Alexander P Lyubartsev

List of Publications by Year
in descending order

174	10,286	34105	37204
papers	citations	52 h-index	96 g-index

180	180	180	8405
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	New approach to Monte Carlo calculation of the free energy: Method of expanded ensembles. Journal of Chemical Physics, 1992, 96, 1776-1783.	3.0	935
2	Calculation of effective interaction potentials from radial distribution functions: A reverse Monte Carlo approach. Physical Review E, 1995, 52, 3730-3737.	2.1	716
3	The inhomogeneous structure of water at ambient conditions. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15214-15218.	7.1	526
4	Derivation and Systematic Validation of a Refined All-Atom Force Field for Phosphatidylcholine Lipids. Journal of Physical Chemistry B, 2012, 116, 3164-3179.	2.6	486
5	An Extension and Further Validation of an All-Atomistic Force Field for Biological Membranes. Journal of Chemical Theory and Computation, 2012, 8, 2938-2948.	5.3	408
6	M.DynaMix â€“ a scalable portable parallel MD simulation package for arbitrary molecular mixtures. Computer Physics Communications, 2000, 128, 565-589.	7.5	374
7	Concentration Effects in Aqueous NaCl Solutions. A Molecular Dynamics Simulation. The Journal of Physical Chemistry, 1996, 100, 16410-16418.	2.9	256
8	Another Piece of the Membrane Puzzle: Extending Slipids Further. Journal of Chemical Theory and Computation, 2013, 9, 774-784.	5.3	237
9	Molecular Dynamics Simulations of Dimethyl Sulfoxide and Dimethyl Sulfoxideâ^'Water Mixture. Journal of Physical Chemistry A, 2001, 105, 1702-1710.	2.5	197
10	Hydration of Li+ ion. An ab initio molecular dynamics simulation. Journal of Chemical Physics, 2001, 114, 3120-3126.	3.0	195
11	Multiscale modeling of lipids and lipid bilayers. European Biophysics Journal, 2005, 35, 53-61.	2.2	146
12	Systematic coarse-graining of molecular models by the Newton inversion method. Faraday Discussions, 2010, 144, 43-56.	3.2	139
13	Theoretical approximations to X-ray absorption spectroscopy of liquid water and ice. Journal of Electron Spectroscopy and Related Phenomena, 2010, 177, 135-157.	1.7	132
14	Recent development in computer simulations of lipid bilayers. Soft Matter, 2011, 7, 25-39.	2.7	132
15	Osmotic and activity coefficients from effective potentials for hydrated ions. Physical Review E, 1997, 55, 5689-5696.	2.1	127
16	New six-site acetonitrile model for simulations of liquid acetonitrile and its aqueous mixtures. Journal of Computational Chemistry, 2007, 28, 2020-2026.	3.3	124
17	On the Competition between Water, Sodium Ions, and Spermine in Binding to DNA: A Molecular Dynamics Computer Simulation Study. Biophysical Journal, 2002, 82, 2860-2875.	0.5	118
18	Toward Atomistic Resolution Structure of Phosphatidylcholine Headgroup and Glycerol Backbone at Different Ambient Conditions. Journal of Physical Chemistry B, 2015, 119, 15075-15088.	2.6	109

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19	Competitive Binding of Mg2+, Ca2+, Na+, and K+ Ions to DNA in Oriented DNA Fibers: Experimental and Monte Carlo Simulation Results. Biophysical Journal, 1999, 77, 2736-2749.	0.5	108
20	Monte Carlo Simulation Study of Ion Distribution and Osmotic Pressure in Hexagonally Oriented DNA. The Journal of Physical Chemistry, 1995, 99, 10373-10382.	2.9	103
21	Exploring the Free Energy Landscape of Solutes Embedded in Lipid Bilayers. Journal of Physical Chemistry Letters, 2013, 4, 1781-1787.	4.6	103
