	23
36	Communication: Estimating the initial biasing potential for Î»-local-elevation umbrella-sampling (Î»-LEUS) simulations via slow growth. Journal of Chemical Physics, 2014, 141, 201101.	3.0	11

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37	Intramolecular hydrogen-bonding in aqueous carbohydrates as a cause or consequence of conformational preferences: a molecular dynamics study of cellobiose stereoisomers. European Biophysics Journal, 2013, 42, 521-537.	2.2	44
38	Calculating the binding free energies of charged species based on explicit-solvent simulations employing lattice-sum methods: An accurate correction scheme for electrostatic finite-size effects. Journal of Chemical Physics, 2013, 139, 184103.	3.0	187
39	Efficient Combination of Environment Change and Alchemical Perturbation within the Enveloping Distribution Sampling (EDS) Scheme: Twin-System EDS and Application to the Determination of Octanolâ€“Water Partition Coefficients. Journal of Chemical Theory and Computation, 2013, 9, 1334-1346.	5.3	14
40	Phase-transition properties of glycerol-monopalmitate lipid bilayers investigated by molecular dynamics simulation: influence of the system size and force-field parameters. Molecular Simulation, 2013, 39, 563-583.	2.0	10
41	New Interaction Parameters for Charged Amino Acid Side Chains in the GROMOS Force Field. Journal of Chemical Theory and Computation, 2012, 8, 3705-3723.	5.3	189
42	Calculation of Derivative Thermodynamic Hydration and Aqueous Partial Molar Properties of Ions Based on Atomistic Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3542-3564.	5.3	13
43	A GROMOS Parameter Set for Vicinal Diether Functions: Properties of Polyethyleneoxide and Polyethyleneglycol. Journal of Chemical Theory and Computation, 2012, 8, 3943-3963.	5.3	61
44	Wilfred van Gunsteren: 35 Years of Biomolecular Simulation. Journal of Chemical Theory and Computation, 2012, 8, 3425-3429.	5.3	1
45	Reoptimized interaction parameters for the peptideâ€backbone model compound Nâ€methylacetamide in the GROMOS force field: Influence on the folding properties of two betaâ€peptides in methanol. Journal of Computational Chemistry, 2012, 33, 1907-1917.	3.3	13
46	Temperature Dependence of the Dielectric Permittivity of Acetic Acid, Propionic Acid and Their Methyl Esters: A Molecular Dynamics Simulation Study. ChemPhysChem, 2012, 13, 1182-1190.	2.1	19
47	New functionalities in the GROMOS biomolecular simulation software. Journal of Computational Chemistry, 2012, 33, 340-353.	3.3	98
48	Enantiomeric Segregation in the Gel Phase of Lipid Bilayers. Journal of the American Chemical Society, 2011, 133, 8464-8466.	13.7	11
49	Calculation of Relative Free Energies for Ligand-Protein Binding, Solvation, and Conformational Transitions Using the GROMOS Software. Journal of Physical Chemistry B, 2011, 115, 13570-13577.	2.6	71
50	Computation of methodology-independent single-ion solvation properties from molecular simulations. III. Correction terms for the solvation free energies, enthalpies, entropies, heat capacities, volumes, compressibilities, and expansivities of solvated ions. Journal of Chemical Physics, 2011, 134, 144103.	3.0	66
51	New Interaction Parameters for Oxygen Compounds in the GROMOS Force Field: Improved Pure-Liquid and Solvation Properties for Alcohols, Ethers, Aldehydes, Ketones, Carboxylic Acids, and Esters. Journal of Chemical Theory and Computation, 2011, 7, 1016-1031.	5.3	112
52	Preferential Affinity of the Components of Liquid Mixtures at a Rigid Nonâ€Polar Surface: Enthalpic and Entropic Driving Forces. ChemPhysChem, 2011, 12, 3214-3223.	2.1	3
53	A reoptimized GROMOS force field for hexopyranoseâ€based carbohydrates accounting for the relative free energies of ring conformers, anomers, epimers, hydroxymethyl rotamers, and glycosidic linkage conformers. Journal of Computational Chemistry, 2011, 32, 998-1032.	3.3	147
54	Computation of methodology-independent single-ion solvation properties from molecular simulations. IV. Optimized Lennard-Jones interaction parameter sets for the alkali and halide ions in water. Journal of Chemical Physics, 2011, 134, 144104.	3.0	136

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55	Residual structure in a peptide fragment of the outer membrane protein X under denaturing conditions: a molecular dynamics study. European Biophysics Journal, 2010, 39, 1421-1432.	2.2	7
