John E Straub

List of Publications by Year
in descending order

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159	9,232	36303	46799
papers	citations	51 h-index	89 g-index

170	170	170	6384
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimerâ€™s Disease, Parkinsonâ€™s Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. Chemical Reviews, 2021, 121, 2545-2647.	47.7	406
2	Classical and modern methods in reaction rate theory. The Journal of Physical Chemistry, 1988, 92, 3711-3725.	2.9	377
3	Monomer adds to preformed structured oligomers of Abeta-peptides by a two-stage dock-lock mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 111-116.	7.1	344
4	Role of Water in Protein Aggregation and Amyloid Polymorphism. Accounts of Chemical Research, 2012, 45, 83-92.	15.6	301
5	Toward a Molecular Theory of Early and Late Events in Monomer to Amyloid Fibril Formation. Annual Review of Physical Chemistry, 2011, 62, 437-463.	10.8	249
6	Novel methods of sampling phase space in the simulation of biological systems. Current Opinion in Structural Biology, 1997, 7, 181-189.	5.7	206
7	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	47.7	205
8	Dynamics of Asp23â^'Lys28 Salt-Bridge Formation in AÎ²10-35Monomers. Journal of the American Chemical Society, 2006, 128, 16159-16168.	13.7	200
9	Entropic Stabilization of Proteins by TMAO. Journal of Physical Chemistry B, 2011, 115, 13401-13407.	2.6	174
10	Nonâ€Markovian activated rate processes: Comparison of current theories with numerical simulation data. Journal of Chemical Physics, 1986, 84, 1788-1794.	3.0	161
11	A Molecular Switch in Amyloid Assembly:â€‰ Met³⁵and Amyloid Î²-Protein Oligomerization. Journal of the American Chemical Society, 2003, 125, 15359-15365.	13.7	158
12	Molecular dynamics study of the photodissociation of carbon monoxide from myoglobin: Ligand dynamics in the first 10 ps. Chemical Physics, 1991, 158, 221-248.	1.9	156
13	Aqueous urea solution destabilizes AÂ16-22 oligomers. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 14760-14765.	7.1	151
14	Generalized simulated annealing algorithms using Tsallis statistics: Application to conformational optimization of a tetrapeptide. Physical Review E, 1996, 53, R3055-R3058.	2.1	149
15	Influence of Preformed Asp23â^'Lys28 Salt Bridge on the Conformational Fluctuations of Monomers and Dimers of AÎ² Peptides with Implications for Rates of Fibril Formation. Journal of Physical Chemistry B, 2009, 113, 1162-1172.	2.6	147
16	Sequence Effects on Size, Shape, and Structural Heterogeneity in Intrinsically Disordered Proteins. Journal of Physical Chemistry B, 2019, 123, 3462-3474.	2.6	125
17	Molecular dynamics study of an isomerizing diatomic in a Lennardâ€Jones fluid. Journal of Chemical Physics, 1988, 89, 4833-4847.	3.0	122
18	The MaxFlux algorithm for calculating variationally optimized reaction paths for conformational transitions in many body systems at finite temperature. Journal of Chemical Physics, 1997, 107, 5000-5006.	3.0	122

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19	Simulation Study of the Structure and Dynamics of the Alzheimerâ€™s Amyloid Peptide Congener in Solution. Biophysical Journal, 2001, 80, 31-44.	0.5	120
20	Dynamics of locking of peptides onto growing amyloid fibrils. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11948-11953.	7.1	116
21	Dynamic friction on rigid and flexible bonds. Journal of Chemical Physics, 1990, 93, 5084-5095.	3.0	115
22	Global energy minimum searches using an approximate solution of the imaginary time Schroedinger equation. The Journal of Physical Chemistry, 1993, 97, 6715-6721.	2.9	115
23	Vibrational energy relaxation in proteins. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6726-6731.	7.1	115
