Yuko Okamoto

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5785628/publications.pdf

Version: 2024-02-01

248	12,855	44069	24982
papers	citations	48 h-index	109 g-index

251	251	251	7316
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Replica-exchange molecular dynamics method for protein folding. Chemical Physics Letters, 1999, 314, 141-151.	2.6	3,978
2	Multidimensional replica-exchange method for free-energy calculations. Journal of Chemical Physics, 2000, 113, 6042-6051.	3.0	775
3	Generalized-ensemble algorithms for molecular simulations of biopolymers. Biopolymers, 2001, 60, 96-123.	2.4	725
4	Prediction of peptide conformation by multicanonical algorithm: New approach to the multiple-minima problem. Journal of Computational Chemistry, 1993, 14, 1333-1338.	3.3	371
5	Generalized-ensemble algorithms: enhanced sampling techniques for Monte Carlo and molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2004, 22, 425-439.	2.4	307
6	Replica-exchange multicanonical algorithm and multicanonical replica-exchange method for simulating systems with rough energy landscape. Chemical Physics Letters, 2000, 329, 261-270.	2.6	287
7	Molecular dynamics, Langevin and hydrid Monte Carlo simulations in a multicanonical ensemble. Chemical Physics Letters, 1996, 259, 321-330.	2.6	282
8	New Monte Carlo algorithms for protein folding. Current Opinion in Structural Biology, 1999, 9, 177-183.	5.7	266
9	Replica-exchange Monte Carlo method for the isobaricâ€“isothermal ensemble. Chemical Physics Letters, 2001, 335, 435-439.	2.6	204
10	Thermodynamics of Helix-Coil Transitions Studied by Multicanonical Algorithms. The Journal of Physical Chemistry, 1995, 99, 11276-11287.	2.9	187
11	Numerical comparisons of three recently proposed algorithms in the protein folding problem. Journal of Computational Chemistry, 1997, 18, 920-933.	3.3	152
12	Comparisons of force fields for proteins by generalized-ensemble simulations. Chemical Physics Letters, 2004, 386, 460-467.	2.6	151
13	Replica-exchange multicanonical and multicanonical replica-exchange Monte Carlo simulations of peptides. I. Formulation and benchmark test. Journal of Chemical Physics, 2003, 118, 6664-6675.	3.0	133
14	Hadronic contributions to the anomalous magnetic moment of the muon. Physical Review D, 1985, 31, 2108-2119.	4.7	120
15	Comparative study of multicanonical and simulated annealing algorithms in the protein folding problem. Physica A: Statistical Mechanics and Its Applications, 1994, 212, 415-437.	2.6	120
16	Structureâ€“function insights into direct lipid transfer between membranes by Mmm1â€“Mdm12 of ERMES. Journal of Cell Biology, 2018, 217, 959-974.	5.2	116
17	Generalized-ensemble Monte Carlo method for systems with rough energy landscape. Physical Review E, 1997, 56, 2228-2233.	2.1	108
18	A prediction of tertiary structures of peptide by the Monte Carlo simulated annealing method. Protein Engineering, Design and Selection, 1989, 3, 85-94.	2.1	105

#	Article	IF	Citations
19	Î±-Helix folding by Monte Carlo simulated annealing in isolated C-peptide of ribonuclease A. Protein Engineering, Design and Selection, 1991, 4, 639-647.	2.1	94
20	Improved Theory of the Muon Anomalous Magnetic Moment. Physical Review Letters, 1984, 52, 717-719.	7.8	91
21	QM/MM free energy simulations: recent progress and challenges. Molecular Simulation, 2016, 42, 1056-1078.	2.0	89
22	Explicit symplectic integrators of molecular dynamics algorithms for rigid-body molecules in the canonical, isobaric-isothermal, and related ensembles. Journal of Chemical Physics, 2007, 126, 084103.	3.0	88
23	Thermodynamic Perspective on the Dockâ^'Lock Growth Mechanism of Amyloid Fibrils. Journal of Physical Chemistry B, 2009, 113, 14421-14430.	2.6	88
24	Secondary-structure preferences of force fields for proteins evaluated by generalized-ensemble simulations. Chemical Physics, 2004, 307, 269-283.	1.9	85
25	Replica-exchange simulated tempering method for simulations of frustrated systems. Chemical Physics Letters, 2000, 332, 131-138.	2.6	83
26	Finite-size scaling of helixâ€"coil transitions in poly-alanine studied by multicanonical simulations. Journal of Chemical Physics, 1999, 110, 1267-1276.	3.0	81
27	N+-C-HÂ·Â·Â·O Hydrogen bonds in protein-ligand complexes. Scientific Reports, 2019, 9, 767.	3.3	81
28	THE GENERALIZED-ENSEMBLE APPROACH FOR PROTEIN FOLDING SIMULATIONS. , 1999, , 129-157.		80
29	First-Principle Determination of Peptide Conformations in Solvents:Â Combination of Monte Carlo Simulated Annealing and RISM Theory. Journal of the American Chemical Society, 1998, 120, 1855-1863.	13.7	79
30	Replica-exchange multicanonical and multicanonical replica-exchange Monte Carlo simulations of peptides. II. Application to a more complex system. Journal of Chemical Physics, 2003, 118, 6676-6688.	3.0	79
31	Eighth-order QED contribution to the anomalous magnetic moment of the muon. Physical Review D, 1990, 41, 593-610.	4.7	74
32	Characteristic temperatures of folding of a small peptide. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 10652-10656.	7.1	72
33	Monte Carlo simulations in generalized ensemble: Multicanonical algorithm versus simulated tempering. Physical Review E, 1996, 54, 5863-5865.	2.1	65
34	The folding funnel landscape for the peptide met-enkephalin. , 1999, 34, 472-483.		64
35	Free energy calculations for DNA base stacking by replica-exchange umbrella sampling. Chemical Physics Letters, 2004, 385, 1-7.	2.6	61
36	Prediction of Î±-Helix Folding of Isolated C-Peptide of Ribonuclease A by Monte Carlo Simulated Annealing. Chemistry Letters, 1991, 20, 213-216.	1.3	60

