

# Peter G Bolhuis

## List of Publications by Year in descending order

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165  
papers

13,966  
citations

31902

53  
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20900

115  
g-index

171  
all docs

171  
docs citations

171  
times ranked

7836  
citing authors

#	ARTICLE	IF	CITATIONS
1	TRANSITIONPATHSAMPLING: Throwing Ropes Over Rough Mountain Passes, in the Dark. Annual Review of Physical Chemistry, 2002, 53, 291-318.	4.8	1,704
2	Transition path sampling and the calculation of rate constants. Journal of Chemical Physics, 1998, 108, 1964-1977.	1.2	925
3	Tracing the phase boundaries of hard spherocylinders. Journal of Chemical Physics, 1997, 106, 666-687.	1.2	708
4	A novel path sampling method for the calculation of rate constants. Journal of Chemical Physics, 2003, 118, 7762-7774.	1.2	434
5	Entropy difference between crystal phases. Nature, 1997, 388, 235-236.	13.7	396
6	Can Polymer Coils Be Modeled as "Soft Colloids"? Physical Review Letters, 2000, 85, 2522-2525.	2.9	374
7	Reaction coordinates of biomolecular isomerization. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 5877-5882.	3.3	370
8	Efficient transition path sampling: Application to Lennard-Jones cluster rearrangements. Journal of Chemical Physics, 1998, 108, 9236-9245.	1.2	313
9	Transition Path Sampling. Advances in Chemical Physics, 2003, , 1-78.	0.3	310
10	Accurate effective pair potentials for polymer solutions. Journal of Chemical Physics, 2001, 114, 4296-4311.	1.2	308
11	On the calculation of reaction rate constants in the transition path ensemble. Journal of Chemical Physics, 1999, 110, 6617-6625.	1.2	292
12	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	1.6	285
13	Sampling ensembles of deterministic transition pathways. Faraday Discussions, 1998, 110, 421-436.	1.6	282
14	Interplay between Structure and Size in a Critical Crystal Nucleus. Physical Review Letters, 2005, 94, 235703.	2.9	275
15	Mean-field fluid behavior of the Gaussian core model. Physical Review E, 2000, 62, 7961-7972.	0.8	241
16	Elaborating transition interface sampling methods. Journal of Computational Physics, 2005, 205, 157-181.	1.9	229
17	Sampling the multiple folding mechanisms of Trp-cage in explicit solvent. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 15859-15864.	3.3	228
18	Transition-path sampling of $\hat{A}$ -hairpin folding. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 12129-12134.	3.3	211

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19	Prediction of an expanded-to-condensed transition in colloidal crystals. <i>Physical Review Letters</i> , 1994, 72, 2211-2214.	2.9	185
20	Influence of Polymer-Excluded Volume on the Phase-Behavior of Colloid-Polymer Mixtures. <i>Physical Review Letters</i> , 2002, 89, 128302.	2.9	182
21	Monte Carlo study of freezing of polydisperse hard spheres. <i>Physical Review E</i> , 1996, 54, 634-643.	0.8	173
22	Numerical study of the phase behavior of rodlike colloids with attractive interactions. <i>Journal of Chemical Physics</i> , 1997, 107, 1551-1564.	1.2	164
23	Isostructural solid-solid transition in crystalline systems with short-ranged interaction. <i>Physical Review E</i> , 1994, 50, 4880-4890.	0.8	155
24	Rate constants for diffusive processes by partial path sampling. <i>Journal of Chemical Physics</i> , 2004, 120, 4055-4065.	1.2	155
25	Hysteresis in Clay Swelling Induced by Hydrogen Bonding: Accurate Prediction of Swelling States. <i>Langmuir</i> , 2006, 22, 1223-1234.	1.6	154
26	Freezing of polydisperse hard spheres. <i>Physical Review E</i> , 1999, 59, 618-622.	0.8	152
27	Polymer induced depletion potentials in polymer-colloid mixtures. <i>Journal of Chemical Physics</i> , 2002, 117, 1893-1907.	1.2	132
28	Rate Constant and Reaction Coordinate of Trp-Cage Folding in Explicit Water. <i>Biophysical Journal</i> , 2008, 95, 4246-4257.	0.2	130
29	Tunable Long Range Forces Mediated by Self-Propelled Colloidal Hard Spheres. <i>Physical Review Letters</i> , 2015, 114, 018302.	2.9	130
30	Colloid-Polymer Mixtures in the Protein Limit. <i>Physical Review Letters</i> , 2003, 90, 068304.	2.9	127
31	Role of the Prestructured Surface Cloud in Crystal Nucleation. <i>Physical Review Letters</i> , 2011, 106, 085701.	2.9	122
32	Transition path sampling of cavitation between molecular scale solvophobic surfaces. <i>Journal of Chemical Physics</i> , 2000, 113, 8154-8160.	1.2	119
33	Numerical study of the phase diagram of a mixture of spherical and rodlike colloids. <i>Journal of Chemical Physics</i> , 1994, 101, 9869-9875.	1.2	118
34	How To Derive and Parameterize Effective Potentials in Colloid-Polymer Mixtures. <i>Macromolecules</i> , 2002, 35, 1860-1869.	2.2	90
35	Kinetic Pathways of $\hat{1}^2$ -Hairpin (Un)folding in Explicit Solvent. <i>Biophysical Journal</i> , 2005, 88, 50-61.	0.2	86
36	Self-assembly of microcapsules via colloidal bond hybridization and anisotropy. <i>Nature</i> , 2016, 534, 364-368.	13.7	86

