

Ulrich H E Hansmann

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173
papers

5,730
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36
h-index

71
g-index

201
ext. papers

6,143
ext. citations

3.5
avg, IF

6.09
L-index

#	Paper	IF	Citations
173	Parallel tempering algorithm for conformational studies of biological molecules. <i>Chemical Physics Letters</i> , 1997 , 281, 140-150	2.5	883
172	Prediction of peptide conformation by multicanonical algorithm: New approach to the multiple-minima problem. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1333-1338	3.5	349
171	Molecular dynamics, Langevin and hybrid Monte Carlo simulations in a multicanonical ensemble. <i>Chemical Physics Letters</i> , 1996 , 259, 321-330	2.5	252
170	New Monte Carlo algorithms for protein folding. <i>Current Opinion in Structural Biology</i> , 1999 , 9, 177-83	8.1	245
169	Optimized parallel tempering simulations of proteins. <i>Journal of Chemical Physics</i> , 2006 , 124, 174903	3.9	193
168	Thermodynamics of Helix-Coil Transitions Studied by Multicanonical Algorithms. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 11276-11287		174
167	Global optimization by energy landscape paving. <i>Physical Review Letters</i> , 2002 , 88, 068105	7.4	160
166	Numerical comparisons of three recently proposed algorithms in the protein folding problem 1997 , 18, 920-933		141
165	[SMMP] A modern package for simulation of proteins. <i>Computer Physics Communications</i> , 2001 , 138, 192-212		110
164	Comparative study of multicanonical and simulated annealing algorithms in the protein folding problem. <i>Physica A: Statistical Mechanics and Its Applications</i> , 1994 , 212, 415-437	3.3	110
163	Generalized-ensemble Monte Carlo method for systems with rough energy landscape. <i>Physical Review E</i> , 1997 , 56, 2228-2233	2.4	104
162	Simulation of an ensemble with varying magnetic field: A numerical determination of the order-order interface tension in the D=2 Ising model. <i>Physical Review B</i> , 1993 , 47, 497-500	3.3	89
161	Generalized ensemble and tempering simulations: a unified view. <i>Physical Review E</i> , 2007 , 75, 026109	2.4	86
160	Parallel tempering simulations of HP-36. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003 , 52, 436-452	4.2	86
159	Finite-size scaling of helix-coil transitions in poly-alanine studied by multicanonical simulations. <i>Journal of Chemical Physics</i> , 1999 , 110, 1267-1276	3.9	78
158	Efficient sampling of protein structures by model hopping. <i>Physical Review Letters</i> , 2005 , 95, 138102	7.4	77
157	THE GENERALIZED-ENSEMBLE APPROACH FOR PROTEIN FOLDING SIMULATIONS 1999 , 129-157		76

156	Partition function zeros and finite size scaling of helix-coil transitions in a polypeptide. <i>Physical Review Letters</i> , 2000 , 84, 1836-9	7.4	70
155	Characteristic temperatures of folding of a small peptide. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1997 , 94, 10652-6	11.5	69
154	Monte Carlo simulations in generalized ensemble: Multicanonical algorithm versus simulated tempering. <i>Physical Review E</i> , 1996 , 54, 5863-5865	2.4	64
153	Energy landscape paving simulations of the trp-cage protein. <i>Journal of Chemical Physics</i> , 2005 , 122, 1943-1951	3.1	61
152	Structure and dynamics of amyloid- β segmental polymorphisms. <i>PLoS ONE</i> , 2012 , 7, e41479	3.7	61
151	The folding funnel landscape for the peptide Met-enkephalin. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 34, 472-83	4.2	57
150	In silico cross seeding of A β and amylin fibril-like oligomers. <i>ACS Chemical Neuroscience</i> , 2013 , 4, 1488-500	5.7	53
149	Optimized explicit-solvent replica exchange molecular dynamics from scratch. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 10386-7	3.4	52
148	Self-assembly of phenylalanine-based molecules. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 1609-15	2.8	50
147	An enhanced version of SMMP open-source software package for simulation of proteins. <i>Computer Physics Communications</i> , 2006 , 174, 422-429	4.2	48
146	Variation of the Energy Landscape of a Small Peptide under a Change from the ECEPP/2 Force Field to ECEPP/3. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 3304-3310	3.4	43
145	The Alzheimer beta-amyloid (A β (1-39)) dimer in an implicit solvent. <i>Journal of Chemical Physics</i> , 2008 , 129, 195102	3.9	43
144	Simulation of Top7-CF β : a transient helix extension guides folding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 8004-7	11.5	42
143	Folding proteins by first-passage-times-optimized replica exchange. <i>Physical Review E</i> , 2008 , 78, 061905	2.4	42
142	Solution effects and the order of the helix-coil transition in polyalanine. <i>Journal of Chemical Physics</i> , 2003 , 118, 2374-2380	3.9	41
141	The stability of cylindrin β -barrel amyloid oligomer models-a molecular dynamics study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013 , 81, 1542-55	4.2	38
140	Support vector machines for prediction of dihedral angle regions. <i>Bioinformatics</i> , 2006 , 22, 3009-15	7.2	38
139	Side-chain hydrophobicity and the stability of A β aggregates. <i>Protein Science</i> , 2012 , 21, 1837-48	6.3	37