22	Computer Simulation Study oftert-Butyl Alcohol. 2. Structure in Aqueous Solution. Journal of Physical Chemistry B, 2000, 104, 9533-9539.	2.6	94
23	A Molecular Dynamics Investigation of the Influence of Hydration and Temperature on Structural and Dynamical Properties of a Dimyristoylphosphatidylcholine Bilayer. Journal of Physical Chemistry B, 2006, 110, 14326-14336.	2.6	92
24	Monte Carlo Simulation Study of DNA Polyelectrolyte Properties in the Presence of Multivalent Polyamine Ions. Journal of Physical Chemistry B, 1997, 101, 4335-4342.	2.6	86
25	Structural Evidence for the Ordered Crystallites of Ionic Liquid in Confined Carbon Nanotubes. Journal of Physical Chemistry C, 2009, 113, 10013-10020.	3.1	82
26	Molecular Dynamics Simulations of DNA in Solution with Different Counter-ions. Journal of Biomolecular Structure and Dynamics, 1998, 16, 579-592.	3.5	81
27	Effective potentials for ionâ€“DNA interactions. Journal of Chemical Physics, 1999, 111, 11207-11215.	3.0	81
28	Electrostatically Induced Polyelectrolyte Association of Rodlike Virus Particles. Physical Review Letters, 1998, 81, 5465-5468.	7.8	80
29	Force Field Development for Lipid Membrane Simulations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2483-2497.	2.6	80
30	Spermine: an â€œinvisibleâ€•component in the crystals of B-DNA. A grand canonical Monte Carlo and molecular dynamics simulation study. Journal of Molecular Biology, 2001, 308, 907-917.	4.2	78
31	On Coarse-Graining by the Inverse Monte Carlo Method: Dissipative Particle Dynamics Simulations Made to a Precise Tool in Soft Matter Modeling. Soft Materials, 2002, 1, 121-137.	1.7	78
32	Molecular Dynamics Simulations of Adsorption of Amino Acid Side Chain Analogues and a Titanium Binding Peptide on the TiO₂ (100) Surface. Journal of Physical Chemistry C, 2015, 119, 18126-18139.	3.1	77
33	Temperature and Concentration Effects on Li+-Ion Hydration. A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2003, 107, 3234-3242.	2.6	76
34	Effect of Local Anesthetic Lidocaine on Electrostatic Properties of a Lipid Bilayer. Biophysical Journal, 2008, 94, 525-531.	0.5	76
35	The polyelectrolyte properties of chromatin. Soft Matter, 2012, 8, 9322.	2.7	76
36	A molecular dynamics simulation study of oriented DNA with polyamine and sodium counterions: diffusion and averaged binding of water and cations. Nucleic Acids Research, 2003, 31, 5971-5981.	14.5	75

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37	Effective macroion-macroion potentials in asymmetric electrolytes. Physical Review E, 2001, 63, 020401.	2.1	71
38	Molecular dynamics simulations of local anesthetic articaine in a lipid bilayer. Biophysical Chemistry, 2010, 153, 27-35.	2.8	69
39	Metal Ion-Induced Lateral Aggregation of Filamentous Viruses fd and M13. Biophysical Journal, 2002, 83, 566-581.	0.5	68
40	Computer Modeling Demonstrates that Electrostatic Attraction of Nucleosomal DNA is Mediated by Histone Tails. Biophysical Journal, 2006, 90, 4305-4316.	0.5	67
41	Solubility of Organic Compounds in Water/Octanol Systems. A Expanded Ensemble Molecular Dynamics Simulation Study of logPParameters. Journal of Physical Chemistry B, 2001, 105, 7775-7782.	2.6	63
42	Modification of the CHARMM force field for DMPC lipid bilayer. Journal of Computational Chemistry, 2008, 29, 2359-2369.	3.3	63
43	Free energy calculations for Lennard-Jones systems and water using the expanded ensemble method A Monte Carlo and molecular dynamics simulation study. Molecular Physics, 1994, 82, 455-471.	1.7	62