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37	Ultrafast Reorientation of Dangling OH Groups at the Air-Water Interface Using Femtosecond Vibrational Spectroscopy. <i>Physical Review Letters</i> , 2011, 107, 116102.	2.9	84
38	Predicting the reaction coordinates of millisecond light-induced conformational changes in photoactive yellow protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 2397-2402.	3.3	83
39	Transverse interlayer order in lyotropic smectic liquid crystals. <i>Physical Review E</i> , 1995, 52, R1277-R1280.	0.8	79
40	Rare events via multiple reaction channels sampled by path replica exchange. <i>Journal of Chemical Physics</i> , 2008, 129, 114108.	1.2	75
41	Accurate Free Energies of Micelle Formation. <i>Journal of Physical Chemistry B</i> , 2005, 109, 6650-6657.	1.2	74
42	Many-body interactions and correlations in coarse-grained descriptions of polymer solutions. <i>Physical Review E</i> , 2001, 64, 021801.	0.8	73
43	Density profiles and surface tension of polymers near colloidal surfaces. <i>Journal of Chemical Physics</i> , 2002, 116, 10547-10556.	1.2	70
44	Reaction coordinates, one-dimensional Smoluchowski equations, and a test for dynamical self-consistency. <i>Journal of Chemical Physics</i> , 2013, 138, 054106.	1.2	70
45	Transition Path Sampling and Other Advanced Simulation Techniques for Rare Events. , 2009, , 167-233.		69
46	Investigating rare events by transition interface sampling. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2004, 340, 395-401.	1.2	68
47	Demixing in hard ellipsoid rod-plate mixtures. <i>Journal of Chemical Physics</i> , 1997, 106, 9270-9275.	1.2	65
48	Transition Path Sampling Simulations of Biological Systems. , 2006, , 291-317.		64
49	Equilibrium and non-equilibrium cluster phases in colloids with competing interactions. <i>Soft Matter</i> , 2014, 10, 4479-4486.	1.2	64
50	Crystallizing hard-sphere glasses by doping with active particles. <i>Soft Matter</i> , 2014, 10, 6609-6613.	1.2	63
51	Folding Dynamics of the Trp-Cage Miniprotein: Evidence for a Native-Like Intermediate from Combined Time-Resolved Vibrational Spectroscopy and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11490-11501.	1.2	60
52	A Molecular Mechanism of Hysteresis in Clay Swelling. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 2650-2652.	7.2	57
53	Multiple state transition path sampling. <i>Journal of Chemical Physics</i> , 2008, 129, 224107.	1.2	56
54	Isostructural solid - solid transitions in systems with a repulsive 'shoulder' potential. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 381-387.	0.7	55