24	On Monte Carlo and molecular dynamics methods inspired by Tsallis statistics: Methodology, optimization, and application to atomic clusters. Journal of Chemical Physics, 1997, 107, 9117-9124.	3.0	112
25	Statistical-Temperature MonteÂCarlo and Molecular Dynamics Algorithms. Physical Review Letters, 2006, 97, 050601.	7.8	111
26	Probing the Initial Stage of Aggregation of the AÎ²10-35-protein: Assessing the Propensity for Peptide Dimerization. Journal of Molecular Biology, 2005, 345, 1141-1156.	4.2	106
27	Energy landscape theory for Alzheimer's amyloid ?-peptide fibril elongation. Proteins: Structure, Function and Bioinformatics, 2001, 42, 217-229.	2.6	104
28	Theoretical study of intramultiplet transitions in collisions of atoms inP3electronic states with structureless targets:Ca(P3)+He. Physical Review A, 1983, 28, 73-82.	2.5	103
29	Time scales and pathways for kinetic energy relaxation in solvated proteins: Application to carbonmonoxy myoglobin. Journal of Chemical Physics, 2000, 113, 7702-7711.	3.0	99
30	Principles governing oligomer formation in amyloidogenic peptides. Current Opinion in Structural Biology, 2010, 20, 187-195.	5.7	97
31	Directed Energy â€œFunneling" Mechanism for Heme Cooling Following Ligand Photolysis or Direct Excitation in Solvated Carbonmonoxy Myoglobin. Journal of Physical Chemistry B, 2001, 105, 7057-7063.	2.6	95
32	Structures of Î²-Amyloid Peptide 1â^'40, 1â^'42, and 1â^'55â€”the 672â^'726 Fragment of APPâ€”in a Membrane Environment with Implications for Interactions with Î³-Secretase. Journal of the American Chemical Society, 2009, 131, 17843-17852.	13.7	95
33	Design, synthesis, and biomedical applications of synthetic sulphated polysaccharides. Chemical Society Reviews, 2019, 48, 2338-2365.	38.1	93
34	Thermodynamic Perspective on the Dockâ^'Lock Growth Mechanism of Amyloid Fibrils. Journal of Physical Chemistry B, 2009, 113, 14421-14430.	2.6	88
35	Orientational potentials extracted from protein structures improve native fold recognition. Protein Science, 2004, 13, 862-874.	7.6	84
36	Dry amyloid fibril assembly in a yeast prion peptide is mediated by long-lived structures containing water wires. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 21459-21464.	7.1	82

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37	Generalized Replica Exchange Method. Journal of Chemical Physics, 2010, 132, 224107.	3.0	80
38	Transmembrane Structures of Amyloid Precursor Protein Dimer Predicted by Replica-Exchange Molecular Dynamics Simulations. Journal of the American Chemical Society, 2009, 131, 3438-3439.	13.7	79
39	Impact of membrane lipid composition on the structure and stability of the transmembrane domain of amyloid precursor protein. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E5281-7.	7.1	74
40	Dynamics in Rugged Energy Landscapes with Applications to the S-Peptide and Ribonuclease A. Journal of the American Chemical Society, 1994, 116, 2049-2063.	13.7	71
41	Structures and Free-Energy Landscapes of the Wild Type and Mutants of the AÎ²21â€“30 Peptide Are Determined by an Interplay between Intrapeptide Electrostatic and Hydrophobic Interactions. Journal of Molecular Biology, 2008, 379, 815-829.	4.2	71
42	Simulated annealing using the classical density distribution. Journal of Chemical Physics, 1994, 101, 533-541.	3.0	70
43	Charge states rather than propensity for Î²-structure determine enhanced fibrillogenesis in wild-type Alzheimer's Î²-amyloid peptide compared to E22Q Dutch mutant. Protein Science, 2009, 11, 1639-1647.	7.6	69
44	Spatial dependence of timeâ€dependent friction for pair diffusion in a simple fluid. Journal of Chemical Physics, 1990, 93, 6804-6812.	3.0	66
45	Probing the Structure and Dynamics of Confined Water in AOT Reverse Micelles. Journal of Physical Chemistry B, 2013, 117, 7345-7351.	2.6	61