44	Application of Polyelectrolyte Theories for Analysis of DNA Melting in the Presence of Na+ and Mg2+ Ions. Biophysical Journal, 1998, 75, 3041-3056.	0.5	61
45	Partial atomic charges and their impact on the free energy of solvation. Journal of Computational Chemistry, 2013, 34, 187-197.	3.3	60
46	Computer Simulation Study oftert-Butyl Alcohol. 1. Structure in the Pure Liquid. Journal of Physical Chemistry B, 2000, 104, 9526-9532.	2.6	59
47	Dynamical and structural properties of charged and uncharged lidocaine in a lipid bilayer. Biophysical Chemistry, 2007, 125, 416-424.	2.8	58
48	Solvation free energies of methane and alkali halide ion pairs: An expanded ensemble molecular dynamics simulation study. Journal of Chemical Physics, 1998, 108, 227-233.	3.0	57
49	A Coarse-Grained DNA Model Parameterized from Atomistic Simulations by Inverse Monte Carlo. Polymers, 2014, 6, 1655-1675.	4.5	55
50	Diffusion and reaction pathways of water near fully hydrated TiO2 surfaces from ab initio molecular dynamics. Journal of Chemical Physics, 2017, 147, 024704.	3.0	55
51	Electrostatic Origin of Salt-Induced Nucleosome Array Compaction. Biophysical Journal, 2010, 99, 1896-1905.	0.5	54
52	MagiC: Software Package for Multiscale Modeling. Journal of Chemical Theory and Computation, 2013, 9, 1512-1520.	5.3	54
53	Curvature sensing by cardiolipin in simulated buckled membranes. Soft Matter, 2019, 15, 792-802.	2.7	54
54	Investigation of Water Clusters Containing OH- and H3O+ Ions in Atmospheric Conditions. A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2002, 106, 6479-6487.	2.6	53

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55	Systematic Optimization of a Force Field for Classical Simulations of TiO₂â€“Water Interfaces. Journal of Physical Chemistry C, 2015, 119, 18110-18125.	3.1	53
56	Transferable force-field for modelling of CO₂, N₂, O₂and Ar in all silica and Na⁺exchanged zeolites. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 045002.	2.0	53
57	Molecular dynamics simulations of water clusters with ions at atmospheric conditions. Journal of Chemical Physics, 2002, 116, 7879-7892.	3.0	52
58	Cholesterol in phospholipid bilayers: positions and orientations inside membranes with different unsaturation degrees. Soft Matter, 2019, 15, 78-93.	2.7	52
59	Molecular Dynamics Simulation Study of Glycerolâ€“Water Liquid Mixtures. Journal of Physical Chemistry B, 2011, 115, 14572-14581.	2.6	51
60	Solvation Structure of Hydroxyl Radical by Carâ€™Parrinello Molecular Dynamics. Journal of Physical Chemistry A, 2005, 109, 378-386.	2.5	49
61	Update to the General Amber Force Field for Small Solutes with an Emphasis on Free Energies of Hydration. Journal of Physical Chemistry B, 2014, 118, 3793-3804.	2.6	47
62	An Advanced Coarse-Grained Nucleosome Core Particle Model for Computer Simulations of Nucleosome-Nucleosome Interactions under Varying Ionic Conditions. PLoS ONE, 2013, 8, e54228.	2.5	46
63	Evaluation of effective ion-ion potentials in aqueous electrolytes. Physical Review E, 2002, 65, 041202.	2.1	45
64	Reply to Soper et al.: Fluctuations in water around a bimodal distribution of local hydrogen-bonded structural motifs. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, .	7.1	44
65	Molecular Dynamics Studies of Liposomes as Carriers for Photosensitizing Drugs: Development, Validation, and Simulations with a Coarse-Grained Model. Journal of Chemical Theory and Computation, 2014, 10, 5-13.	5.3	44