56	Conformational properties of glucose-based disaccharides investigated using molecular dynamics simulations with local elevation umbrella sampling. Carbohydrate Research, 2010, 345, 1781-1801.	2.3	125
57	Interaction of the disaccharides trehalose and gentiobiose with lipid bilayers: A comparative molecular dynamics study. Journal of Molecular Graphics and Modelling, 2010, 29, 331-346.	2.4	33
58	Using the local elevation method to construct optimized umbrella sampling potentials: Calculation of the relative free energies and interconversion barriers of glucopyranose ring conformers in water. Journal of Computational Chemistry, 2010, 31, 1-23.	3.3	104
59	Interaction of alginate single-chain polyguluronate segments with mono- and divalent metal cations: a comparative molecular dynamics study. Molecular Simulation, 2010, 36, 778-795.	2.0	26
60	Enhanced Conformational Sampling in Molecular Dynamics Simulations of Solvated Peptides: Fragment-Based Local Elevation Umbrella Sampling. Journal of Chemical Theory and Computation, 2010, 6, 2598-2621.	5.3	25
61	Theoretical Investigation of Solvent Effects on Glycosylation Reactions: Stereoselectivity Controlled by Preferential Conformations of the Intermediate Oxacarbenium-Counterion Complex. Journal of Chemical Theory and Computation, 2010, 6, 1783-1797.	5.3	137
62	Molecular dynamics simulations of the interaction between polyhydroxylated compounds and Lennard-Jones walls: preferential affinity/exclusion effects and their relevance for bioprotection. Molecular Simulation, 2010, 36, 708-728.	2.0	6
63	Ball-and-Stick Local Elevation Umbrella Sampling: Molecular Simulations Involving Enhanced Sampling within Conformational or Alchemical Subspaces of Low Internal Dimensionalities, Minimal Irrelevant Volumes, and Problem-Adapted Geometries. Journal of Chemical Theory and Computation, 2010, 6, 2622-2646.	5.3	29
64	Simulating the Transition between Gel and Liquid-Crystal Phases of Lipid Bilayers: Dependence of the Transition Temperature on the Hydration Level. Journal of Chemical Theory and Computation, 2010, 6, 2488-2500.	5.3	26
65	In the eye of the beholder: Inhomogeneous distribution of high-resolution shapes within the random-walk ensemble. Journal of Chemical Physics, 2009, 130, 214904.	3.0	2
66	Absolute Single-Molecule Entropies from Quasi-Harmonic Analysis of Microsecond Molecular Dynamics: Correction Terms and Convergence Properties. Journal of Chemical Theory and Computation, 2009, 5, 3150-3160.	5.3	75
67	Molecular Dynamics Simulations of a Reversibly Folding Î²-Heptapeptide in Methanol: Influence of the Treatment of Long-Range Electrostatic Interactions. Journal of Physical Chemistry B, 2009, 113, 3112-3128.	2.6	72
68	Molecular dynamics simulation of highly charged proteins: Comparison of the particle-particle particle-mesh and reaction field methods for the calculation of electrostatic interactions. Protein Science, 2009, 12, 2161-2172.	7.6	42
69	Martini Coarse-Grained Force Field: Extension to Carbohydrates. Journal of Chemical Theory and Computation, 2009, 5, 3195-3210.	5.3	363
70	Effect of Trehalose on a Phospholipid Membrane under Mechanical Stress. Biophysical Journal, 2008, 95, 3525-3534.	0.5	43
71	Carâ€“Parrinello Molecular Dynamics Simulations of CaCl₂ Aqueous Solutions. Journal of Chemical Theory and Computation, 2008, 4, 779-789.	5.3	66
72	The influence of polyhydroxylated compounds on a hydrated phospholipid bilayer: a molecular dynamics study. Molecular Simulation, 2008, 34, 403-420.	2.0	36

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73	Conformation, dynamics and ion-binding properties of single-chain polyuronates: a molecular dynamics study. Molecular Simulation, 2008, 34, 421-446.	2.0	34
74	Explicit-solvent molecular dynamics simulations of a DNA tetradecanucleotide duplex: lattice-sum versus reaction-field electrostatics. Molecular Simulation, 2008, 34, 491-499.	2.0	15
75	Explicit-Solvent Molecular Dynamics Simulations of the Polysaccharide Schizophyllan in Water. Biophysical Journal, 2007, 93, 442-455.	0.5	61
76	Molecular dynamics simulations of the native and partially folded states of ubiquitin: Influence of methanol cosolvent, pH, and temperature on the protein structure and dynamics. Protein Science, 2007, 16, 1101-1118.	7.6	51
77	On the relative stabilities of the alkali cations 222 cryptates in the gas phase and in water-methanol solution. Journal of Molecular Modeling, 2007, 13, 1017-1025.	1.8	8