138	Ground-state properties of the three-dimensional Ising spin glass. <i>Physical Review B</i> , 1994 , 50, 16444-16452	3.5	37
137	Replica exchange molecular dynamics of the thermodynamics of fibril growth of Alzheimer's A β 2 peptide. <i>Journal of Chemical Physics</i> , 2011 , 135, 065101	3.9	35
136	All-atom generalized-ensemble simulations of small proteins. <i>Journal of Molecular Graphics and Modelling</i> , 2004 , 22, 397-403	2.8	35
135	Solvation model dependency of helix-coil transition in polyalanine. <i>Biophysical Journal</i> , 2002 , 82, 3269-76	2.9	34
134	Effects of Side-Chain Charges on β -Helix Stability in C-Peptide of Ribonuclease A Studied by Multicanonical Algorithm. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 1595-1604	3.4	34
133	Multicanonical Study of the 3D Ising Spin Glass. <i>Europhysics Letters</i> , 1993 , 22, 63-68	1.6	34
132	LOCUSTRA: accurate prediction of local protein structure using a two-layer support vector machine approach. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 1903-8	6.1	32
131	Dynamics and optimal number of replicas in parallel tempering simulations. <i>Physical Review E</i> , 2007 , 76, 065701	2.4	32
130	Tertiary Structure Prediction of C-Peptide of Ribonuclease A by Multicanonical Algorithm. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 653-656	3.4	32
129	Mutations and seeding of amylin fibril-like oligomers. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 16076-85	3.4	27
128	Helix formation and folding in an artificial peptide. <i>Journal of Chemical Physics</i> , 2002 , 117, 2337-2343	3.9	27
127	Folding simulations of the A and B domains of protein G. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 6645-53	3.5	26
126	Effective way for determination of multicanonical weights. <i>Physical Review E</i> , 1997 , 56, 6200-6203	2.4	26
125	Temperature dependence of distributions of conformations of a small peptide. <i>Journal of Molecular Graphics and Modelling</i> , 1998 , 16, 226-38, 262-3	2.8	25
124	Optimizing replica exchange moves for molecular dynamics. <i>Physical Review E</i> , 2007 , 76, 057102	2.4	25
123	Comment on "Monte Carlo Simulation of a First-Order Transition for Protein Folding". <i>The Journal of Physical Chemistry</i> , 1995 , 99, 2236-2237		25
122	Inter-species cross-seeding: stability and assembly of rat-human amylin aggregates. <i>PLoS ONE</i> , 2014 , 9, e97051	3.7	24
121	Velocity-scaling optimized replica exchange molecular dynamics of proteins in a hybrid explicit/implicit solvent. <i>Journal of Chemical Physics</i> , 2011 , 135, 084115	3.9	24