66	Cation-induced polyelectrolyteâ€“polyelectrolyte attraction in solutions of DNA and nucleosome core particles. Advances in Colloid and Interface Science, 2010, 158, 32-47.	14.7	43
67	Implicit inclusion of atomic polarization in modeling of partitioning between water and lipid bilayers. Physical Chemistry Chemical Physics, 2013, 15, 4677.	2.8	43
68	2D to 3D crossover of the magnetic properties in ordered arrays of iron oxide nanocrystals. Nanoscale, 2013, 5, 953-960.	5.6	43
69	A systematic analysis of nucleosome core particle and nucleosome-nucleosome stacking structure. Scientific Reports, 2018, 8, 1543.	3.3	43
70	Determination of solvation free energies by adaptive expanded ensemble molecular dynamics. Journal of Chemical Physics, 2004, 120, 3770-3776.	3.0	41
71	Multiscale coarse-grained simulations of ionic liquids: comparison of three approaches to derive effective potentials. Physical Chemistry Chemical Physics, 2013, 15, 7701.	2.8	41
72	Extension of the Slipids Force Field to Polyunsaturated Lipids. Journal of Physical Chemistry B, 2016, 120, 12826-12842.	2.6	39

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73	Determination of Free Energy from Chemical Potentials: Application of the Expanded Ensemble Method. Molecular Simulation, 1996, 18, 43-58.	2.0	38
74	Modeling DNA Flexibility: Comparison of Force Fields from Atomistic to Multiscale Levels. Journal of Physical Chemistry B, 2020, 124, 38-49.	2.6	37
75	Modelling chromatin structure and dynamics: status and prospects. Current Opinion in Structural Biology, 2012, 22, 151-159.	5.7	36
76	Effective solvent mediated potentials of Na+ and Clâ^' ions in aqueous solution: temperature dependence. Physical Chemistry Chemical Physics, 2011, 13, 5722.	2.8	35
77	Optimization of Slipids Force Field Parameters Describing Headgroups of Phospholipids. Journal of Physical Chemistry B, 2020, 124, 8784-8793.	2.6	35
78	Path-integral Monte Carlo method in quantum statistics for a system ofNidentical fermions. Physical Review A, 1993, 48, 4075-4083.	2.5	34
79	Systematic hierarchical coarse-graining with the inverse Monte Carlo method. Journal of Chemical Physics, 2015, 143, 243120.	3.0	33
80	A molecular dynamics simulation study of polyamine? and sodium?DNA. Interplay between polyamine binding and DNA structure. European Biophysics Journal, 2004, 33, 671-682.	2.2	31
81	Molecular dynamics simulation study of oriented polyamine- and Na-DNA: Sequence specific interactions and effects on DNA structure. Biopolymers, 2004, 73, 542-555.	2.4	31
82	Experimental and Monte Carlo Simulation Studies on the Competitive Binding of Li+, Na+, and K+Ions to DNA in Oriented DNA Fibersâ€. Journal of Physical Chemistry B, 1999, 103, 9008-9019.	2.6	30
83	Simulation of excited states and the sign problem in the path integral Monte Carlo method. Journal of Physics A, 2005, 38, 6659-6674.	1.6	30
84	NMR investigations of interactions between anesthetics and lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 2604-2611.	2.6	30
85	McMillanâ€“Mayer theory for solvent effects in inhomogeneous systems: Calculation of interaction pressure in aqueous electrical double layers. Journal of Chemical Physics, 2001, 114, 9565-9577.	3.0	29
86	Determination of effective pair potentials from ab initio simulations: application to liquid water. Chemical Physics Letters, 2000, 325, 15-21.	2.6	28