78	Conformation, dynamics, solvation and relative stabilities of selected Î²-hexopyranoses in water: a molecular dynamics study with the gromos 45A4 force field. Carbohydrate Research, 2007, 342, 2097-2124.	2.3	79
79	Computation of methodology-independent ionic solvation free energies from molecular simulations. I. The electrostatic potential in molecular liquids. Journal of Chemical Physics, 2006, 124, 124106.	3.0	140
80	Computation of methodology-independent ionic solvation free energies from molecular simulations. II. The hydration free energy of the sodium cation. Journal of Chemical Physics, 2006, 124, 224501.	3.0	176
81	Development of a lattice-sum method emulating nonperiodic boundary conditions for the treatment of electrostatic interactions in molecular simulations: A continuum-electrostatics study. Journal of Chemical Physics, 2006, 124, 124108.	3.0	13
82	Comparison of Atomic-Level and Coarse-Grained Models for Liquid Hydrocarbons from Molecular Dynamics Configurational Entropy Estimates. Journal of Physical Chemistry B, 2006, 110, 8464-8473.	2.6	60
83	Conformational and Dynamical Properties of Disaccharides in Water: a Molecular Dynamics Study. Biophysical Journal, 2006, 90, 4337-4344.	0.5	97
84	The Transition between the B and Z Conformations of DNA Investigated by Targeted Molecular Dynamics Simulations with Explicit Solvation. Biophysical Journal, 2006, 91, 2976-2990.	0.5	47
85	Configurational Entropies of Lipids in Pure and Mixed Bilayers from Atomic-Level and Coarse-Grained Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 15602-15614.	2.6	58
86	Interaction of the Sugars Trehalose, Maltose and Glucose with a Phospholipid Bilayer:Â A Comparative Molecular Dynamics Study. Journal of Physical Chemistry B, 2006, 110, 15572-15581.	2.6	94
87	Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092.	13.8	503
88	A multiple time step algorithm compatible with a large number of distance classes and an arbitrary distance dependence of the time step size for the fast evaluation of nonbonded interactions in molecular simulations. Journal of Computational Chemistry, 2006, 27, 1163-1176.	3.3	7
89	Measuring 1Hâ€“1H and 1Hâ€“13C RDCs in methyl groups: example of pulse sequences with numerically optimized coherence transfer schemes. Journal of Magnetic Resonance, 2005, 172, 36-47.	2.1	3
90	An improved nucleic acid parameter set for the GROMOS force field. Journal of Computational Chemistry, 2005, 26, 725-737.	3.3	161

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91	A new GROMOS force field for hexopyranose-based carbohydrates. Journal of Computational Chemistry, 2005, 26, 1400-1412.	3.3	286
92	The GROMOS software for biomolecular simulation: GROMOS05. Journal of Computational Chemistry, 2005, 26, 1719-1751.	3.3	592
93	Combining the lattice-sum and reaction-field approaches for evaluating long-range electrostatic interactions in molecular simulations. Journal of Chemical Physics, 2005, 123, 034107.	3.0	47
94	Molecular Dynamics Simulations of Phospholipid Bilayers:â€‰ Influence of Artificial Periodicity, System Size, and Simulation Time. Journal of Physical Chemistry B, 2005, 109, 11643-11652.	2.6	66
95	Use of Molecular Dynamics in the Design and Structure Determination of a Photoinducible Î²-Hairpin. Journal of the American Chemical Society, 2005, 127, 4935-4942.	13.7	29
96	Trehalose-protein interaction in aqueous solution. Proteins: Structure, Function and Bioinformatics, 2004, 55, 177-186.	2.6	204
97	A fast pairlist-construction algorithm for molecular simulations under periodic boundary conditions. Journal of Computational Chemistry, 2004, 25, 1474-1486.	3.3	50
98	Explicit-Solvent Molecular Dynamics Simulations of the Î²(1â†'3)- and Î²(1â†'6)-Linked Disaccharides Î²-Laminarabiose and Î²-Gentiobiose in Water. Journal of Physical Chemistry B, 2004, 108, 5815-5826.	2.6	32
99	pH-Dependent Stability of a Decalysine Î±-Helix Studied by Explicit-Solvent Molecular Dynamics Simulations at Constant pH. Journal of Physical Chemistry B, 2004, 108, 13551-13559.	2.6	50
100	Influence of Artificial Periodicity and Ionic Strength in Molecular Dynamics Simulations of Charged Biomolecules Employing Lattice-Sum Methods. Journal of Physical Chemistry B, 2004, 108, 774-788.	2.6	121
101	Interaction of the Disaccharide Trehalose with a Phospholipid Bilayer: A Molecular Dynamics Study. Biophysical Journal, 2004, 86, 2273-2285.	0.5	156