#	Article	IF	Citations
37	Exploration of Conformational Spaces of Highâ€Mannoseâ€Type Oligosaccharides by an NMRâ€Validated Simulation. Angewandte Chemie - International Edition, 2014, 53, 10941-10944.	13.8	60
38	Enhanced Sampling Algorithms. Methods in Molecular Biology, 2013, 924, 153-195.	0.9	59
39	Monte Carlo simulations in multibaricâ€“multithermal ensemble. Chemical Physics Letters, 2004, 383, 391-396.	2.6	57
40	Conformational effects of N-glycan core fucosylation of immunoglobulin G Fc region on its interaction with FcÎ³ receptor IIIa. Scientific Reports, 2017, 7, 13780.	3.3	57
41	Solvation structure and stability of peptides in aqueous solutions analyzed by the reference interaction site model theory. Journal of Chemical Physics, 1997, 107, 1586-1599.	3.0	56
42	Cooperative folding mechanism of a Î²-hairpin peptide studied by a multicanonical replica-exchange molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2006, 66, 846-859.	2.6	56
43	Temperature and Pressure Dependence of Alanine Dipeptide Studied by Multibaricâ^'Multithermal Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 12038-12049.	2.6	55
44	Monte Carlo simulations in generalized isobaric-isothermal ensembles. Physical Review E, 2004, 70, 026702.	2.1	54
45	Molecular dynamics simulations in the multibaricâ€“multithermal ensemble. Chemical Physics Letters, 2004, 391, 248-253.	2.6	54
46	Replica-exchange extensions of simulated tempering method. Journal of Chemical Physics, 2004, 121, 2491.	3.0	53
47	Multibaric-multithermal ensemble molecular dynamics simulations. Journal of Computational Chemistry, 2006, 27, 379-395.	3.3	53
48	Ab Initio prediction of proteinâ€“ligand binding structures by replicaâ€exchange umbrella sampling simulations. Journal of Computational Chemistry, 2011, 32, 2810-2821.	3.3	53
49	Multidimensional generalized-ensemble algorithms for complex systems. Journal of Chemical Physics, 2009, 130, 214105.	3.0	52
50	Multioverlap simulations for transitions between reference configurations. Physical Review E, 2003, 68, 036126.	2.1	49
51	Analysis on conformational stability of C-peptide of ribonuclease A in water using the reference interaction site model theory and Monte Carlo simulated annealing. Journal of Chemical Physics, 1999, 110, 4090-4100.	3.0	47
52	Amyloid-Î²(29â^'42) Dimer Formations Studied by a Multicanonicalâ^'Multioverlap Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 2767-2770.	2.6	47
53	Helix-coil transitions of amino-acid homo-oligomers in aqueous solution studied by multicanonical simulations. Journal of Chemical Physics, 2000, 112, 10638-10647.	3.0	46
54	Replica-exchange method in van der Waals radius space: Overcoming steric restrictions for biomolecules. Journal of Chemical Physics, 2010, 132, 134105.	3.0	46

#	Article	IF	Citations
55	Dependence on the dielectric model and pH in a synthetic helical peptide studied by Monte Carlo simulated annealing. Biopolymers, 1994, 34, 529-539.	2.4	45
56	Ab initio replica-exchange Monte Carlo method for cluster studies. Chemical Physics Letters, 2001, 333, 199-206.	2.6	43
57	Communication: Simulated tempering with fast on-the-fly weight determination. Journal of Chemical Physics, 2013, 138, 061102.	3.0	43
58	Residual entropy of ordinary ice from multicanonical simulations. Physical Review B, 2007, 75, .	3.2	41
59	Entropy of planar random surfaces on the lattice. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1983, 130, 415-419.	4.1	40
60	Peptide Conformations in Alcohol and Water:Â Analyses by the Reference Interaction Site Model Theory. Journal of the American Chemical Society, 2000, 122, 2773-2779.	13.7	40
61	Hydrophobic Core Formation and Dehydration in Protein Folding Studied by Generalized-Ensemble Simulations. Biophysical Journal, 2010, 99, 1637-1644.	0.5	40
62	Calculation of solvation free energy using RISM theory for peptide in salt solution. Journal of Computational Chemistry, 1998, 19, 1724-1735.	3.3	39
63	Calculation of hydration free energy for a solute with many atomic sites using the RISM theory: A robust and efficient algorithm. Journal of Computational Chemistry, 1997, 18, 1320-1326.	3.3	38
64	Tertiary Structure Prediction of C-Peptide of Ribonuclease A by Multicanonical Algorithm. Journal of Physical Chemistry B, 1998, 102, 653-656.	2.6	38
65	Effects of Side-Chain Charges on Î±-Helix Stability in C-Peptide of Ribonuclease A Studied by Multicanonical Algorithm. Journal of Physical Chemistry B, 1999, 103, 1595-1604.	2.6	38
66	Prediction of Low-Energy Structures of Met-Enkephalin by Monte Carlo Simulated Annealing. Chemistry Letters, 1992, 21, 1275-1278.	1.3	37
67	Multibaricâ€“Multithermal Molecular Dynamics Simulation of Alanine Dipeptide in Explicit Water. Bulletin of the Chemical Society of Japan, 2007, 80, 1114-1123.	3.2	37
68	Multi-overlap molecular dynamics methods for biomolecular systems. Chemical Physics Letters, 2004, 400, 308-313.	2.6	36
69	Multicanonical algorithm combined with the RISM theory for simulating peptides in aqueous solution. Chemical Physics Letters, 2000, 329, 295-303.	2.6	35
70	Prediction of membrane protein structures by replica-exchange Monte Carlo simulations: Case of two helices. Journal of Chemical Physics, 2004, 120, 10837-10847.	3.0	35
71	From multidimensional replica-exchange method to multidimensional multicanonical algorithm and simulated tempering. Physical Review E, 2009, 79, 047701.	2.1	35
72	Twoâ€dimensional replicaâ€exchange method for predicting proteinâ€“ligand binding structures. Journal of Computational Chemistry, 2013, 34, 2601-2614.	3.3	35