120	Simulated annealing with Tsallis weights a numerical comparison. <i>Physica A: Statistical Mechanics and Its Applications</i> , 1997 , 242, 250-257	3.3	24
119	Yang-Dee zeros and the helix-coil transition in a continuum model of polyalanine. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2001 , 292, 509-518	3.3	24
118	The Alzheimer β amyloid (A β 1-39) monomer in an implicit solvent. <i>Journal of Chemical Physics</i> , 2008 , 128, 165102	3.9	22
117	Simulating Protein Fold Switching by Replica Exchange with Tunneling. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 5656-5666	6.4	21
116	Ring-like N-fold Models of A β fibrils. <i>Scientific Reports</i> , 2017 , 7, 6588	4.9	21
115	Helix versus sheet formation in a small peptide. <i>Physical Review E</i> , 2003 , 68, 041911	2.4	21
114	Stability of Iowa mutant and wild type A β peptide aggregates. <i>Journal of Chemical Physics</i> , 2014 , 141, 175101	3.9	20
113	Folding and self-assembly of a small protein complex. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3416-3422	6.4	20
112	Microcanonical replica exchange molecular dynamics simulation of proteins. <i>Physical Review E</i> , 2009 , 80, 056703	2.4	20
111	Understanding protein folding: small proteins in silico. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2008 , 1784, 252-8	4	20
110	Thermodynamics and kinetics of folding of a small peptide. <i>Journal of Chemical Physics</i> , 2001 , 115, 1601-1606	3.9	20
109	Dispersion terms and analysis of size- and charge dependence in an enhanced Poisson-Boltzmann approach. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 8910-8	3.4	19
108	SMMP v. 3.0: Simulating proteins and protein interactions in Python and Fortran. <i>Computer Physics Communications</i> , 2008 , 178, 459-470	4.2	19
107	Short-time dynamics of the helix-coil transition in polypeptides. <i>Physical Review E</i> , 2006 , 73, 040902	2.4	19
106	Aggregation of beta-amyloid fragments. <i>Journal of Chemical Physics</i> , 2007 , 126, 014706	3.9	19
105	Exploring protein energy landscapes with hierarchical clustering. <i>International Journal of Quantum Chemistry</i> , 2005 , 105, 826-830	2.1	19
104	Fibril-Barrel Transitions in Cylindrin Amyloids. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3936-3944	6.4	18
103	Extension of UNRES force field to treat polypeptide chains with D-amino-acid residues. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 4746-4757	6.4	18