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55	Nonlinear reaction coordinate analysis in the reweighted path ensemble. <i>Journal of Chemical Physics</i> , 2010, 133, 174110.	1.2	55
56	Statics and Dynamics of Free and Hydrogen-Bonded OH Groups at the Air/Water Interface. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9467-9481.	1.2	53
57	Transition path sampling: throwing ropes over mountains in the dark. <i>Journal of Physics Condensed Matter</i> , 2000, 12, A147-A152.	0.7	52
58	Transition path sampling on diffusive barriers. <i>Journal of Physics Condensed Matter</i> , 2003, 15, S113-S120.	0.7	52
59	Prediction of an Autocatalytic Replication Mechanism for Micelle Formation. <i>Physical Review Letters</i> , 2006, 97, 018302.	2.9	52
60	The reweighted path ensemble. <i>Journal of Chemical Physics</i> , 2010, 133, 174109.	1.2	49
61	Unbiased atomistic insight in the competing nucleation mechanisms of methane hydrates. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 19305-19310.	3.3	49
62	Practical and conceptual path sampling issues. <i>European Physical Journal: Special Topics</i> , 2015, 224, 2409-2427.	1.2	48
63	OpenPathSampling: A Python Framework for Path Sampling Simulations. 1. Basics. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 813-836.	2.3	45
64	Sampling the kinetic pathways of a micelle fusion and fission transition. <i>Journal of Chemical Physics</i> , 2007, 126, 244703.	1.2	43
65	Foundations and latest advances in replica exchange transition interface sampling. <i>Journal of Chemical Physics</i> , 2017, 147, 152722.	1.2	43
66	Phase Transition to Bundles of Flexible Supramolecular Polymers. <i>Physical Review Letters</i> , 2008, 100, 188301.	2.9	41
67	Temperature-sensitive colloidal phase behavior induced by critical Casimir forces. <i>Journal of Chemical Physics</i> , 2013, 139, 094903.	1.2	41
68	Reaction coordinates for the crystal nucleation of colloidal suspensions extracted from the reweighted path ensemble. <i>Journal of Chemical Physics</i> , 2011, 135, 154110.	1.2	40
69	Rotational diffusion affects the dynamical self-assembly pathways of patchy particles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 15308-15313.	3.3	39
70	Dynamics of Hydration Water around Native and Misfolded $\beta$ -Lactalbumin. <i>Journal of Physical Chemistry B</i> , 2016, 120, 4756-4766.	1.2	39
71	Primary Fibril Nucleation of Aggregation Prone Tau Fragments $\langle i \rangle$ PHF6 $\langle /i \rangle$ and $\langle i \rangle$ PHF6 $\langle /i \rangle^*$ . <i>Journal of Physical Chemistry B</i> , 2017, 121, 3250-3261.	1.2	39
72	The Asakura-Oosawa model in the protein limit: the role of many-body interactions. <i>Journal of Physics Condensed Matter</i> , 2003, 15, S3429-S3442.	0.7	38

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73	Simultaneous computation of free energies and kinetics of rare events. <i>Physical Review E</i> , 2005, 71, 056709.	0.8	38
74	Elucidating the Locking Mechanism of Peptides onto Growing Amyloid Fibrils through Transition Path Sampling. <i>Biophysical Journal</i> , 2012, 103, 1296-1304.	0.2	37
75	Primary Nucleation Kinetics of Short Fibril-Forming Amyloidogenic Peptides. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12568-12579.	1.2	37
76	Can purely repulsive soft potentials predict micelle formation correctly?. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 941-948.	1.3	34
77	OpenPathSampling: A Python Framework for Path Sampling Simulations. 2. Building and Customizing Path Ensembles and Sample Schemes. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 837-856.	2.3	34
78	Transition Path Sampling as Markov Chain Monte Carlo of Trajectories: Recent Algorithms, Software, Applications, and Future Outlook. <i>Advanced Theory and Simulations</i> , 2021, 4, 2000237.	1.3	34
79	Activation Energies from Transition Path Sampling Simulations. <i>Molecular Simulation</i> , 2004, 30, 795-799.	0.9	33
80	Prediction of solvent dependent $\beta$ -roll formation of a self-assembling silk-like protein domain. <i>Soft Matter</i> , 2009, 5, 2658.	1.2	32
81	Confinement-Induced States in the Folding Landscape of the Trp-cage Miniprotein. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11872-11880.	1.2	32
82	Coarse-graining polymers as soft colloids. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2002, 306, 251-261.	1.2	31
83	Combining molecular dynamics with mesoscopic Green's function reaction dynamics simulations. <i>Journal of Chemical Physics</i> , 2015, 143, 214102.	1.2	31
84	Multiple state transition interface sampling of alanine dipeptide in explicit solvent. <i>Journal of Chemical Physics</i> , 2011, 135, 145102.	1.2	30
85	Transition path sampling of protein conformational changes. <i>Chemical Physics</i> , 2012, 396, 30-44.	0.9	30
86	Interplay between Folding and Assembly of Fibril-Forming Polypeptides. <i>Physical Review Letters</i> , 2013, 111, 058101.	2.9	30
87	A replica exchange transition interface sampling method with multiple interface sets for investigating networks of rare events. <i>Journal of Chemical Physics</i> , 2014, 141, 044101.	1.2	30
88	An extended autoencoder model for reaction coordinate discovery in rare event molecular dynamics datasets. <i>Journal of Chemical Physics</i> , 2021, 155, 064103.	1.2	29
89	Effects of a Mutation on the Folding Mechanism of a $\beta$ -Hairpin. <i>Journal of Physical Chemistry B</i> , 2009, 113, 16184-16196.	1.2	28
90	A one-way shooting algorithm for transition path sampling of asymmetric barriers. <i>Journal of Chemical Physics</i> , 2016, 145, 164112.	1.2	28