#	Article	IF	Citations
73	Helix-forming tendencies of nonpolar amino acids predicted by Monte Carlo simulated annealing. Proteins: Structure, Function and Bioinformatics, 1994, 19, 14-23.	2.6	34
74	Generalized-ensemble algorithms for molecular dynamics simulations. Molecular Simulation, 2007, 33, 47-56.	2.0	33
75	Conformational Change of Amyloid-Î² 40 in Association with Binding to GM1-Glycan Cluster. Scientific Reports, 2019, 9, 6853.	3.3	33
76	Generalized-Ensemble Algorithms for the Isobaricâ€“Isothermal Ensemble. Journal of the Physical Society of Japan, 2010, 79, 074003.	1.6	32
77	Optimization of protein force-field parameters with the Protein Data Bank. Chemical Physics Letters, 2003, 382, 626-636.	2.6	31
78	Molecular Mechanism for Stabilizing a Short Helical Peptide Studied by Generalized-Ensemble Simulations with Explicit Solvent. Biophysical Journal, 2005, 88, 3180-3190.	0.5	31
79	Comment on "Monte Carlo Simulation of a First-Order Transition for Protein Folding". The Journal of Physical Chemistry, 1995, 99, 2236-2237.	2.9	30
80	Combination of the Replica-Exchange Monte Carlo Method and the Reference Interaction Site Model Theory for Simulating a Peptide Molecule in Aqueous Solution. Journal of Physical Chemistry B, 2004, 108, 19002-19012.	2.6	30
81	Theoretical studies of transition states by the multioverlap molecular dynamics methods. Journal of Chemical Physics, 2006, 124, 104103.	3.0	29
82	Liquidâ€“Gas Phase Transitions Studied by Multibaricâ€“Multithermal Monte Carlo Simulations. Journal of the Physical Society of Japan, 2004, 73, 3304-3311.	1.6	28
83	Prediction of Proteinâ€“Ligand Binding Structures by Replica-Exchange Umbrella Sampling Simulations: Application to Kinase Systems. Journal of Chemical Theory and Computation, 2013, 9, 4660-4671.	5.3	28
84	Prediction of transmembrane helix configurations by replica-exchange simulations. Chemical Physics Letters, 2004, 383, 397-402.	2.6	26
85	Structures of a peptide fragment of Î²2-microglobulin studied by replica-exchange molecular dynamics simulations - Towards the understanding of the mechanism of amyloid formation. FEBS Letters, 2005, 579, 5425-5429.	2.8	26
86	Temperature dependence of distributions of conformations of a small peptide. Journal of Molecular Graphics and Modelling, 1998, 16, 226-238.	2.4	25
87	Self-assembly of transmembrane helices of bacteriorhodopsin by a replica-exchange Monte Carlo simulation. Chemical Physics Letters, 2004, 392, 168-175.	2.6	25
88	Effective sampling in the configurational space of a small peptide by the multicanonical-multioverlap algorithm. Physical Review E, 2007, 76, 026705.	2.1	23
89	Replica-Exchange Molecular Dynamics Simulations for Various Constant Temperature Algorithms. Journal of the Physical Society of Japan, 2010, 79, 074001.	1.6	23
90	Asymptotic photon propagator in massive QED and the muon anomalous magnetic moment. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1991, 254, 235-240.	4.1	22