46	Smart Darting Monte Carlo. Journal of Chemical Physics, 2001, 114, 6994-7000.	3.0	60
47	A rapid method for determining rate constants by molecular dynamics. Journal of Chemical Physics, 1985, 83, 1138-1139.	3.0	59
48	Long Time Dynamic Simulations:â€‰Exploring the Folding Pathways of an Alzheimer's Amyloid AÎ²-Peptide. Accounts of Chemical Research, 2002, 35, 473-481.	15.6	59
49	Energy equipartitioning in the classical timeâ€dependent Hartree approximation. Journal of Chemical Physics, 1991, 94, 6737-6739.	3.0	58
50	Approximate solution of the classical Liouville equation using Gaussian phase packet dynamics: Application to enhanced equilibrium averaging and global optimization. Journal of Chemical Physics, 1993, 99, 4024-4035.	3.0	57
51	A Study of Vibrational Relaxation of B-State Carbon Monoxide in the Heme Pocket of Photolyzed Carboxymyoglobin. Biophysical Journal, 1999, 77, 70-84.	0.5	55
52	Propensity to Form Amyloid Fibrils Is Encoded as Excitations in the Free Energy Landscape of Monomeric Proteins. Journal of Molecular Biology, 2014, 426, 2653-2666.	4.2	55
53	Characterizing the structural ensemble of Î³-secretase using a multiscale molecular dynamics approach. Chemical Science, 2017, 8, 5576-5584.	7.4	55
54	Shortcomings of current theories of nonâ€Markovian activated rate processes. Journal of Chemical Physics, 1985, 83, 3172-3174.	3.0	52

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55	Transmembrane Fragment Structures of Amyloid Precursor Protein Depend on Membrane Surface Curvature. Journal of the American Chemical Society, 2014, 136, 854-857.	13.7	52
56	A statistical theory for the effect of nonadiabatic transitions on activated processes. Journal of Chemical Physics, 1987, 87, 6111-6116.	3.0	51
57	Simulation study of the collapse of linear and ring homopolymers. Journal of Chemical Physics, 1995, 103, 2615-2624.	3.0	51
58	Molecular Dynamics Simulation Study of the B-States of Solvated Carbon Monoxymyoglobin. Journal of the American Chemical Society, 1997, 119, 2541-2551.	13.7	51
59	Energy diffusion in manyâ€dimensional Markovian systems: The consequences of competition between interâ€and intramolecular vibrational energy transfer. Journal of Chemical Physics, 1986, 85, 2999-3006.	3.0	50
60	Simulating Vibrational Energy Flow in Proteins:Â Relaxation Rate and Mechanism for Heme Cooling in Cytochrome c. Journal of Physical Chemistry B, 2003, 107, 12339-12345.	2.6	50
61	Time-dependent perturbation theory for vibrational energy relaxation and dephasing in peptides and proteins. Journal of Chemical Physics, 2006, 124, 144910.	3.0	50
62	Generalized parallel sampling. Physica A: Statistical Mechanics and Its Applications, 2002, 305, 157-171.	2.6	49
63	Efforts toward Developing Direct Probes of Protein Dynamics. Journal of the American Chemical Society, 2006, 128, 6028-6029.	13.7	49
64	Differences in the free energies between the excited states of A Î² 40 and A Î² 42 monomers encode their aggregation propensities. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 19926-19937.	7.1	49
65	Structural and dynamical analysis of the hydration of the Alzheimer's Î²-amyloid peptide. Journal of Computational Chemistry, 2003, 24, 143-153.	3.3	48
66	Direct computation of long time processes in peptides and proteins: Reaction path study of the coil-to-helix transition in polyalanine. Proteins: Structure, Function and Bioinformatics, 1999, 36, 249-261.	2.6	47
67	Statistical temperature molecular dynamics: Application to coarse-grained Î²-barrel-forming protein models. Journal of Chemical Physics, 2007, 126, 135101.	3.0	46
68	Molecular Dynamics Study on the Solvent Dependent Heme Cooling Following Ligand Photolysis in Carbonmonoxy Myoglobin. Journal of Physical Chemistry B, 2007, 111, 3243-3250.	2.6	46