102	Free-energy-driven folding and thermodynamics of the 67-residue protein GS-alpha3W--a large-scale Monte Carlo study. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1642-8	3.5	18
101	Numerical comparison of two approaches for the study of phase transitions in small systems. <i>Physical Review E</i> , 2002 , 65, 036110	2.4	18
100	Sampling of Protein Folding Transitions: Multicanonical Versus Replica Exchange Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9,	6.4	17
99	Stability of amyloid oligomers. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014 , 96, 113-41	5.3	17
98	Velocity scaling for optimizing replica exchange molecular dynamics. <i>Journal of Chemical Physics</i> , 2011 , 134, 044124	3.9	17
97	Systematic study of the boundary composition in Poisson Boltzmann calculations. <i>Journal of Computational Chemistry</i> , 2007 , 28, 2538-44	3.5	17
96	Folding of proteins with diverse folds. <i>Biophysical Journal</i> , 2006 , 91, 3573-8	2.9	17
95	Generalized-ensemble simulations of the human parathyroid hormone fragment PTH(1-34). <i>Journal of Chemical Physics</i> , 2004 , 120, 417-22	3.9	17
94	Stability of a Recently Found Triple-Stranded A β -42 Fibril Motif. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 4548-57	3.4	17
93	Stability of Osaka Mutant and Wild-Type Fibril Models. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 13063-70	3.0	16
92	Out-of-Register A β Assemblies as Models for Neurotoxic Oligomers and Fibrils. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1099-1110	6.4	16
91	Sampling Ground-State Configurations of a Peptide by Multicanonical Annealing. <i>Journal of the Physical Society of Japan</i> , 1994 , 63, 3945-3949	1.5	16
90	Computational assessment of the entropy of solvation of small-sized hydrophobic entities. <i>Physical Chemistry Chemical Physics</i> , 2006 , 8, 5515-21	3.6	15
89	Multifunnel Landscape of the Fold-Switching Protein RfaH-CTD. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 1600-1607	3.4	14
88	Replica-exchange-with-tunneling for fast exploration of protein landscapes. <i>Journal of Chemical Physics</i> , 2015 , 143, 224102	3.9	14
87	On the lack of polymorphism in A β peptide aggregates derived from patient brains. <i>Protein Science</i> , 2015 , 24, 923-35	6.3	14
86	A New Look at the 2D Ising Model from Exact Partition Function Zeros for Large Lattice Sizes. <i>International Journal of Modern Physics C</i> , 1997 , 08, 1063-1071	1.1	14
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82	Short-time dynamics of polypeptides. <i>Journal of Chemical Physics</i> , 2007 , 126, 045107	3.9	12
81	Protein-folding simulations in generalized ensembles. <i>International Journal of Quantum Chemistry</i> , 2002 , 90, 1515-1521	2.1	12
80	Modeling Structural Flexibility of Proteins with Go-Models. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2127-2133	6.4	11
79	Internal and environmental effects on folding and dimerization of the Alzheimer β amyloid peptide. <i>Molecular Simulation</i> , 2011 , 37,	2	11
78	Caching of a chameleon segment facilitates folding of a protein with end-to-end beta-sheet. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 15134-9	3.4	11
77	Protein simulations combining an all-atom force field with a Go term. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 285215	1.8	11
76	On the helix-coil transition in alanine based polypeptides in gas phase. <i>Journal of Chemical Physics</i> , 2007 , 126, 204307	3.9	11
75	Parallel tempering molecular dynamics folding simulation of a signal peptide in explicit water. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 68, 662-9	4.2	10
74	NUMERICAL COMPARISON OF WANG-ANDAU SAMPLING AND PARALLEL TEMPERING FOR MET-ENKEPHALIN. <i>International Journal of Modern Physics C</i> , 2006 , 17, 817-824	1.1	10
73	Partition function zeros and leading-order scaling correction of the 3D Ising model from multicanonical simulations. <i>Journal of Physics A</i> , 2000 , 33, 7489-7498		10
72	The van Hemmen spin glass revisited. <i>Journal of Statistical Physics</i> , 1993 , 73, 775-788	1.5	10
71	Side-chain and backbone ordering in a polypeptide. <i>Journal of Chemical Physics</i> , 2006 , 125, 164902	3.9	9
70	Helix Propensities of Amino Acids Studied by Multicanonical Algorithm. <i>Chemistry Letters</i> , 1995 , 24, 391-392	1.7	9
69	Tackling the protein folding problem by a generalized-ensemble approach with Tsallis statistics. <i>Brazilian Journal of Physics</i> , 1999 , 29,	1.2	9
68	Presence of a SARS-CoV-2 Protein Enhances Amyloid Formation of Serum Amyloid A. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 9155-9167	3.4	9
67	A numerical investigation into possible mechanisms by that the A629P mutant of ATP7A causes Menkes Disease. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 11390-7	3.6	8

66	Molecular dynamics simulations of early steps in RNA-mediated conversion of prions. <i>Protein Science</i> , 2017 , 26, 1524-1534	6.3	7
65	Cleavage, Downregulation, and Aggregation of Serum Amyloid A. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 1009-1019	3.4	7
64	Effect of single point mutations in a form of systemic amyloidosis. <i>Protein Science</i> , 2015 , 24, 1451-62	6.3	7
63	DETECTING SECONDARY BOTTLENECKS IN PARALLEL QUANTUM CHEMISTRY APPLICATIONS USING MPI. <i>International Journal of Modern Physics C</i> , 2008 , 19, 1-13	1.1	7
62	Simulations of a small protein in a specifically designed generalized ensemble. <i>Physical Review E</i> , 2004 , 70, 012902	2.4	7
61	Structural transitions in biomolecules - a numerical comparison of two approaches for the study of phase transitions in small systems. <i>International Journal of Molecular Sciences</i> , 2002 , 3, 17-29	6.3	7
60	Conversion between parallel and antiparallel β sheets in wild-type and Iowa mutant A β fibrils. <i>Journal of Chemical Physics</i> , 2018 , 148, 045103	3.9	6
59	Folding and association of a homotetrameric protein complex in an all-atom Go model. <i>Physical Review E</i> , 2013 , 87, 014701	2.4	6
58	Chameleonicity and folding of the C-fragment of TOP7. <i>Europhysics Letters</i> , 2012 , 97, 68003	1.6	6
57	Generalized-ensemble simulations of all-atom protein models. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2005 , 350, 28-37	3.3	6
56	Structure determination of organic molecules from diffraction data by simulated annealing. <i>Physical Review E</i> , 2001 , 64, 056707	2.4	6
55	d-Retro Inverso Amylin and the Stability of Amylin Fibrils. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5358-5368	6.4	6
54	Stability of the N-Terminal Helix and Its Role in Amyloid Formation of Serum Amyloid A. <i>ACS Omega</i> , 2018 , 3, 16184-16190	3.9	6
53	Large fatty acid-derived A β 2 oligomers form ring-like assemblies. <i>Journal of Chemical Physics</i> , 2019 , 150, 075101	3.9	5
52	Pearl-Necklace-Like Local Ordering Drives Polypeptide Collapse. <i>Macromolecules</i> , 2019 , 52, 5491-5498	5.5	5
51	All-atom Simulation of Amyloid Aggregates. <i>Physics Procedia</i> , 2015 , 68, 61-68		5
50	Ring polymer simulations with global radius of curvature. <i>Physical Review E</i> , 2007 , 75, 051803	2.4	5
49	New algorithms and the physics of proteins. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2003 , 321, 152-163	3.3	5