#	Article	IF	Citations
91	Free-Energy Calculations in Protein Folding by Generalized-Ensemble Algorithms. Lecture Notes in Computational Science and Engineering, 2002, , 304-332.	0.3	22
92	Asymptotic photon propagator and higher-order QED Callan-Symanzik Î² function. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1991, 260, 193-198.	4.1	20
93	Replica-ExchangeMonte Carlo Method for Ar Fluid. Progress of Theoretical Physics Supplement, 2000, 138, 270-271.	0.1	20
94	PROTEIN FORCE-FIELD PARAMETERS OPTIMIZED WITH THE PROTEIN DATA BANK II: COMPARISONS OF FORCE FIELDS BY FOLDING SIMULATIONS OF SHORT PEPTIDES. Journal of Theoretical and Computational Chemistry, 2004, 03, 359-378.	1.8	20
95	Sampling Ground-State Configurations of a Peptide by Multicanonical Annealing. Journal of the Physical Society of Japan, 1994, 63, 3945-3949.	1.6	19
96	Î²-sheet folding of fragment (16â€“36) of bovine pancreatic trypsin inhibitor as predicted by Monte Carlo simulated annealing. Protein Engineering, Design and Selection, 1992, 5, 495-503.	2.1	18
97	Molecular dynamics of C-peptide of ribonuclease A studied by replica-exchange Monte Carlo method and diffusion theory. Chemical Physics Letters, 2003, 380, 609-619.	2.6	18
98	PROTEIN FORCE-FIELD PARAMETERS OPTIMIZED WITH THE PROTEIN DATA BANK I: FORCE-FIELD OPTIMIZATIONS. Journal of Theoretical and Computational Chemistry, 2004, 03, 339-358.	1.8	18
99	On Existence of Non-Renormalizable Field Theory: Pure SU(2) Lattice Gauge Theory in Five Dimensions. Progress of Theoretical Physics, 1992, 88, 341-350.	2.0	17
100	Stochastic dynamics simulations in a new generalized ensemble. Chemical Physics Letters, 1998, 297, 374-382.	2.6	17
101	Replica-exchange molecular dynamics simulation of small peptide in water and in ethanol. Chemical Physics Letters, 2005, 412, 280-284.	2.6	16
102	Protein structure predictions by parallel simulated annealing molecular dynamics using genetic crossover. Journal of Computational Chemistry, 2011, 32, 1353-1360.	3.3	16
103	Phase Behavior of a Lipid Bilayer System Studied by a Replica-Exchange Molecular Dynamics Simulation. Journal of the Physical Society of Japan, 2012, 81, 024002.	1.6	16
104	Conformational Dynamics of Oligosaccharides Characterized by Paramagnetism-Assisted NMR Spectroscopy in Conjunction with Molecular Dynamics Simulation. Advances in Experimental Medicine and Biology, 2015, 842, 217-230.	1.6	16
105	Î±-Helix structure of parathyroid hormone fragment (1-34) predicted by Monte Carlo simulated annealing. International Journal of Peptide and Protein Research, 1993, 42, 300-303.	0.1	15
106	A novel algorithm for calculation of the extreme eigenvalues of large Hermitian matrices. Computer Physics Communications, 1993, 76, 191-202.	7.5	14
107	Î±-Helix propensities of homo-oligomers in aqueous solution studied by multicanonical algorithm. Chemical Physics Letters, 1999, 309, 95-100.	2.6	14
108	Secondary-Structure Design of Proteins by a Backbone Torsion Energy. Journal of the Physical Society of Japan, 2006, 75, 054802.	1.6	14

#	Article	IF	Citations
109	Î²-sheet formation in BPTI(16â€“36) by Monte Carlo simulated annealing. Chemical Physics Letters, 1999, 299, 17-24.	2.6	13
110	Dynamic structure of the polytheonamide B channel studied by normal mode analysis. Molecular Simulation, 2011, 37, 975-985.	2.0	13
111	Replica-exchange molecular dynamics simulation of a lipid bilayer system with a coarse-grained model. Molecular Simulation, 2012, 38, 437-441.	2.0	13
112	Î±-Helix Propensities of Amino Acids Studied by Multicanonical Algorithm. Chemistry Letters, 1995, 24, 391-392.	1.3	12
113	New approach to the first-order phase transition of Lennard-Jones fluids. Journal of Chemical Physics, 2004, 120, 7557-7563.	3.0	12
114	Analysis of Helix-Helix Interactions of Bacteriorhodopsin by Replica-Exchange Simulations. Biophysical Journal, 2009, 96, 765-776.	0.5	12
115	Prediction of Ligand Binding Affinity by the Combination of Replica-Exchange Method and Double-Decoupling Method. Journal of Chemical Theory and Computation, 2014, 10, 3563-3569.	5.3	12
116	Tackling the protein folding problem by a generalized-ensemble approach with Tsallis statistics. Brazilian Journal of Physics, 1999, 29, .	1.4	12
117	Generalized Einstein theory on solar and galactic scales. Physical Review D, 1993, 48, 578-582.	4.7	11
118	Solvent effects on conformational stability of peptides: RISM analyses. Journal of Molecular Liquids, 2001, 90, 195-204.	4.9	11
119	Folding simulations of gramicidin A into the Î²-helix conformations: Simulated annealing molecular dynamics study. Journal of Chemical Physics, 2009, 131, 165103.	3.0	11
120	Residual entropy of ordinary ice calculated from multicanonical Monte Carlo simulations. Molecular Simulation, 2012, 38, 856-860.	2.0	11
121	Free-energy analyses of a proton transfer reaction by simulated-tempering umbrella sampling and first-principles molecular dynamics simulations. Physical Review E, 2013, 87, 023301.	2.1	11
122	Optimisation of OPLSâ€“UA force-field parameters for protein systems using protein data bank. Molecular Simulation, 2010, 36, 1148-1156.	2.0	10
123	Conformational changes of ubiquitin under high pressure conditions: A pressure simulated tempering molecular dynamics study. Journal of Computational Chemistry, 2017, 38, 1167-1173.	3.3	10
124	Implementation of replica-exchange umbrella sampling in GAMESS. Computer Physics Communications, 2018, 228, 152-162.	7.5	10
125	Monte Carlo Simulated Annealing Prediction for Î±-Helix Propensity of Amino Acid Homopolymers. Chemistry Letters, 1991, 20, 1279-1282.	1.3	9
126	Classification and Prediction of Low-Energy Membrane Protein Helix Configurations by Replica-Exchange Monte Carlo Method. Journal of the Physical Society of Japan, 2004, 73, 2571-2585.	1.6	9