69	Probing the Origins of Increased Activity of the E22Q â€œDutchâ€•Mutant Alzheimer's Î²-Amyloid Peptide. Biophysical Journal, 2001, 81, 697-709.	0.5	45
70	Influence of Nanoparticle Size and Shape on Oligomer Formation of an Amyloidogenic Peptide. Journal of Physical Chemistry Letters, 2011, 2, 1171-1177.	4.6	45
71	Critical size dependence of domain formation observed in coarse-grained simulations of bilayers composed of ternary lipid mixtures. Journal of Chemical Physics, 2017, 147, 095101.	3.0	43
72	Sequence and Crowding Effects in the Aggregation of a 10-Residue Fragment Derived from Islet Amyloid Polypeptide. Biophysical Journal, 2009, 96, 4552-4560.	0.5	42

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73	Empirical Maps For The Calculation of Amide I Vibrational Spectra of Proteins From Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2014, 118, 7848-7855.	2.6	41
74	Quantum dynamics of N-methylacetamide studied by the vibrational configuration interaction method. Chemical Physics Letters, 2007, 443, 6-11.	2.6	40
75	Structural Heterogeneity in Transmembrane Amyloid Precursor Protein Homodimer Is a Consequence of Environmental Selection. Journal of the American Chemical Society, 2014, 136, 9619-9626.	13.7	40
76	Analysis of the role of attractive forces in self-diffusion of a simple fluid. Molecular Physics, 1992, 76, 373-385.	1.7	39
77	Structure of APP-C991â€“99 and implications for role of extra-membrane domains in function and oligomerization. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1698-1708.	2.6	38
78	Membrane-wrapped nanoparticles probe divergent roles of GM3 and phosphatidylserine in lipid-mediated viral entry pathways. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E9041-E9050.	7.1	38
79	Vibrational Energy Relaxation of â€œTailoredâ€•Hemes in Myoglobin Following Ligand Photolysis Supports Energy Funneling Mechanism of Heme â€œCoolingâ€• Journal of Physical Chemistry B, 2003, 107, 10634-10639.	2.6	37
80	Replica Exchange Statistical Temperature Molecular Dynamics Algorithm. Journal of Physical Chemistry B, 2012, 116, 8646-8653.	2.6	37
81	Regimes of Complex Lipid Bilayer Phases Induced by Cholesterol Concentration in MD Simulation. Biophysical Journal, 2018, 115, 2167-2178.	0.5	37
82	Communication: Iteration-free, weighted histogram analysis method in terms of intensive variables. Journal of Chemical Physics, 2011, 135, 061103.	3.0	36
83	Specific Binding of Cholesterol to C99 Domain of Amyloid Precursor Protein Depends Critically on Charge State of Protein. Journal of Physical Chemistry Letters, 2016, 7, 3535-3541.	4.6	35
84	Vibrational Frequency Shifts and Relaxation Rates for a Selected Vibrational Mode in Cytochrome c. Biophysical Journal, 2003, 85, 1429-1439.	0.5	32
85	Cellular prion protein targets amyloid-Î² fibril ends via its C-terminal domain to prevent elongation. Journal of Biological Chemistry, 2017, 292, 16858-16871.	3.4	32
86	Monte Carlo simulations of polyalanine using a reduced model and statistics-based interaction potentials. Journal of Chemical Physics, 2005, 122, 024904.	3.0	31
87	Resilience of the Iron Environment in Heme Proteins. Biophysical Journal, 2008, 95, 5874-5889.	0.5	31
88	Mode-Specific Vibrational Energy Relaxation of Amide Iâ€² and IIâ€² Modes in N-Methylacetamide/Water Clusters: Intra- and Intermolecular Energy Transfer Mechanisms. Journal of Physical Chemistry A, 2009, 113, 3051-3060.	2.5	30
89	Vibrational energy flow across hemeâ€“cytochrome c and cytochrome câ€“water interfaces. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	30
90	Extracting the Energy Barrier Distribution of a Disordered System from the Instantaneous Normal Mode Density of States: Applications to Peptides and Proteins. The Journal of Physical Chemistry, 1994, 98, 10978-10987.	2.9	29

