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	Dynamical Models of Chemical Exchange in Nuclear Magnetic Resonance Spectroscopy. The Biophysicist, 2022, 3, 13-34.	0.3	1
2	On Computing Equilibrium Binding Constants for Proteinâ€“Protein Association in Membranes. Journal of Chemical Theory and Computation, 2022, 18, 3961-3971.	5.3	8
3	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
4	Direct Observation of Cholesterol Dimers and Tetramers in Lipid Bilayers. Journal of Physical Chemistry B, 2021, 125, 1825-1837.	2.6	25
5	New and notable: A multiscale coarse-grained model of the SARS-CoV-2 virion. Biophysical Journal, 2021, 120, 975-976.	0.5	2
6	Addressing the Excessive Aggregation of Membrane Proteins in the MARTINI Model. Journal of Chemical Theory and Computation, 2021, 17, 2513-2521.	5.3	23
7	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
8	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
9	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
10	2020 JCP Emerging Investigator Special Collection. Journal of Chemical Physics, 2021, 155, 230401.	3.0	1
11	JCP Emerging Investigator Special Collection 2019. Journal of Chemical Physics, 2020, 153, 110402.	3.0	2
12	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
13	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
14	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
15	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	47.7	205
16	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
17	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
18	Sequence Effects on Size, Shape, and Structural Heterogeneity in Intrinsically Disordered Proteins. Journal of Physical Chemistry B, 2019, 123, 3462-3474.	2.6	125

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19	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
20	Design, synthesis, and biomedical applications of synthetic sulphated polysaccharides. Chemical Society Reviews, 2019, 48, 2338-2365.	38.1	93
21	Enhanced sampling method in molecular simulations using genetic algorithm for biomolecular systems. Journal of Computational Chemistry, 2019, 40, 475-481.	3.3	3
22	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
23	Influence of membrane lipid composition on the structure and activity of Î³-secretase. Physical Chemistry Chemical Physics, 2018, 20, 27294-27304.	2.8	20
24	Regimes of Complex Lipid Bilayer Phases Induced by Cholesterol Concentration in MD Simulation. Biophysical Journal, 2018, 115, 2167-2178.	0.5	37
25	Characterization of dynamics and mechanism in the self-assembly of AOT reverse micelles. Journal of Chemical Physics, 2018, 149, 144901.	3.0	6
26	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
27	Molecular Insights into Human Hereditary Apolipoprotein A-I Amyloidosis Caused by the Glu34Lys Mutation. Biochemistry, 2018, 57, 5738-5747.	2.5	9
28	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
29	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
30	Exploring the structure and stability of cholesterol dimer formation in multicomponent lipid bilayers. Journal of Computational Chemistry, 2017, 38, 1479-1488.	3.3	25
31	Characterizing the structural ensemble of Î³-secretase using a multiscale molecular dynamics approach. Chemical Science, 2017, 8, 5576-5584.	7.4	55
32	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
33	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
34	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
35	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
36	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

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37	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
38	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
39	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
40	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
41	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
42	Limit of Metastability for Liquid and Vapor Phases of Water. Physical Review Letters, 2014, 112, 157802.	7.8	17
43	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
44	Membraneâ€"Protein Interactions Are Key to Understanding Amyloid Formation. Journal of Physical Chemistry Letters, 2014, 5, 633-635.	4.6	25
45	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
46	Vibrational energy flow across hemeâ€"cytochrome c and cytochrome câ€"water interfaces. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	30
47	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
48	Probing the Structure and Dynamics of Confined Water in AOT Reverse Micelles. Journal of Physical Chemistry B, 2013, 117, 7345-7351.	2.6	61
49	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
50	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
51	Spatio-temporal hierarchy in the dynamics of a minimalist protein model. Journal of Chemical Physics, 2013, 139, 215101.	3.0	5
52	Role of Water in Protein Aggregation and Amyloid Polymorphism. Accounts of Chemical Research, 2012, 45, 83-92.	15.6	301
53	Dynamics of Methionine Ligand Rebinding in Cytochrome c. Journal of Physical Chemistry B, 2012, 116, 6980-6990.	2.6	5
54	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