87	Spatial distribution functions as a tool in the analysis of ribonucleic acids hydration â€” molecular dynamics studies. Computers & Chemistry, 2000, 24, 451-457.	1.2	26
88	Computer Modeling Reveals that Modifications of the Histone Tail Charges Define Salt-Dependent Interaction of the Nucleosome Core Particles. Biophysical Journal, 2009, 96, 2082-2094.	0.5	26
89	Computer simulation of lipid membranes: Methodology and achievements. Polymer Science - Series C, 2013, 55, 162-180.	1.7	26
90	A multiscale model of protein adsorption on a nanoparticle surface. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 084003.	2.0	26

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91	Efficient Production of Solar Hydrogen Peroxide Using Piezoelectric Polarization and Photoinduced Charge Transfer of Nanopiezoelectrics Sensitized by Carbon Quantum Dots. Advanced Science, 2022, 9, e2105792.	11.2	26
92	Competitive substitution of hexammine cobalt(III) for Na+ and K+ ions in oriented DNA fibers. Biopolymers, 2001, 58, 268-278.	2.4	25
93	A multiscale analysis of DNA phase separation: from atomistic to mesoscale level. Nucleic Acids Research, 2019, 47, 5550-5562.	14.5	24
94	First principles characterisation of bioâ€“nano interface. Physical Chemistry Chemical Physics, 2021, 23, 13473-13482.	2.8	24
95	Molecular Dynamics Investigation of23Na NMR Relaxation in Oligomeric DNA Aqueous Solution. Journal of Physical Chemistry B, 2004, 108, 16295-16302.	2.6	22
96	Hierarchical Multiscale Modelling Scheme from First Principles to Mesoscale. Journal of Computational and Theoretical Nanoscience, 2009, 6, 951-959.	0.4	22
97	Molecular dynamics simulations demonstrate the regulation of DNAâ€DNA attraction by H4 histone tail acetylations and mutations. Biopolymers, 2014, 101, 1051-1064.	2.4	22
98	Magic v.3: An integrated software package for systematic structure-based coarse-graining. Computer Physics Communications, 2019, 237, 263-273.	7.5	22
99	Bottom-Up Coarse-Grained Modeling of DNA. Frontiers in Molecular Biosciences, 2021, 8, 645527.	3.5	22
100	Self-Diffusion and Association of Li+, Cs+, and H2O in Oriented DNA Fibers. An NMR and MD Simulation Study. Journal of Physical Chemistry B, 1998, 102, 10636-10642.	2.6	21
101	Electrostatic Background of Chromatin Fiber Stretching. Journal of Biomolecular Structure and Dynamics, 2004, 22, 215-226.	3.5	21
102	AMBER-ii: New Combining Rules and Force Field for Perfluoroalkanes. Journal of Physical Chemistry B, 2015, 119, 14563-14573.	2.6	21
103	Effect of lipid saturation on amyloid-beta peptide partitioning and aggregation in neuronal membranes: molecular dynamics simulations. European Biophysics Journal, 2019, 48, 813-824.	2.2	21
104	Entropic sampling of flexible polyelectrolytes within the Wang-Landau algorithm. Physical Review E, 2007, 75, 016705.	2.1	20
105	A new AMBER-compatible force field parameter set for alkanes. Journal of Molecular Modeling, 2014, 20, 2143.	1.8	19
106	Multiscale coarse-grained modelling of chromatin components: DNA and the nucleosome. Advances in Colloid and Interface Science, 2016, 232, 36-48.	14.7	19
107	Computing Curvature Sensitivity of Biomolecules in Membranes by Simulated Buckling. Journal of Chemical Theory and Computation, 2018, 14, 1643-1655.	5.3	19
108	Entropic sampling in the path integral Monte Carlo method. Journal of Physics A, 2003, 36, 685-693.	1.6	18