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91	Mean First-Passage Time Calculations for the Coil-to-Helix Transition:Â The Active Helix Ising Modelâ€. Journal of Physical Chemistry B, 2001, 105, 6684-6697.	2.6	29
92	Bicelles Rich in both Sphingolipids and Cholesterol and Their Use in Studies of Membrane Proteins. Journal of the American Chemical Society, 2020, 142, 12715-12729.	13.7	29
93	The influence of intramolecular vibrational relaxation on the pressure dependence of unimolecular rate constants. Journal of Chemical Physics, 1986, 85, 146-149.	3.0	28
94	Theoretical probes of conformational fluctuations in S-peptide and RNase A/3â€²-UMP enzyme product complex. Proteins: Structure, Function and Bioinformatics, 1993, 15, 360-373.	2.6	27
95	Continuous anisotropic representation of coarse-grained potentials for proteins by spherical harmonics synthesis. Journal of Molecular Graphics and Modelling, 2004, 22, 441-450.	2.4	27
96	Combined Molecular Dynamics Simulations and Experimental Studies of the Structure and Dynamics of Poly-Amido-Saccharides. Journal of the American Chemical Society, 2016, 138, 6532-6540.	13.7	27
97	Vibrational Energy Relaxation of Isotopically Labeled Amide I Modes in Cytochrome c:â€‰ Theoretical Investigation of Vibrational Energy Relaxation Rates and Pathways. Journal of Physical Chemistry B, 2007, 111, 12017-12023.	2.6	26
98	Generalized simulated tempering for exploring strong phase transitions. Journal of Chemical Physics, 2010, 133, 154101.	3.0	26
99	Simulated annealing using coarse grained classical dynamics: Smoluchowski dynamics in the Gaussian density approximation. Journal of Chemical Physics, 1995, 103, 1574-1581.	3.0	25
100	Orientation-dependent coarse-grained potentials derived by statistical analysis of molecular structural databases. Polymer, 2004, 45, 597-608.	3.8	25
101	Replica exchange statistical temperature Monte Carlo. Journal of Chemical Physics, 2009, 130, 124112.	3.0	25
102	Membraneâ€“Protein Interactions Are Key to Understanding Amyloid Formation. Journal of Physical Chemistry Letters, 2014, 5, 633-635.	4.6	25
103	Exploring the structure and stability of cholesterol dimer formation in multicomponent lipid bilayers. Journal of Computational Chemistry, 2017, 38, 1479-1488.	3.3	25
104	Direct Observation of Cholesterol Dimers and Tetramers in Lipid Bilayers. Journal of Physical Chemistry B, 2021, 125, 1825-1837.	2.6	25
105	Aerosol-OT Surfactant Forms Stable Reverse Micelles in Apolar Solvent in the Absence of Water. Journal of Physical Chemistry B, 2019, 123, 2546-2557.	2.6	23
106	Addressing the Excessive Aggregation of Membrane Proteins in the MARTINI Model. Journal of Chemical Theory and Computation, 2021, 17, 2513-2521.	5.3	23
107	Finding the needle in the haystack: Algorithms for conformational optimization. Computers in Physics, 1996, 10, 449.	0.5	22
108	Global optimization using bad derivatives: Derivative-free method for molecular energy minimization. Journal of Computational Chemistry, 1998, 19, 1445-1455.	3.3	22

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109	Quantum and classical vibrational relaxation dynamics of Nâ€methylacetamide on ab initio potential energy surfaces. International Journal of Quantum Chemistry, 2009, 109, 2047-2057.	2.0	22
110	Coarse-Grained Model of Coil-to-Helix Kinetics Demonstrates the Importance of Multiple Nucleation Sites in Helix Folding. Journal of Chemical Theory and Computation, 2006, 2, 674-684.	5.3	20
111	Influence of membrane lipid composition on the structure and activity of Î³-secretase. Physical Chemistry Chemical Physics, 2018, 20, 27294-27304.	2.8	20
112	OPTIMIZATION TECHNIQUES WITH APPLICATIONS TO PROTEINS. Advanced Series in Physical Chemistry, 1996, , 137-196.	1.5	20