#	Article	IF	Citations
127	Replica-exchange methods and predictions of helix configurations of membrane proteins. Molecular Simulation, 2006, 32, 791-801.	2.0	9
128	Controlling the secondary-structure-forming tendencies of proteins by a backbone torsion-energy term. Molecular Simulation, 2010, 36, 138-158.	2.0	9
129	Helix-Hairpin Transitions of a Designed Peptide Studied by a Generalized-Ensemble Simulation. Journal of Chemical Theory and Computation, 2010, 6, 979-983.	5.3	9
130	Simulated tempering and magnetizing: Application of two-dimensional simulated tempering to the two-dimensional Ising model and its crossover. Physical Review E, 2012, 86, 056705.	2.1	9
131	Two polyhedral frameworks of an M12L24 spherical complex revealed by replica-exchange molecular dynamics simulations. Chemical Physics Letters, 2019, 714, 185-189.	2.6	9
132	Protein folding simulations and structure predictions. Computer Physics Communications, 2001, 142, 55-63.	7.5	8
133	Generalized-ensemble simulations of spin systems and protein systems. Computer Physics Communications, 2002, 146, 69-76.	7.5	8
134	Effects of the fixed end in single-molecule imaging techniques: A replica-exchange molecular dynamics simulation study. Chemical Physics Letters, 2005, 414, 449-455.	2.6	8
135	Electrostatic effects on the Î±-helix and Î²-strand formation of BPTI(16-36) studied by Monte Carlo simulated annealing. Chemical Biology and Drug Design, 2008, 54, 230-236.	1.1	8
136	Generalized-Ensemble Algorithms for Protein Folding Simulations. , 2008, , 369-407.		8
137	Folding simulations of three proteins having all Î±-helix, all Î²-strand and Î±/Î²-structures. Molecular Simulation, 2010, 36, 302-310.	2.0	8
138	A Conformational Search Method for Protein Systems Using Genetic Crossover and Metropolis Criterion. Journal of Physics: Conference Series, 2014, 487, 012003.	0.4	8
139	Conformational properties of an artificial GM1 glycan cluster based on a metal-ligand complex. Journal of Chemical Physics, 2018, 149, 135101.	3.0	8
140	On Existence of Non-Renormalizable Field Theory. Progress of Theoretical Physics, 1992, 88, 341-350.	2.0	8
141	An Analysis on Protein Folding Problem by Replica-Exchange Method. Progress of Theoretical Physics Supplement, 2000, 138, 402-403.	0.1	7
142	MOLECULAR DYNAMICS SIMULATIONS OF DNA DIMERS BASED ON REPLICA-EXCHANGE UMBRELLA SAMPLING I: TEST OF SAMPLING EFFICIENCY. Journal of Theoretical and Computational Chemistry, 2005, 04, 411-432.	1.8	7
143	Replica-exchange molecular dynamics simulation for understanding the initial process of amyloid peptide aggregation. Molecular Simulation, 2015, 41, 1041-1044.	2.0	7
144	Modeling 15N NMR chemical shift changes in protein backbone with pressure. Journal of Chemical Physics, 2016, 145, 085104.	3.0	7

#	Article	IF	Citations
145	Computational analysis for selectivity of histone deacetylase inhibitor by replica-exchange umbrella sampling molecular dynamics simulations. Journal of Chemical Physics, 2018, 148, 125102.	3.0	7
146	Protein Folding Simulations by Generalized-Ensemble Algorithms. Advances in Experimental Medicine and Biology, 2014, 805, 1-27.	1.6	7
147	Singular behavior of the reference interaction site model theory observed for peptide in salt solution. Chemical Physics Letters, 1998, 297, 433-438.	2.6	6
148	TACKLING THE MULTIPLE-MINIMA PROBLEM IN PROTEIN FOLDING BY MONTE CARLO SIMULATED ANNEALING AND GENERALIZED-ENSEMBLE ALGORITHMS. International Journal of Modern Physics C, 1999, 10, 1571-1582.	1.7	6
149	Dependency of ligand free energy landscapes on charge parameters and solvent models. Journal of Computer-Aided Molecular Design, 2010, 24, 699-712.	2.9	6
150	Multi-dimensional multicanonical algorithm, simulated tempering, replica-exchange method, and all that. Physics Procedia, 2010, 4, 89-105.	1.2	6
151	Ligand Docking Simulations by Generalized-Ensemble Algorithms. Advances in Protein Chemistry and Structural Biology, 2013, 92, 63-91.	2.3	6
152	Implementation of replica-exchange umbrella sampling in the DFTB<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si6.gif" display="inline" overflow="scroll"><mml:mo>+</mml:mo></mml:math> semiempirical quantum chemistry package. Computer Physics Communications, 2016, 204, 1-10.	7.5	6
153	Determination of the structural ensemble of the molten globule state of a protein by computer simulations. Proteins: Structure, Function and Bioinformatics, 2019, 87, 635-645.	2.6	6
154	Efficient simulation protocol for determining the density of states: Combination of replica-exchange Wang-Landau method and multicanonical replica-exchange method. Physical Review E, 2019, 100, 043304.	2.1	6
155	Structural Characteristics of Monomeric AÎ²42 on Fibril in the Early Stage of Secondary Nucleation Process. ACS Chemical Neuroscience, 2020, 11, 2989-2998.	3.5	6
156	Generalized-Ensemble Algorithms for Simulations of Complex Molecular Systems. , 2012, , 69-101.		6
157	The E6 âŠ— SO(10) preon model based on global SU(18) color-flavor. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1985, 162, 333-334.	4.1	5
158	Amino-acid-dependent main-chain torsion-energy terms for protein systems. Journal of Chemical Physics, 2013, 138, 064103.	3.0	5
159	Predictions of Tertiary Structures of Î±-Helical Membrane Proteins by Replica-Exchange Method with Consideration of Helix Deformations. Journal of the Physical Society of Japan, 2015, 84, 084802.	1.6	5
160	Designed-walk replica-exchange method for simulations of complex systems. Computer Physics Communications, 2015, 196, 380-383.	7.5	5
161	Two major stable structures of amyloid-forming peptides: amorphous aggregates and amyloid fibrils. Molecular Simulation, 2017, 43, 1370-1376.	2.0	5
162	Calculation of the residual entropy of Ice Ih by Monte Carlo simulation with the combination of the replica-exchange Wangâ€“Landau algorithm and multicanonical replica-exchange method. Journal of Chemical Physics, 2021, 154, 044503.	3.0	5