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109	Systematic implicit solvent coarse graining of dimyristoylphosphatidylcholine lipids. Journal of Computational Chemistry, 2014, 35, 1208-1218.	3.3	18
110	Reactive wetting properties of TiO₂ nanoparticles predicted by ab initio molecular dynamics simulations. Nanoscale, 2016, 8, 13385-13398.	5.6	18
111	Free Energy Calculations by Expanded Ensemble Method for Lattice and Continuous Polymers. The Journal of Physical Chemistry, 1996, 100, 1153-1158.	2.9	16
112	Anesthetics mechanism on a DMPC lipid membrane model: Insights from molecular dynamics simulations. Biophysical Chemistry, 2017, 226, 1-13.	2.8	16
113	All-Atom MD Simulation of DNA Condensation Using Ab Initio Derived Force Field Parameters of Cobalt(III)-Hexammine. Journal of Physical Chemistry B, 2017, 121, 7761-7770.	2.6	16
114	Molecular dynamics simulations of ubiquinone; a survey over torsional potentials and hydrogen bonds. Molecular Physics, 2001, 99, 1795-1804.	1.7	15
115	Application of the Poisson Boltzmann Polyelectrolyte Model for Analysis of Equilibria Between Single-, Double-, and Triple-Stranded Polynucleotides in the Presence of K⁺, Na⁺, and Mg²⁺ions. Journal of Biomolecular Structure and Dynamics, 2002, 20, 275-290.	3.5	15
116	Application of the Poisson Boltzmann polyelectrolyte model for analysis of thermal denaturation of DNA in the presence of Na+ and polyamine cations. Biophysical Chemistry, 2003, 104, 55-66.	2.8	15
117	Base sequence specificity of counterion binding to DNA: what can MD simulations tell us?. Canadian Journal of Chemistry, 2016, 94, 1181-1188.	1.1	15
118	Monte Carlo-Self Consistent Field Study of the Symmetrical Models of Polyelectrolytes. Molecular Simulation, 1992, 9, 285-306.	2.0	14
119	Topological and spatial aspects of the hydration of solutes of extreme solvation entropy. Physical Review E, 1999, 60, 4482-4495.	2.1	14
120	Entropic Sampling of Free and Ring Polymer Chains. Macromolecular Theory and Simulations, 2005, 14, 491-504.	1.4	14
121	Multiscale Modelling of Bionano Interface. Advances in Experimental Medicine and Biology, 2017, 947, 173-206.	1.6	14
122	Prediction of Chronic Inflammation for Inhaled Particles: the Impact of Material Cycling and Quarantining in the Lung Epithelium. Advanced Materials, 2020, 32, e2003913.	21.0	14
123	Conformational characteristics of single flexible polyelectrolyte chain. European Physical Journal E, 2009, 30, 341-50.	1.6	13
124	Monte-Carlo - Self Consistent Field Method in the Polyelectrolyte Theory. Journal of Biomolecular Structure and Dynamics, 1989, 7, 739-747.	3.5	12
125	Computer modeling of melting of ionized ice microcrystals. Journal of Chemical Physics, 2003, 119, 10237-10246.	3.0	12
126	Atomistic Perspective on Biomolecular Adsorption on Functionalized Carbon Nanomaterials under Ambient Conditions. Journal of Physical Chemistry B, 2021, 125, 416-430.	2.6	12

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127	A Bottom-Up Coarse-Grained Model for Nucleosomeâ€“Nucleosome Interactions with Explicit Ions. Journal of Chemical Theory and Computation, 2022, 18, 3948-3960.	5.3	12
128	Reconstruction of pair interaction potentials from radial distribution functions. Computer Physics Communications, 1999, 121-122, 57-59.	7.5	11
129	First and Second Hydration Shell of Ni2+ Studied by Molecular Dynamics Simulations. Theoretical Chemistry Accounts, 2006, 115, 170-176.	1.4	11