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91	Multiscale simulations of anisotropic particles combining molecular dynamics and Greenâ€™s function reaction dynamics. <i>Journal of Chemical Physics</i> , 2017, 146, 114106.	1.2	28
92	Adaptive single replica multiple state transition interface sampling. <i>Journal of Chemical Physics</i> , 2013, 139, 044105.	1.2	27
93	Molecular Understanding of Homogeneous Nucleation of CO <sub>2</sub> Hydrates Using Transition Path Sampling. <i>Journal of Physical Chemistry B</i> , 2021, 125, 338-349.	1.2	27
94	Microscopic and mesoscopic simulation of entropic micelles. <i>Physica A: Statistical Mechanics and Its Applications</i> , 1997, 244, 45-58.	1.2	26
95	The influence of micelle formation on the stability of colloid surfactant mixtures. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14789.	1.3	26
96	A method of incorporating rate constants as kinetic constraints in molecular dynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	26
97	Predicting the Signaling State of Photoactive Yellow Protein. <i>Biophysical Journal</i> , 2005, 88, 3525-3535.	0.2	25
98	Effect of excluded volume interactions on the interfacial properties of colloid-polymer mixtures. <i>Journal of Chemical Physics</i> , 2008, 128, 024904.	1.2	24
99	On the Relation Between Projections of the Reweighted Path Ensemble. <i>Journal of Statistical Physics</i> , 2011, 145, 841-859.	0.5	24
100	Sampling the equilibrium kinetic network of Trp-cage in explicit solvent. <i>Journal of Chemical Physics</i> , 2014, 140, 195102.	1.2	24
101	The Trigger Factor Chaperone Encapsulates and Stabilizes Partial Folds of Substrate Proteins. <i>PLoS Computational Biology</i> , 2015, 11, e1004444.	1.5	24
102	Nested Transition Path Sampling. <i>Physical Review Letters</i> , 2018, 120, 250601.	2.9	24
103	Water structure and dynamics in the hydration layer of a type III anti-freeze protein. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6996-7006.	1.3	23
104	Revealing pseudorotation and ring-opening reactions in colloidal organic molecules. <i>Nature Communications</i> , 2021, 12, 2810.	5.8	23
105	Rate Prediction for Homogeneous Nucleation of Methane Hydrate at Moderate Supersaturation Using Transition Interface Sampling. <i>Journal of Physical Chemistry B</i> , 2020, 124, 8099-8109.	1.2	22
106	Switching Colloidal Superstructures by Critical Casimir Forces. <i>Advanced Materials</i> , 2017, 29, 1700819.	11.1	21
107	Stabilization of Nanoparticle Shells by Competing Interactions. <i>Journal of Physical Chemistry C</i> , 2010, 114, 7780-7786.	1.5	20
108	The intrinsic rate constants in diffusion-influenced reactions. <i>Faraday Discussions</i> , 2016, 195, 421-441.	1.6	19