#	Article	IF	Citations
163	A method for calculating the eigenvalues of large Hermitian matrices by second-order recursion formulae. Computer Physics Communications, 1996, 96, 217-231.	7.5	4
164	Classification of Low-Energy Conformations of Met-Enkephalin in the Gas Phase and in a Model Solvent Based on the Extended Scaled Particle Theory. Bulletin of the Chemical Society of Japan, 1999, 72, 1717-1729.	3.2	4
165	Metropolis Algorithms in Generalized Ensemble. AIP Conference Proceedings, 2003, , .	0.4	4
166	Normal Mode Analysis of Polytheonamide B. Journal of the Physical Society of Japan, 2007, 76, 094801.	1.6	4
167	Determination method of the balance of the secondary-structure-forming tendencies of force fields. Molecular Simulation, 2010, 36, 159-165.	2.0	4
168	Molecular simulations in generalised ensemble. Molecular Simulation, 2012, 38, 1282-1296.	2.0	4
169	Application of simulated tempering and magnetizing to a two-dimensional Potts model. Journal of Statistical Mechanics: Theory and Experiment, 2013, 2013, P02039.	2.3	4
170	Observation of helix associations for insertion of a retinal molecule and distortions of helix structures in bacteriorhodopsin. Journal of Chemical Physics, 2015, 143, 235101.	3.0	4
171	Protein structure predictions by enhanced conformational sampling methods. Biophysics and Physicobiology, 2019, 16, 344-366.	1.0	4
172	Recent Applications of Replica-Exchange Molecular Dynamics Simulations of Biomolecules. Current Physical Chemistry, 2012, 2, 401-412.	0.2	4
173	A grand unification preon model with E6 metacolor. Nuclear Physics B, 1986, 268, 397-405.	2.5	3
174	On possible global symmetries in superstring inspired supersymmetric models. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1987, 191, 103-108.	4.1	3
175	Protein Folding Simulations by Simulated Annealing and Generalized-Ensemble Algorithms. Progress of Theoretical Physics Supplement, 2000, 138, 301-310.	0.1	3
176	A pH-dependent variation in ?-helix structure of the S-peptide of ribonuclease A studied by Monte Carlo simulated annealing. Biopolymers, 2002, 63, 273-279.	2.4	3
177	MOLECULAR DYNAMICS SIMULATIONS OF DNA DIMERS BASED ON REPLICA-EXCHANGE UMBRELLA SAMPLING II: FREE ENERGY ANALYSIS. Journal of Theoretical and Computational Chemistry, 2005, 04, 433-448.	1.8	3
178	Monte Carlo Study of First-Order Phase Transitions of a Bulk Lennardâ€“Jones Fluid System in the Isobaricâ€“Multithermal Ensemble. Bulletin of the Chemical Society of Japan, 2008, 81, 697-702.	3.2	3
179	Salt effects on hydrophobicâ€core formation in folding of a helical miniprotein studied by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 933-943.	2.6	3
180	Conformational search simulations of Trp-cage using genetic crossover. Molecular Simulation, 2015, 41, 1045-1049.	2.0	3