113	Sequence Determines the Switch in the Fibril Forming Regions in the Low-Complexity FUS Protein and Its Variants. Journal of Physical Chemistry Letters, 2021, 12, 9026-9032.	4.6	19
114	Numerical simulation of rate constants for a two degree of freedom system in the weak collision limit. Journal of Chemical Physics, 1987, 86, 4296-4297.	3.0	18
115	Relationship between protein folding thermodynamics and the energy landscape. Physical Review E, 2009, 79, 030902.	2.1	18
116	Exploring the impact of proteins on the line tension of a phase-separating ternary lipid mixture. Journal of Chemical Physics, 2019, 150, 204702.	3.0	18
117	Direct evidence for mode-specific vibrational energy relaxation from quantum time-dependent perturbation theory. I. Five-coordinate ferrous iron porphyrin model. Journal of Chemical Physics, 2009, 130, 025102.	3.0	17
118	Exploring the Solidâ€“Liquid Phase Change of an Adapted Dzugutov Model Using Generalized Replica Exchange Method. Journal of Physical Chemistry B, 2012, 116, 8654-8661.	2.6	17
119	Limit of Metastability for Liquid and Vapor Phases of Water. Physical Review Letters, 2014, 112, 157802.	7.8	17
120	Optimal replica exchange method combined with Tsallis weight sampling. Journal of Chemical Physics, 2009, 130, 144114.	3.0	16
121	Structural Basis for Lipid Binding and Function by an Evolutionarily Conserved Protein, Serum Amyloid A. Journal of Molecular Biology, 2020, 432, 1978-1995.	4.2	16
122	Energy minimization using the classical density distribution: Application to sodium chloride clusters. Physical Review B, 1996, 53, 13857-13863.	3.2	15
123	Order parameter free enhanced sampling of the vapor-liquid transition using the generalized replica exchange method. Journal of Chemical Physics, 2013, 138, 104119.	3.0	15
124	Extension of a protein docking algorithm to membranes and applications to amyloid precursor protein dimerization. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2170-2185.	2.6	15
125	Diversity of Solvent Dependent Energy Transfer Pathways in Heme Proteins. Journal of Physical Chemistry B, 2009, 113, 825-830.	2.6	14
126	Computational methods inspired by Tsallis statistics: Monte Carlo and molecular dynamics algorithms for the simulation of classical and quantum systems. Brazilian Journal of Physics, 1999, 29, 179-186.	1.4	14

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127	Simulation Analysis of the Binding Interactions in the RNase A/3'-UMP Enzyme-Product Complex as a Function of pH. Journal of the American Chemical Society, 1994, 116, 2591-2599.	13.7	13
128	Exploring the role of hydration and confinement in the aggregation of amyloidogenic peptides AÎ²16â˜’22 and Sup357â˜’13 in AOT reverse micelles. Journal of Chemical Physics, 2014, 141, 22D530.	3.0	13
129	The interpretation of site-directed mutagenesis experiments by linear free energy relations. Protein Engineering, Design and Selection, 1990, 3, 673-675.	2.1	12
130	An efficient Monte Carlo algorithm for overcoming broken ergodicity in the simulation of spin systems. Physica A: Statistical Mechanics and Its Applications, 1997, 247, 553-558.	2.6	11
131	Investigating the solid-liquid phase transition of water nanofilms using the generalized replica exchange method. Journal of Chemical Physics, 2014, 141, 18C525.	3.0	11
132	Finite-Size Effects and Optimal System Sizes in Simulations of Surfactant Micelle Self-Assembly. Journal of Physical Chemistry B, 2021, 125, 5068-5077.	2.6	11
133	Interfacial hydration determines orientational and functional dimorphism of sterol-derived Raman tags in lipid-coated nanoparticles. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	10
134	Role of Charge and Solvation in the Structure and Dynamics of Alanine-Rich Peptide AKA2 in AOT Reverse Micelles. Journal of Physical Chemistry B, 2015, 119, 9084-9090.	2.6	9