48	Proteinlike behavior of a spin system near the transition between a ferromagnet and a spin glass. <i>Physical Review E</i> , 2001 , 64, 052903	2.4	5
47	COMPUTER SIMULATION OF BIOLOGICAL MACROMOLECULES IN GENERALIZED ENSEMBLES. <i>International Journal of Modern Physics C</i> , 1999 , 10, 1521-1530	1.1	5
46	The effect of retro-inverse D-amino acid Aβ-peptides on Aβ-fibril formation. <i>Journal of Chemical Physics</i> , 2019 , 150, 095101	3.9	4
45	Folding and self-assembly of a small heterotetramer. <i>Journal of Chemical Physics</i> , 2014 , 140, 105103	3.9	4
44	Multicanonical Molecular Dynamics Simulations of the N-terminal Domain of Protein L9. <i>Europhysics Letters</i> , 2014 , 105, 30008	1.6	4
43	Temperature random walk sampling of protein configurations. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2010 , 389, 1400-1404	3.3	4
42	A Simple Ansatz to Describe Thermodynamic Quantities of Peptides and Proteins at Low Temperatures. <i>International Journal of Modern Physics C</i> , 1997 , 08, 1085-1093	1.1	4
41	Side-chain and backbone ordering in homopolymers. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 4244-50	3.4	4
40	Protein energy landscapes as studied by a generalized-ensemble approach with Tsallis statistics. <i>Chaos, Solitons and Fractals</i> , 2002 , 13, 507-512	9.3	4
39	Energy landscape paving for X-ray structure determination of organic molecules. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2002 , 58, 259-64		4
38	A simple hydrophobicity-based score for profiling protein structures. <i>Journal of Physics Condensed Matter</i> , 2005 , 17, S1595-S1606	1.8	4
37	Stability of Human Serum Amyloid A Fibrils. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 10708-10717	3.4	4
36	Bifurcated Hydrogen Bonds and the Fold Switching of Lymphotoxin. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 6555-6564	3.4	4
35	Binding of ACE-inhibitors to in vitro and patient-derived amyloid-β-fibril models. <i>Journal of Chemical Physics</i> , 2016 , 144, 015101	3.9	4
34	Stability differences in the NMR ensembles of amyloid β-fibrils. <i>Journal of Theoretical and Computational Chemistry</i> , 2016 , 15, 1650059	1.8	3
33	Global minimum configuration of a small peptide for the ECEPP/2 and ECEPP/3 force fields. <i>Chemical Physics Letters</i> , 1997 , 268, 86-92	2.5	3
32	Solution Effects and the Folding of an Artificial Peptide. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 10284-10293	3.4	3
31	GLASS TRANSITION TEMPERATURE AND FRACTAL DIMENSION OF PROTEIN FREE ENERGY LANDSCAPES. <i>International Journal of Modern Physics C</i> , 2000 , 11, 301-308	1.1	3