#	Article	IF	Citations
181	Structural Analysis of a Trimer of Î²2-Microgloblin Fragment by Molecular Dynamics Simulations. Biophysical Journal, 2019, 116, 781-790.	0.5	3
182	Enhanced sampling method in molecular simulations using genetic algorithm for biomolecular systems. Journal of Computational Chemistry, 2019, 40, 475-481.	3.3	3
183	Molecular movie of nucleotide binding to a motor protein. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129654.	2.4	3
184	Mega Process Genetic Algorithm Using Grid MP. Lecture Notes in Computer Science, 2005, , 152-170.	1.3	3
185	Constraint on â€™t Hooft indices in preon models with complementarity. Physical Review D, 1986, 34, 3923-3924.	4.7	2
186	MÃ¶bius and super-MÃ¶bius gauge fixing for the closed string amplitudes on the desk. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1988, 213, 160-164.	4.1	2
187	Thermodynamics of two lattice ice models in three dimensions. Physical Review E, 2008, 78, 041113.	2.1	2
188	Monte Carlo simulation in the isobaric-multithermal ensemble of a bulk Lennard-Jones fluid system: Thermodynamic quantities for pressure fromPâ^—=2.42to 7.25. Physical Review E, 2008, 77, 051201.	2.1	2
189	Drug Design by Generalized-Ensemble Simulations. Current Pharmaceutical Design, 2011, 17, 1758-1772.	1.9	2
190	Generalised-ensemble algorithms for studying temperature and pressure dependence of complex systems. Molecular Simulation, 2012, 38, 452-457.	2.0	2
191	Improvement of the backbone-torsion-energy term in the force field for protein systems by the double Fourier series expansion. Molecular Simulation, 2013, 39, 85-93.	2.0	2
192	Deterministic replica-exchange method without pseudo random numbers for simulations of complex systems. Computer Physics Communications, 2015, 197, 128-135.	7.5	2
193	A MULTICANONICAL STUDY OF THE PROTEIN FOLDING PROBLEM. International Journal of Modern Physics C, 1994, 05, 271-273.	1.7	1
194	Multicanonical approach in statistical mechanics of peptides. Nuclear Physics, Section B, Proceedings Supplements, 1995, 42, 914-916.	0.4	1
195	Thermodynamics of helix-coil transitions in amino-acid homopolymers studied by multicanonical algorithms. Nuclear Physics, Section B, Proceedings Supplements, 1996, 47, 842-845.	0.4	1
196	Towards the prediction of protein tertiary structures from first principles. Physica A: Statistical Mechanics and Its Applications, 1998, 254, 7-14.	2.6	1
197	Molecular simulations in the multibaric-multithermal ensembles. Computer Physics Communications, 2005, 169, 317-321.	7.5	1
198	Simulated Tempering and Magnetizing Simulations of the Ising Model. Physics Procedia, 2012, 34, 100-104.	1.2	1

#	Article	IF	Citations
199	Protein Force Field Improved by using a New Backbone-Torsion-Energy Term. Biophysical Journal, 2012, 102, 171a.	0.5	1
200	Molecular Dynamics Simulations to Clarify the Concentration Dependency of Protein Aggregation. , 2015, , .		1
201	Equilibrium Molecular Thermodynamics from Kirkwood Sampling. Journal of Physical Chemistry B, 2015, 119, 6155-6169.	2.6	1
202	Study of Ligand Binding Selectivity of Histone Deacetylases by Replica-Exchange Umbrella Sampling Molecular Dynamics Simulations. Biophysical Journal, 2016, 110, 544a-545a.	0.5	1
203	Quantum chemical replica-exchange umbrella sampling molecular dynamics simulations reveal the formation mechanism of iron phthalocyanine from iron and phthalonitrile. Journal of Chemical Physics, 2018, 149, 072332.	3.0	1
204	Analysis of liquids, gases, and supercritical fluids by a two-dimensional replica-exchange Monte Carlo method in temperature and chemical potential space. Journal of Chemical Physics, 2020, 152, 194108.	3.0	1
205	Optimizations of Protein Force Fields. Springer Series in Bio-/neuroinformatics, 2014, , 195-247.	0.1	1
206	Simulations for Tertiary Structure Predicition. Seibutsu Butsuri, 2000, 40, 308-309.	0.1	1
207	Are â€™t Hooft indices constrained in preon models with complementarity?. Physical Review D, 1989, 39, 1798-1801.	4.7	0
208	Approaching the protein folding problem. Nuclear Physics, Section B, Proceedings Supplements, 1994, 34, 792-794.	0.4	0
209	First-Principles Protein Folding Simulations. Molecular Simulation, 2000, 24, 351-368.	2.0	0
210	Free energy calculations of the stacked and unstacked states for DNA dimers by replica-exchange umbrella sampling. AIP Conference Proceedings, 2004, , .	0.4	0
211	Generalized-Ensemble Monte Carlo Algorithms for Simulations of Proteins. AIP Conference Proceedings, 2004, , .	0.4	0
212	Multibaricâ€“Multithermal Ensemble Simulation for Simple Liquids. Molecular Simulation, 2004, 30, 847-852.	2.0	0
213	Multibaricâ€“multithermal ensemble simulations for fluid systems. Physica A: Statistical Mechanics and Its Applications, 2005, 350, 150-158.	2.6	0
214	1P584 Amyloid Î²-peptides studied by the multicanonical-multioverlap algorithm(27. Molecular dynamics) Tj ETQq0 0 0 rgBT /Overlock 1 S292.	0.1	0
215	1P585 Explicit Symplectic Molecular Dynamics Simulation for Rigid-Body Molecules in the Canonical Ensemble(27. Molecular dynamics simulation,Poster Session,Abstract,Meeting Program of EABS &) Tj ETQq1 1 0.784314 rgBT /Ov		
216	Multibaricâ€“multithermal molecular dynamics simulation: generalized NosÃ©â€“PoincarÃ©â€“Andersen method. Molecular Simulation, 2007, 33, 91-96.	2.0	0