102	Influence of cut-off truncation and artificial periodicity of electrostatic interactions in molecular simulations of solvated ions: A continuum electrostatics study. Journal of Chemical Physics, 2003, 119, 9129-9144.	3.0	67
103	A fast-Fourier transform method to solve continuum-electrostatics problems with truncated electrostatic interactions: Algorithm and application to ionic solvation and ionâ€“ion interaction. Journal of Chemical Physics, 2003, 119, 12205-12223.	3.0	32
104	Effect of mutations involving charged residues on the stability of staphylococcal nuclease: a continuum electrostatics study. Protein Engineering, Design and Selection, 2003, 16, 831-840.	2.1	8
105	Calculation of the group-based pressure in molecular simulations. II. Numerical tests and application to liquid water. Journal of Chemical Physics, 2002, 116, 6898-6909.	3.0	11
106	Solving the Poisson equation for soluteâ€“solvent systems using fast Fourier transforms. Journal of Chemical Physics, 2002, 116, 7434-7451.	3.0	26
107	Calculation of the group-based pressure in molecular simulations. I. A general formulation including Ewald and particle-particleâ€“particle-mesh electrostatics. Journal of Chemical Physics, 2002, 116, 6880-6897.	3.0	45
108	Molecular dynamics simulations of a double unit cell in a protein crystal: Volume relaxation at constant pressure and correlation of motions between the two unit cells. Proteins: Structure, Function and Bioinformatics, 2002, 48, 327-340.	2.6	23

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109	Comparison of four methods to compute the dielectric permittivity of liquids from molecular dynamics simulations. Journal of Chemical Physics, 2001, 115, 1125-1136.	3.0	327
110	Explicit-solvent molecular dynamics simulation at constant pH: Methodology and application to small amines. Journal of Chemical Physics, 2001, 114, 9706-9719.	3.0	114
111	Computational Analysis of PKAâˆ'Balanol Interactions. Journal of Medicinal Chemistry, 2001, 44, 1530-1539.	6.4	33
112	Comparison of different schemes to treat long-range electrostatic interactions in molecular dynamics simulations of a protein crystal. Proteins: Structure, Function and Bioinformatics, 2001, 43, 509-519.	2.6	51
113	A fast SHAKE algorithm to solve distance constraint equations for small molecules in molecular dynamics simulations. Journal of Computational Chemistry, 2001, 22, 501-508.	3.3	959
114	Molecular Dynamics Simulations of a Polyalanine Octapeptide under Ewald Boundary Conditions:Â Influence of Artificial Periodicity on Peptide Conformation. Journal of Physical Chemistry B, 2000, 104, 3668-3675.	2.6	274
115	Optimal charge-shaping functions for the particleâ€"particleâ€"particleâ€"mesh (P3M) method for computing electrostatic interactions in molecular simulations. Journal of Chemical Physics, 2000, 113, 10464-10476.	3.0	69
116	Polarization around an ion in a dielectric continuum with truncated electrostatic interactions. Journal of Chemical Physics, 1999, 110, 10679-10692.	3.0	34
117	Ewald artifacts in computer simulations of ionic solvation and ionâ€"ion interaction: A continuum electrostatics study. Journal of Chemical Physics, 1999, 110, 1856-1872.	3.0	325
118	The GROMOS Biomolecular Simulation Program Package. Journal of Physical Chemistry A, 1999, 103, 3596-3607.	2.5	1,354
119	Determinants of Ligand Binding to cAMP-Dependent Protein Kinaseâ€. Biochemistry, 1999, 38, 2358-2366.	2.5	83
120	Molecular dynamics simulations of the hyperthermophilic protein sac7d from Sulfolobus acidocaldarius : contribution of salt bridges to thermostability 1 1Edited by B. Honig. Journal of Molecular Biology, 1999, 285, 1811-1830.	4.2	108
121	Lattice-sum methods for computing electrostatic interactions in molecular simulations. , 1999, , .		36
122	Empirical Classical Force Fields for Molecular Systems. Lecture Notes in Quantum Chemistry II, 1999, , 177-214.	0.3	7
123	Alternative schemes for the inclusion of a reaction-field correction into molecular dynamics simulations: Influence on the simulated energetic, structural, and dielectric properties of liquid water. Journal of Chemical Physics, 1998, 108, 6117-6134.	3.0	122
124	Experimental and Theoretical Approach to Hydrogen-Bonded Diastereomeric Interactions in a Model Complex. Journal of the American Chemical Society, 1997, 119, 7533-7544.	13.7	29
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126	Thermostat Algorithms for Molecular Dynamics Simulations. Advances in Polymer Science, 0, , 105-149.	0.8	394