30	Altering the Solubility of the Antibiotic Candidate Nisin-A Computational Study. <i>ACS Omega</i> , 2020 , 5, 24854-24863	3.9	3
29	BETTY: prediction of beta-strand type from sequence. <i>In Silico Biology</i> , 2007 , 7, 535-42	2	3
28	Mutations Alter RNA-Mediated Conversion of Human Prions. <i>ACS Omega</i> , 2018 , 3, 3936-3944	3.9	2
27	Stability of A β Fibril fragments in the presence of fatty acids. <i>Protein Science</i> , 2019 , 28, 1973-1981	6.3	2
26	Multicanonical Monte Carlo simulations of a de novo designed protein with end-to-end β sheet. <i>Journal of Chemical Physics</i> , 2014 , 140, 065101	3.9	2
25	Sampling Protein Energy Landscapes ¶The Quest for Efficient Algorithms 2011 , 209-230		2
24	Toward reliable simulations of protein folding, misfolding and aggregation. <i>Progress in Molecular Biology and Translational Science</i> , 2008 , 84, 39-55	4	2
23	Protein structure prediction by tempering spatial constraints. <i>Journal of Computer-Aided Molecular Design</i> , 2005 , 19, 603-8	4.2	2
22	Groundstates of the 3d Edwards-Anderson spin glass model. <i>Nuclear Physics, Section B, Proceedings Supplements</i> , 1995 , 42, 905-907		2
21	Multimagnetical simulation of the Ising model. <i>Nuclear Physics, Section B, Proceedings Supplements</i> , 1993 , 30, 285-288		2
20	Enhanced Sampling for Biomolecular Simulations. <i>Springer Series in Bio-/neuroinformatics</i> , 2014 , 249-267		1
19	Generalized ensembles: A new way of simulating proteins. <i>Physica A: Statistical Mechanics and Its Applications</i> , 1998 , 254, 15-23	3.3	1
18	Multicanonical approach in statistical mechanics of peptides. <i>Nuclear Physics, Section B, Proceedings Supplements</i> , 1995 , 42, 914-916		1
17	Thermodynamics of helix-coil transitions in amino-acid homopolymers studied by multicanonical algorithms. <i>Nuclear Physics, Section B, Proceedings Supplements</i> , 1996 , 47, 842-845		1
16	SPIN GLASS GROUNDSTATE INVESTIGATION BY MULTICANONICAL ENSEMBLE. <i>International Journal of Modern Physics C</i> , 1994 , 05, 263-265	1.1	1
15	A MULTICANONICAL STUDY OF THE PROTEIN FOLDING PROBLEM. <i>International Journal of Modern Physics C</i> , 1994 , 05, 271-273	1.1	1
14	Cleavage, down-regulation and aggregation of serum amyloid A		1
13	Effect of Lauric Acid on the Stability of A β Oligomers. <i>ACS Omega</i> , 2021 , 6, 5795-5804	3.9	1

- 12 Small Peptides for Inhibiting Serum Amyloid A Aggregation. *ACS Medicinal Chemistry Letters*, **2021**, 12, 1613-1621 4.3 ○
- 11 Enhanced Sampling for Biomolecular Simulations. *Springer Series on Bio- and Neurosystems*, **2019**, 257-280.5 ○
- 10 Interconversion between Serum Amyloid A Native and Fibril Conformations.. *ACS Omega*, **2022**, 7, 121863, 121920
- 9 Protein Folding in Silico □The Quest for Better Algorithms **2005**, 275-296
- 8 On the protein folding problem. *Nuclear Physics, Section B, Proceedings Supplements*, **1996**, 47, 188-195
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- 5 Thermodynamics of Protein Folding □The Generalized-Ensemble Approach. *Nonconvex Optimization and Its Applications*, **2000**, 91-105
- 4 New Algorithms and the Physics of Protein Folding **2004**, 173-192
- 3 Recent Results from Protein-Folding Simulations in Generalized Ensembles. *Springer Proceedings in Physics*, **1999**, 62-67 0.2
- 2 Proteins Studied by Computer Simulations. *Lecture Notes in Computer Science*, **2012**, 56-65 0.9
- 1 Response to "Comment on □Replica-exchange-with-tunneling for fast exploration of protein landscapes" [J. Chem. Phys. 145, 057101 (2016)]. *Journal of Chemical Physics*, **2016**, 145, 057102 3.9