#	Article	IF	Citations
217	2P113 Simulated Annealing Molecular Dynamics Simulations of Gramicidin A in the Low-Dielectric Environment(Proteins-stability, folding, and other physicochemical properties,Poster Presentations). Seibutsu Butsuri, 2007, 47, S141.	0.1	0
218	3P043 Role of Glycines on Amyloidogenesis of Alzheimer's Amyloid-Beta Peptide Fragments(Proteins-stability, folding, and other physicochemical properties,Poster Presentations). Seibutsu Butsuri, 2007, 47, S213.	0.1	0
219	3P-056 A simulated annealing molecular dynamics simulation with a genetic crossover for protein systems(Protein:Property,The 47th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2009, 49, S160.	0.1	0
220	1P235 1I1325 Phase behavior of DPPC bilayer studied by REMD with coarse-grained model(Biol & Artifi) Tj ETQq0 0 0 rgBT /Overlock 10	0.1	0
221	3P018 A Simulated Annealing Molecular Dynamics Using Genetic Crossover with Knot Theory(Protein:) Tj ETQq1 1 0.784314 rgBT /Over S148.	0.1	0
222	3P075 Pressure dependence of protein conformations studied by generalized simulated tempering molecular dynamics simulations(Protein: Property,The 48th Annual Meeting of the Biophysical Society) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.1	0
223	3G1346 Protein Structure Predictions by Simulated Annealing Molecular Dynamics Using Genetic Crossover(3G Protein: Structure 4,The 49th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2011, 51, S131.	0.1	0
224	1H1336 Conformations of ubiquitin at high pressure studied by isobaric-isothermal simulated tempering simulations(Protein: Property 2,The 49th Annual Meeting of the Biophysical Society of) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.1	0
225	1A1412 Phase Transition Behavior of Lipid Bilayer Studied by REMD with a Coarse-Grained Model(Biol &) Tj ETQq1 1 0.784314 rgBT /Ov	0.1	0
226	3PT224 First principles molecular simulation with a generalized-ensemble algorithm for studying chemical reactions of biomolecular systems(The 50th Annual Meeting of the Biophysical Society of) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.1	0
227	1PT132 Development of a force field of backbone dihedral angles for each amino acid using Protein Data Bank(The 50th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2012, 52, S91.	0.1	0
228	Pressure-Induced Denaturation of Proteins Studied by Generalized-Ensemble Molecular Simulations. Biophysical Journal, 2012, 102, 736a.	0.5	0
229	Generalized-Ensemble Algorithms for Protein Folding and Unfolding. Current Physical Chemistry, 2012, 2, 92-106.	0.2	0
230	A Proposal for Amino Acid Dependent Main-Chain Torsion-Energy Terms for Protein Force Fields. Biophysical Journal, 2013, 104, 507a.	0.5	0
231	2P016 Optimization of force-field parameters for protein systems by an energy-based reweighting approach(01A. Protein: Structure,Poster). Seibutsu Butsuri, 2013, 53, S161.	0.1	0
232	1P128 Calculation of proton transfer in malonaldehyde using DFTB and REUS(06.Electronic) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 147 T S127.	0.1	0
233	Computer Simulations for Predicting Membrane Protein Structures with the Replica-Exchange Methods and Implicit Membrane Model of a Restricted Configurational Space. Biophysical Journal, 2014, 106, 655a.	0.5	0
234	Salt Effects on Folding of a Helical Mini Protein Villin Headpiece Subdomain HP36 Studied by Generalized-Ensemble Simulations. Biophysical Journal, 2014, 106, 672a.	0.5	0

#	Article	IF	Citations
235	2P008 Parameter dependency of an optimized force field for each amino acid(01A.) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 74 Seibutsu Butsuri, 2014, 54, S196.	0.1	0
236	Implementation of Replica-Exchange Umbrella Sampling to the DFTB+ Simulation Package. Biophysical Journal, 2015, 108, 159a.	0.5	0
237	New Implementations of Replica-exchange Method for Simulations of Complex Systems: Designed-walk and Deterministic Replica-exchange Methods. Physics Procedia, 2015, 68, 100-104.	1.2	0
238	Structural Studies of Fibril Formations of Tetrapeptides Using Replica Exchange Molecular Dynamics Simulations. Biophysical Journal, 2016, 110, 323a-324a.	0.5	0
239	Two-dimensional simulated tempering for the isobaricâ€“isothermal ensemble with fast on-the-fly weight determination. Molecular Physics, 2021, 119, .	1.7	0
240	Protein Folding Simulations by Monte Carlo Simulated Annealing and Multicanonical Algorithm. Nonconvex Optimization and Its Applications, 2000, , 73-90.	0.1	0
241	Optimizations of Protein Force-Field Parameters with Protein Data Bank. Seibutsu Butsuri, 2005, 45, 145-148.	0.1	0
242	3P-054 Molecular dynamics study of temperature and pressure effects on a biomolecule with generalized-ensemble algorithms(Protein:Property,The 47th Annual Meeting of the Biophysical Society) Tj ETQq0 0 0 rgBT /Overlock 10	0.1	0
243	Folding Simulation of a Mini Protein with a Hydrophobic Core and .ALPHA.-helices. Seibutsu Butsuri, 2012, 52, 022-023.	0.1	0
244	Structural Fluctuations of Proteins in Folding and Ligand Docking Studied by Replica-Exchange Simulations. , 2016, , 183-204.		0
245	10.1063/1.5045310.1. , 2018, , .		0
246	Optimizations of Protein Force Fields. Springer Series on Bio- and Neurosystems, 2019, , 203-256.	0.2	0
247	Distribution and Structure Analysis of Fibril-Forming Peptides Focusing on Concentration Dependency. ACS Omega, 2022, 7, 10012-10021.	3.5	0
248	Combination of genetic algorithm and generalised-ensemble algorithms for biomolecular simulations. Frontiers of Nanoscience, 2022, , 93-109.	0.6	0