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55	Replica Exchange Statistical Temperature Molecular Dynamics Algorithm. Journal of Physical Chemistry B, 2012, 116, 8646-8653.	2.6	37
56	Entropic Stabilization of Proteins by TMAO. Journal of Physical Chemistry B, 2011, 115, 13401-13407.	2.6	174
57	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
58	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
59	Communication: Iteration-free, weighted histogram analysis method in terms of intensive variables. Journal of Chemical Physics, 2011, 135, 061103.	3.0	36
60	Principles governing oligomer formation in amyloidogenic peptides. Current Opinion in Structural Biology, 2010, 20, 187-195.	5.7	97
61	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
62	Generalized simulated tempering for exploring strong phase transitions. Journal of Chemical Physics, 2010, 133, 154101.	3.0	26
63	Generalized Replica Exchange Method. Journal of Chemical Physics, 2010, 132, 224107.	3.0	80
64	Relationship between protein folding thermodynamics and the energy landscape. Physical Review E, 2009, 79, 030902.	2.1	18
65	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
66	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
67	Replica exchange statistical temperature Monte Carlo. Journal of Chemical Physics, 2009, 130, 124112.	3.0	25
68	Optimal replica exchange method combined with Tsallis weight sampling. Journal of Chemical Physics, 2009, 130, 144114.	3.0	16
69	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
70	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
71	Thermodynamic Perspective on the Dockâ"Lock Growth Mechanism of Amyloid Fibrils. Journal of Physical Chemistry B, 2009, 113, 14421-14430.	2.6	88
72	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

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73	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
74	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
75	Diversity of Solvent Dependent Energy Transfer Pathways in Heme Proteins. Journal of Physical Chemistry B, 2009, 113, 825-830.	2.6	14
76	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
77	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
78	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
79	Resilience of the Iron Environment in Heme Proteins. Biophysical Journal, 2008, 95, 5874-5889.	0.5	31
80	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
81	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
82	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
83	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
84	Statistical temperature molecular dynamics: Application to coarse-grained Î²-barrel-forming protein models. Journal of Chemical Physics, 2007, 126, 135101.	3.0	46
85	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
86	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
87	Quantum dynamics of N-methylacetamide studied by the vibrational configuration interaction method. Chemical Physics Letters, 2007, 443, 6-11.	2.6	40
88	Dynamics of Asp23â^'Lys28 Salt-Bridge Formation in AÎ²10-35Monomers. Journal of the American Chemical Society, 2006, 128, 16159-16168.	13.7	200
89	Statistical-Temperature MonteÂCarlo and Molecular Dynamics Algorithms. Physical Review Letters, 2006, 97, 050601.	7.8	111
90	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

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91	Efforts toward Developing Direct Probes of Protein Dynamics. Journal of the American Chemical Society, 2006, 128, 6028-6029.	13.7	49
92	Time-dependent perturbation theory for vibrational energy relaxation and dephasing in peptides and proteins. Journal of Chemical Physics, 2006, 124, 144910.	3.0	50
93	1SD04 Time scales to attain local ergodicity through vibrational relaxation in proteins. Seibutsu Butsuri, 2005, 45, S6.	0.1	0
94	Vibrational Energy Relaxation (Ver) of a CD Stretching Mode in Cytochrome c. Advances in Chemical Physics, 2005, , 179-203.	0.3	8
95	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
96	Monte Carlo simulations of polyalanine using a reduced model and statistics-based interaction potentials. Journal of Chemical Physics, 2005, 122, 024904.	3.0	31
97	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
98	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
99	Orientational potentials extracted from protein structures improve native fold recognition. Protein Science, 2004, 13, 862-874.	7.6	84
100	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
101	Orientation-dependent coarse-grained potentials derived by statistical analysis of molecular structural databases. Polymer, 2004, 45, 597-608.	3.8	25
102	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
103	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
104	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
105	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
106	Vibrational Frequency Shifts and Relaxation Rates for a Selected Vibrational Mode in Cytochrome c. Biophysical Journal, 2003, 85, 1429-1439.	0.5	32
107	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
108	Gravitational smoothing as a global optimization strategy. Journal of Computational Chemistry, 2002, 23, 1100-1103.	3.3	4