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109	Attractive double layer forces from hard-core correlations. <i>Journal of Chemical Physics</i> , 1993, 98, 8096-8104.	1.2	18
110	Simulation and theory of fluid-fluid interfaces in binary mixtures of hard spheres and hard rods. <i>Journal of Physics Condensed Matter</i> , 2003, 15, S3421-S3428.	0.7	18
111	Prediction of a stable associated liquid of short amyloidogenic peptides. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10556-10567.	1.3	18
112	Protonation of the Chromophore in the Photoactive Yellow Protein. <i>Journal of Physical Chemistry B</i> , 2007, 111, 3765-3773.	1.2	17
113	Exposure of thiol groups in the heat-induced denaturation of $\beta^2$ -lactoglobulin. <i>Molecular Simulation</i> , 2015, 41, 1006-1014.	0.9	17
114	Approximating free energy and committor landscapes in standard transition path sampling using virtual interface exchange. <i>Journal of Chemical Physics</i> , 2019, 151, 174111.	1.2	17
115	The self-assembly mechanism of fibril-forming silk-based block copolymers. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10457.	1.3	16
116	Equilibrium Kinetic Network of the Villin Headpiece in Implicit Solvent. <i>Biophysical Journal</i> , 2015, 108, 368-378.	0.2	16
117	(Un)Folding Mechanisms of the FBP28 WW Domain in Explicit Solvent Revealed by Multiple Rare Event Simulation Methods. <i>Biophysical Journal</i> , 2010, 98, 646-656.	0.2	15
118	The HAMP Signal Relay Domain Adopts Multiple Conformational States through Collective Piston and Tilt Motions. <i>PLoS Computational Biology</i> , 2013, 9, e1002913.	1.5	15
119	Non-adiabatic reactions: general discussion. <i>Faraday Discussions</i> , 2016, 195, 311-344.	1.6	15
120	Numerical study of freezing in polydisperse colloidal suspensions. <i>Journal of Physics Condensed Matter</i> , 1996, 8, 9627-9631.	0.7	14
121	The role of multivalency in the association kinetics of patchy particle complexes. <i>Journal of Chemical Physics</i> , 2017, 146, 234901.	1.2	14
122	Tuning Patchy Bonds Induced by Critical Casimir Forces. <i>Materials</i> , 2017, 10, 1265.	1.3	14
123	Atomistic insight into the kinetic pathways for Watson-Crick to Hoogsteen transitions in DNA. <i>Nucleic Acids Research</i> , 2019, 47, 11069-11076.	6.5	14
124	Multiscale modelling. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10399.	1.3	13
125	Stability and growth mechanism of self-assembling putative antifreeze cyclic peptides. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19032-19042.	1.3	13
126	Light scattering and sedimentation equilibrium of a concentrated multicomponent hard rod dispersion. <i>Physica A: Statistical Mechanics and Its Applications</i> , 1993, 196, 375-388.	1.2	12



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127	Reordering Hydrogen Bonds Using Hamiltonian Replica Exchange Enhances Sampling of Conformational Changes in Biomolecular Systems. <i>Journal of Physical Chemistry B</i> , 2009, 113, 6484-6494.	1.2	12
128	The opposing effects of isotropic and anisotropic attraction on association kinetics of proteins and colloids. <i>Journal of Chemical Physics</i> , 2017, 147, 155101.	1.2	12
129	Revealing Polymerization Kinetics with Colloidal Dipatch Particles. <i>Physical Review Letters</i> , 2021, 127, 108001.	2.9	11
130	Hydrophobic Collapse of Trigger Factor Monomer in Solution. <i>PLoS ONE</i> , 2013, 8, e59683.	1.1	11
131	Solvation of p-Coumaric Acid in Water. <i>Journal of Physical Chemistry B</i> , 2007, 111, 13591-13599.	1.2	10
132	Role of Fluctuations in Ligand Binding Cooperativity of Membrane Receptors. <i>Physical Review Letters</i> , 2011, 106, 168103.	2.9	10
133	Anisotropic aggregation in a simple model of isotropically polymer-coated nanoparticles. <i>Physical Review E</i> , 2013, 88, 012303.	0.8	10
134	Rate constants for proteins binding to substrates with multiple binding sites using a generalized forward flux sampling expression. <i>Journal of Chemical Physics</i> , 2018, 148, 124109.	1.2	10
135	Unbiased Atomistic Insight into the Mechanisms and Solvent Role for Globular Protein Dimer Dissociation. <i>Journal of Physical Chemistry B</i> , 2019, 123, 1883-1895.	1.2	10
136	A maximum caliber approach for continuum path ensembles. <i>European Physical Journal B</i> , 2021, 94, 1.	0.6	10
137	Liquid-Like Behavior in Solids. <i>Molecular Simulation</i> , 1996, 16, 127-137.	0.9	9
138	Microscopic Picture of the Aqueous Solvation of Glutamic Acid. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 898-907.	2.3	9
139	A simple coarse-grained model for self-assembling silk-like protein fibers. <i>Faraday Discussions</i> , 2010, 144, 127-141.	1.6	9
140	Homogenous nucleation rate of CO <sub>2</sub> hydrates using transition interface sampling. <i>Journal of Chemical Physics</i> , 2021, 154, 164507.	1.2	9
141	Transition path sampling for non-equilibrium dynamics without predefined reaction coordinates. <i>Journal of Chemical Physics</i> , 2020, 152, 044108.	1.2	9
142	Two-state protein folding kinetics through all-atom molecular dynamics based sampling. <i>Frontiers in Bioscience - Landmark</i> , 2009, Volume, 2801.	3.0	8
143	The magnitude of the intrinsic rate constant: How deep can association reactions be in the diffusion limited regime?. <i>Journal of Chemical Physics</i> , 2017, 147, 184108.	1.2	8
144	Ratchet-induced variations in bulk states of an active ideal gas. <i>Journal of Chemical Physics</i> , 2018, 149, 174910.	1.2	8