135	Molecular Insights into Human Hereditary Apolipoprotein A-I Amyloidosis Caused by the Glu34Lys Mutation. Biochemistry, 2018, 57, 5738-5747.	2.5	9
136	Impact of Cholesterol Concentration and Lipid Phase on Structure and Fluctuation of Amyloid Precursor Protein. Journal of Physical Chemistry B, 2020, 124, 10173-10185.	2.6	9
137	Vibrational Energy Relaxation (Ver) of a CD Stretching Mode in Cytochrome c. Advances in Chemical Physics, 2005, , 179-203.	0.3	8
138	â€œStrange Kineticsâ€•in the Temperature Dependence of Methionine Ligand Rebinding Dynamics in Cytochrome c. Journal of Physical Chemistry B, 2013, 117, 7190-7202.	2.6	8
139	On Computing Equilibrium Binding Constants for Proteinâ€“Protein Association in Membranes. Journal of Chemical Theory and Computation, 2022, 18, 3961-3971.	5.3	8
140	On the use of mass scaling for stable and efficient simulated tempering with molecular dynamics. Journal of Computational Chemistry, 2016, 37, 2017-2028.	3.3	6
141	Characterization of dynamics and mechanism in the self-assembly of AOT reverse micelles. Journal of Chemical Physics, 2018, 149, 144901.	3.0	6
142	Simulation of quantum systems using path integrals in a generalized ensemble. Chemical Physics Letters, 2001, 346, 274-282.	2.6	5
143	Dynamics of Methionine Ligand Rebinding in Cytochrome c. Journal of Physical Chemistry B, 2012, 116, 6980-6990.	2.6	5
144	Spatio-temporal hierarchy in the dynamics of a minimalist protein model. Journal of Chemical Physics, 2013, 139, 215101.	3.0	5

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145	Uncertainty of path integral averages at low temperature. Journal of Chemical Physics, 2001, 115, 6834-6840.	3.0	4
146	Gravitational smoothing as a global optimization strategy. Journal of Computational Chemistry, 2002, 23, 1100-1103.	3.3	4
147	Response to â€˜â€˜Comment on a proposed method for finding barrier height distributionsâ€™â€™ [J. Chem. Phys. 103, 1235 (1995)]. Journal of Chemical Physics, 1995, 103, 1237-1238.	3.0	3
148	Freezing Transitions of Nanoconfined Coarse-Grained Water Show Subtle Dependence on Confining Environment. Journal of Physical Chemistry B, 2016, 120, 2517-2525.	2.6	3
149	Enhanced sampling method in molecular simulations using genetic algorithm for biomolecular systems. Journal of Computational Chemistry, 2019, 40, 475-481.	3.3	3
150	Direct computation of long time processes in peptides and proteins: Reaction path study of the coilâ€toâ€helix transition in polyalanine. Proteins: Structure, Function and Bioinformatics, 1999, 36, 249-261.	2.6	3
151	Direct evidence for mode-specific vibrational energy relaxation from quantum time-dependent perturbation theory. III. The Î½4 and Î½7 modes of nonplanar nickel porphyrin models. Journal of Chemical Physics, 2009, 130, 215101.	3.0	2
152	JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402.	3.0	2
153	New and notable: A multiscale coarse-grained model of the SARS-CoV-2 virion. Biophysical Journal, 2021, 120, 975-976.	0.5	2
154	Energy landscape theory for Alzheimer's amyloid Î²-peptide fibril elongation. , 2001, 42, 217.		2
155	Dynamical Models of Chemical Exchange in Nuclear Magnetic Resonance Spectroscopy. The Biophysicist, 2022, 3, 13-34.	0.3	1
156	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	3.0	1
157	1SD04 Time scales to attain local ergodicity through vibrational relaxation in proteins. Seibutsu Butsuri, 2005, 45, S6.	0.1	0
158	3P018 The Structure of Amyloid Î² Peptide 1-40 in the membrane and the 672-726 fragment of of APP(Proteins-structure and structure-function relationship,Poster Presentations). Seibutsu Butsuri, 2007, 47, S207.	0.1	0
159	3P-090 The dimer conformation of amyloid Î² precursor protein fragment in membrane(The 46th Annual) Tj ETQq1 1 0.784314 rgBT /Ov	0.1	0