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109	Generalized parallel sampling. Physica A: Statistical Mechanics and Its Applications, 2002, 305, 157-171.	2.6	49
110	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
111	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
112	Smart Darting Monte Carlo. Journal of Chemical Physics, 2001, 114, 6994-7000.	3.0	60
113	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
114	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
115	Energy landscape theory for Alzheimer's amyloid ?-peptide fibril elongation. Proteins: Structure, Function and Bioinformatics, 2001, 42, 217-229.	2.6	104
116	Simulation of quantum systems using path integrals in a generalized ensemble. Chemical Physics Letters, 2001, 346, 274-282.	2.6	5
117	Uncertainty of path integral averages at low temperature. Journal of Chemical Physics, 2001, 115, 6834-6840.	3.0	4
118	Energy landscape theory for Alzheimer's amyloid Î²-peptide fibril elongation. , 2001, 42, 217.		2
119	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
120	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
121	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
122	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
123	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
124	Global optimization using bad derivatives: Derivative-free method for molecular energy minimization. Journal of Computational Chemistry, 1998, 19, 1445-1455.	3.3	22
125	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
126	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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127	Novel methods of sampling phase space in the simulation of biological systems. Current Opinion in Structural Biology, 1997, 7, 181-189.	5.7	206
128	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
129	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
130	Finding the needle in the haystack: Algorithms for conformational optimization. Computers in Physics, 1996, 10, 449.	0.5	22
131	Energy minimization using the classical density distribution: Application to sodium chloride clusters. Physical Review B, 1996, 53, 13857-13863.	3.2	15
132	Generalized simulated annealing algorithms using Tsallis statistics: Application to conformational optimization of a tetrapeptide. Physical Review E, 1996, 53, R3055-R3058.	2.1	149
133	OPTIMIZATION TECHNIQUES WITH APPLICATIONS TO PROTEINS. Advanced Series in Physical Chemistry, 1996, , 137-196.	1.5	20
134	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
135	Simulation study of the collapse of linear and ring homopolymers. Journal of Chemical Physics, 1995, 103, 2615-2624.	3.0	51
136	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
137	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
138	Simulated annealing using the classical density distribution. Journal of Chemical Physics, 1994, 101, 533-541.	3.0	70
139	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
140	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
141	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
142	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
143	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
144	Analysis of the role of attractive forces in self-diffusion of a simple fluid. Molecular Physics, 1992, 76, 373-385.	1.7	39

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145	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
146	Energy equipartitioning in the classical timeâ€dependent Hartree approximation. Journal of Chemical Physics, 1991, 94, 6737-6739.	3.0	58
147	Dynamic friction on rigid and flexible bonds. Journal of Chemical Physics, 1990, 93, 5084-5095.	3.0	115
148	Spatial dependence of timeâ€dependent friction for pair diffusion in a simple fluid. Journal of Chemical Physics, 1990, 93, 6804-6812.	3.0	66
149	The interpretation of site-directed mutagenesis experiments by linear free energy relations. Protein Engineering, Design and Selection, 1990, 3, 673-675.	2.1	12
150	Classical and modern methods in reaction rate theory. The Journal of Physical Chemistry, 1988, 92, 3711-3725.	2.9	377
151	Molecular dynamics study of an isomerizing diatomic in a Lennardâ€Jones fluid. Journal of Chemical Physics, 1988, 89, 4833-4847.	3.0	122
152	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
153	A statistical theory for the effect of nonadiabatic transitions on activated processes. Journal of Chemical Physics, 1987, 87, 6111-6116.	3.0	51
154	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
155	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
156	Nonâ€Markovian activated rate processes: Comparison of current theories with numerical simulation data. Journal of Chemical Physics, 1986, 84, 1788-1794.	3.0	161
157	A rapid method for determining rate constants by molecular dynamics. Journal of Chemical Physics, 1985, 83, 1138-1139.	3.0	59
158	Shortcomings of current theories of nonâ€Markovian activated rate processes. Journal of Chemical Physics, 1985, 83, 3172-3174.	3.0	52
159	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