130	Assessing the electric-field approximation to IR and Raman spectra of dilute HOD in D2O. Journal of Chemical Physics, 2009, 131, 034501.	3.0	11
131	Centroid molecular dynamics: Comparison with exact results for model systems. Journal of Chemical Physics, 2010, 133, 194103.	3.0	11
132	Molecular Dynamics Investigation of Dipeptide - Transition Metal Salts in Aqueous Solutions. Journal of Physical Chemistry B, 2010, 114, 16632-16640.	2.6	11
133	Modelling of interactions between AÎ²(25â€“35) peptide and phospholipid bilayers: effects of cholesterol and lipid saturation. RSC Advances, 2020, 10, 3902-3915.	3.6	11
134	Phase transitions and thermodynamic properties of dense assemblies of truncated nanocubes and cuboctahedra. Nanoscale, 2012, 4, 4765.	5.6	10
135	Multiscale modelling of nucleosome core particle aggregation. Journal of Physics Condensed Matter, 2015, 27, 064111.	1.8	10
136	Bead-Fourier path integral molecular dynamics. Physical Review E, 2003, 67, 066710.	2.1	9
137	Path-integralâ€“expanded-ensemble Monte Carlo method in treatment of the sign problem for fermions. Physical Review E, 2009, 80, 066702.	2.1	9
138	Simulation of polymers by the Monte Carlo method using the Wang-Landau algorithm. Polymer Science - Series A, 2010, 52, 742-760.	1.0	9
139	Soluteâ€“Solvent Interactions in Aqueous Glycylglycineâ€“CuCl2 Solutions: Acoustical and Molecular Dynamics Perspective. Journal of Solution Chemistry, 2011, 40, 1657-1671.	1.2	9
140	Binding energy calculations for heveinâ€“carbohydrate interactions using expanded ensemble molecular dynamics simulations. Journal of Computer-Aided Molecular Design, 2015, 29, 13-21.	2.9	9
141	Coarse-Grained Simulation of Rodlike Higher-Order Quadruplex Structures at Different Salt Concentrations. ACS Omega, 2017, 2, 386-396.	3.5	8
142	Computationally based analysis of the energy efficiency of a CO2 capture process. Chemical Engineering Science, 2017, 174, 174-188.	3.8	8
143	Parallel molecular dynamics simulations of biomolecular systems. Lecture Notes in Computer Science, 1998, , 296-303.	1.3	7
144	Molecular Dynamics Simulations of Furfural and 5-Hydroxymethylfurfural at Ambient and Hydrothermal Conditions. Journal of Physical Chemistry B, 2018, 122, 8416-8428.	2.6	7

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145	Molecular Conformations in a Phospholipid Bilayer Extracted from Dipolar Couplings:Â A Computer Simulation Study. Journal of Physical Chemistry B, 2007, 111, 13638-13644.	2.6	6
146	Bond orientation properties in lipid molecules of membranes: molecular dynamics simulations. Journal of Physics: Conference Series, 2014, 510, 012022.	0.4	6
147	Quantum chemical and molecular dynamics modelling of hydroxylated polybrominated diphenyl ethers. Physical Chemistry Chemical Physics, 2017, 19, 28263-28274.	2.8	6
148	Stress Relief and Reactivity Loss of Hydrated Anatase (001) Surface. Journal of Physical Chemistry C, 2018, 122, 22407-22417.	3.1	6
149	Pressure-induced amorphization of noble gas clathrate hydrates. Physical Review B, 2021, 103, .	3.2	6
150	DNAâ€“DNA Interactions. , 0, , 209-237.		5
151	Improved Sampling in Ab Initio Free Energy Calculations of Biomolecules at Solidâ€“Liquid Interfaces: Tight-Binding Assessment of Charged Amino Acids on TiO2 Anatase (101). Computation, 2020, 8, 12.	2.0	5
152	Structural investigation of three distinct amorphous forms of Ar hydrate. RSC Advances, 2021, 11, 30744-30754.	3.6	5