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145	A temperature-dependent critical Casimir patchy particle model benchmarked onto experiment. <i>Journal of Chemical Physics</i> , 2021, 155, 034902.	1.2	8
146	Liquid-like behavior in colloidal crystals. <i>Physica B: Condensed Matter</i> , 1996, 228, 33-39.	1.3	7
147	Competition between surface adsorption and folding of fibril-forming polypeptides. <i>Physical Review E</i> , 2015, 91, 022711.	0.8	7
148	Modelling critical Casimir force induced self-assembly experiments on patchy colloidal dumbbells. <i>Soft Matter</i> , 2017, 13, 4903-4915.	1.2	7
149	Generalised expressions for the association and dissociation rate constants of molecules with multiple binding sites. <i>Molecular Physics</i> , 2018, 116, 3042-3054.	0.8	7
150	Helix formation is a dynamical bottleneck in the recovery reaction of Photoactive Yellow Protein. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 72, 136-149.	1.5	6
151	Revealing viscoelastic bending relaxation dynamics of isolated semiflexible colloidal polymers. <i>Soft Matter</i> , 2021, 17, 8291-8299.	1.2	6
152	On the efficiency of biased sampling of the multiple state path ensemble. <i>Journal of Chemical Physics</i> , 2010, 133, 034101.	1.2	5
153	Numerical study of the effect of thiol-disulfide exchange in the cluster phase of $\beta^2$ -lactoglobulin aggregation. <i>Faraday Discussions</i> , 2012, 158, 461.	1.6	4
154	Application to large systems: general discussion. <i>Faraday Discussions</i> , 2016, 195, 671-698.	1.6	4
155	Trigger sequence can influence final morphology in the self-assembly of asymmetric telechelic polymers. <i>Soft Matter</i> , 2016, 12, 2095-2107.	1.2	3
156	New methods: general discussion. <i>Faraday Discussions</i> , 2016, 195, 521-556.	1.6	2
157	Fundamentals: general discussion. <i>Faraday Discussions</i> , 2016, 195, 139-169.	1.6	2
158	Predicting the Reaction Coordinates of Millisecond Light-Induced Conformational Changes in Photoactive Yellow Protein. <i>Biophysical Journal</i> , 2010, 98, 174a.	0.2	1
159	Predicting the Mechanism and Kinetics of the Watson-Crick to Hoogsteen Base Pairing Transition. <i>Biophysical Journal</i> , 2016, 110, 563a-564a.	0.2	1
160	Path Sampling Simulations of the Mechanisms and Rates of Transitions between Watson-Crick and Hoogsteen Base Pairing in DNA. <i>Biophysical Journal</i> , 2017, 112, 214a.	0.2	1
161	Fiber Formation of Silk-Like Proteins. <i>Biophysical Journal</i> , 2010, 98, 649a-650a.	0.2	0
162	Trp Cage Folding in Confinement. <i>Biophysical Journal</i> , 2011, 100, 211a.	0.2	0

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163	Exploring Signal Transduction Mechanism of HAMP Domains via Molecular Dynamics and Metadynamics. <i>Biophysical Journal</i> , 2011, 100, 195a.	0.2	0
164	A Molecular Dynamics Study of the Flexibility and Protein-Binding of the Trigger Factor Chaperone in Solution. <i>Biophysical Journal</i> , 2013, 104, 571a.	0.2	0
165	Exploring the Phase Space of Alpha-Synuclein with Replica Exchange Simulations. <i>Biophysical Journal</i> , 2015, 108, 63a.	0.2	0