153	Twoâ€Đimensional Wangâ€“Landau Algorithm for Osmotic Pressure Calculations in a Polyelectrolyteâ€“Membrane System. Macromolecular Theory and Simulations, 2011, 20, 496-509.	1.4	4
154	Implicit solvent systematic coarse-graining of dioleoylphosphatidylethanolamine lipids: From the inverted hexagonal to the bilayer structure. PLoS ONE, 2019, 14, e0214673.	2.5	4
155	Computational insight into the hydrogenation of CO2 and carbamic acids to methanol by a ruthenium(II)-based catalyst: The role of amino (NH) ligand group. Molecular Catalysis, 2021, 506, 111544.	2.0	4
156	Atomistic Molecular Dynamics Simulations of Lipids Near TiO₂ Nanosurfaces. Journal of Physical Chemistry B, 2021, 125, 8048-8059.	2.6	4
157	Internal Structure and Dynamics of the Decamer D(ATGCAGTCAG) 2 In Li + -H 2 O Solution: A molecular Dynamics Simulation Study. Molecular Simulation, 2003, 29, 47-62.	2.0	3
158	Path integral method in quantum statistics problems: generalized ensemble Monte Carlo and density functional approach. Journal of Physics A, 2006, 39, 4711-4716.	1.6	3
159	Solvating, manipulating, damaging, and repairing DNA in a computer. International Journal of Quantum Chemistry, 2007, 107, 279-291.	2.0	3
160	Modeling a Boltzmann Distribution: Simbo (Simulated Boltzmann). Journal of Chemical Education, 2003, 80, 109.	2.3	2
161	Simulations of one- and two-electron systems by Bead-Fourier path integral molecular dynamics. Journal of Chemical Physics, 2005, 123, 034105.	3.0	2
162	Interacting electrons in one dimension: a path integral Monte Carlo study. Journal of Physics A: Mathematical and Theoretical, 2007, 40, 7151-7157.	2.1	2

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163	M.DynaMix Studies of Solvation, Solubility and Permeability. , 2012, , .		2
164	Unperturbed hydrocarbon chains and liquid phase bilayer lipid chains: a computer simulation study. European Biophysics Journal, 2018, 47, 109-130.	2.2	2
165	Exploring High-Pressure Transformations in Low-Z (H2, Ne) Hydrates at Low Temperatures. Crystals, 2022, 12, 9.	2.2	2
166	Calculation of Canonical Properties and Excited States by Path Integral Numerical Methods. Contributions To Plasma Physics, 2011, 51, 382-385.	1.1	1
167	Advanced characterizations for stabilization/solidification technologies. , 2022, , 497-516.		1
168	Electrostatically Induced Bundle Formation of Rodlike Polyelectrolytes: Comparison of Predictions from Monte Carlo Simulations with Experiments on Fd And M13 Virus Particles.. Materials Research Society Symposia Proceedings, 1997, 489, 61.	0.1	0
169	Molecular dynamics investigations of local anesthetic lidocaine in DMPC lipid bilayer. Chemistry and Physics of Lipids, 2007, 149, S30.	3.2	0
170	One dimensional model for water and aqueous solutions. Part V. Monte Carlo simulation of dilute solutions of hard rod in waterlike particles. Journal of Chemical Physics, 2009, 131, 204507.	3.0	0
171	Interactions and Stacking in Ordered Mononucleosomes and Folded Chromatin: Effects of Histone Tail Modifications. Biophysical Journal, 2014, 106, 74a.	0.5	0
172	To the fast calculation of the solvation free energy. Combining expanded ensembles with L2MC. Journal of Computational Chemistry, 2021, 42, 787-792.	3.3	0
173	DNA Counterion Distributions: Molecular Simulations. , 2014, , 1193-1204.		0
174	Disease Prediction: Prediction of Chronic Inflammation for Inhaled Particles: the Impact of Material Cycling and Quarantining in the Lung Epithelium (Adv. Mater. 47/2020). Advanced Materials, 2020, 32, .	21.0	0