Christoph Dellago

List of Publications by Year in Descending Order

192 papers	10,664 citations	46 h-index	100 g-index
199 ext. papers	11,621 ext. citations	4.7 avg, IF	6.52 L-index

#	Paper	IF	Citations
192	Cation interstitial diffusion in lead telluride and cadmium telluride studied by means of neural network potential based molecular dynamics simulations. *Journal of Physics Condensed Matter*, **2021**, 33, 015901	1.8	3
191	Improved description of atomic environments using low-cost polynomial functions with compact support. *Machine Learning: Science and Technology*, **2021**, 2, 035026	5.1	3
190	The microscopic mechanism of bulk melting of ice. *Journal of Chemical Physics*, **2021**, 155, 124501	3.9	1
189	Weak scaling of the contact distance between two fluctuating interfaces with system size. *Physical Review E*, **2020**, 102, 062801	2.4	1
188	Hierarchical self-assembly of patchy colloidal platelets. *Soft Matter*, **2020**, 16, 2774-2785	3.6	12
187	Protein design under competing conditions for the availability of amino acids. *Scientific Reports*, **2020**, 10, 2684	4.9	1
186	The generic unfolding of a biomimetic polymer during force spectroscopy. *Soft Matter*, **2020**, 16, 3941-3951	3.6	0
185	Enhancing transport by shaping barriers. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 2238-2240	11.5	1
184	How patchiness controls the properties of chain-like assemblies of colloidal platelets. *Journal of Physics Condensed Matter*, **2020**, 32, 204001	1.8	2
183	Origin of mean-field behavior in an elastic Ising model. *Physical Review B*, **2020**, 102,	3.3	2
182	Catalytic Mechanism of Processive GlfT2: Transition Path Sampling Investigation of Substrate Translocation. *ACS Omega*, **2020**, 5, 21374-21384	3.9	1
181	Identification of Protein Functional Regions. *ChemPhysChem*, **2020**, 21, 335-347	3.2	0
180	Ab initio structure and thermodynamics of the RPBE-D3 water/vapor interface by neural-network molecular dynamics. *Journal of Chemical Physics*, **2020**, 153, 144710	3.9	13
179	Phase stability of the ice XVII-based CO chiral hydrate from molecular dynamics simulations. *Journal of Chemical Physics*, **2019**, 151, 104502	3.9	3
178	Consequences of Lattice Mismatch for Phase Equilibrium in Heterostructured Solids. *Physical Review Letters*, **2019**, 123, 135701	7.4	6
177	Library-Based LAMMPS Implementation of High-Dimensional Neural Network Potentials. *Journal of Chemical Theory and Computation*, **2019**, 15, 1827-1840	6.4	94
176	Parallel Multistream Training of High-Dimensional Neural Network Potentials. *Journal of Chemical Theory and Computation*, **2019**, 15, 3075-3092	6.4	61

175	An efficient method to reconstruct free energy profiles for diffusive processes in transition interface sampling and forward flux sampling simulations. *Journal of Chemical Physics*, **2019**, 150, 094114	2.9	1
174	General Methodology to Identify the Minimum Alphabet Size for Heteropolymer Design. *Advanced Theory and Simulations*, **2019**, 2, 1900031	3.5	5
173	Design of Patchy Rhombi: From Close-Packed Tilings to Open Lattices. *Nano Letters*, **2019**, 19, 7806-7815	11.5	13
172	A High Coordination of Cross-Links Is Beneficial for the Strength of Cross-Linked Fibers. *Biomimetics*, **2019**, 4,	3.7	11
171	Ab initio thermodynamics of liquid and solid water. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 1110-1115	11.5	130
170	Design of Protein-Protein Binding Sites Suggests a Rationale for Naturally Occurring Contact Areas. *Journal of Chemical Theory and Computation*, **2019**, 15, 1383-1392	6.4	3
169	Calibration and energy measurement of optically levitated nanoparticle sensors. *Review of Scientific Instruments*, **2018**, 89, 033111	1.7	29
168	Nanocrystals: A Shape-Induced Orientation Phase within 3D Nanocrystal Solids (Adv. Mater. 32/2018). *Advanced Materials*, **2018**, 30, 1870235	24	
167	Rigid-lattice Monte Carlo study of nucleation kinetics in dilute bcc Fe-Cu alloys using statistical sampling techniques. *Acta Materialia*, **2018**, 159, 429-438	8.4	6
166	Theoretical prediction of the homogeneous ice nucleation rate: disentangling thermodynamics and kinetics. *Physical Chemistry Chemical Physics*, **2018**, 20, 28732-28740	3.6	20
165	Melting Si: Beyond Density Functional Theory. *Physical Review Letters*, **2018**, 121, 195701	7.4	33
164	State-dependent diffusion coefficients and free energies for nucleation processes from Bayesian trajectory analysis. *Molecular Physics*, **2018**, 116, 2987-2997	1.7	3
163	Heteropolymer Design and Folding of Arbitrary Topologies Reveals an Unexpected Role of Alphabet Size on the Knot Population. *Macromolecules*, **2018**, 51, 8346-8356	5.5	5
162	Density anomaly of water at negative pressures from first principles. *Journal of Physics Condensed Matter*, **2018**, 30, 254005	1.8	7
161	Theoretical Prediction of Thermal Polarization. *Physical Review Letters*, **2018**, 120, 226001	7.4	4
160	A Shape-Induced Orientation Phase within 3D Nanocrystal Solids. *Advanced Materials*, **2018**, 30, e1802078	24	3
159	Long-Range Dispersion Effects on the Water/Vapor Interface Simulated Using the Most Common Models. *Journal of Physical Chemistry B*, **2017**, 121, 3798-3803	3.4	28
158	Numerical evidence for thermally induced monopoles. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 4911-4914	11.5	7

157	Crystallization and flow in active patch systems. *Soft Matter*, **2017**, 13, 930-936	3.6	6
156	Direct measurement of Kramers turnover with a levitated nanoparticle. *Nature Nanotechnology*, **2017**, 12, 1130-1133	28.7	69
155	Interplay of fast and slow dynamics in rare transition pathways: The disk-to-slab transition in the 2d Ising model. *Journal of Chemical Physics*, **2017**, 147, 152714	3.9	8
154	The role of directional interactions in the designability of generalized heteropolymers. *Scientific Reports*, **2017**, 7, 4986	4.9	14
153	Role of Water in the Selection of Stable Proteins at Ambient and Extreme Thermodynamic Conditions. *Physical Review X*, **2017**, 7,	9.1	12
152	Perspectives on the Future of Ice Nucleation Research: Research Needs and Unanswered Questions Identified from Two International Workshops. *Atmosphere*, **2017**, 8, 138	2.7	43
151	Pathways to self-organization: Crystallization via nucleation and growth. *European Physical Journal E*, **2016**, 39, 77	1.5	29
150	Direct Measurement of Photon Recoil from a Levitated Nanoparticle. *Physical Review Letters*, **2016**, 116, 243601	7.4	176
149	Avoiding traps in trajectory space: Metadynamics enhanced transition path sampling. *European Physical Journal: Special Topics*, **2016**, 225, 1609-1620	2.3	4
148	Molecular mechanism for cavitation in water under tension. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 13582-13587	11.5	78
147	S-shooting: a Bennett-Chandler-like method for the computation of rate constants from committor trajectories. *Faraday Discussions*, **2016**, 195, 345-364	3.6	7
146	How van der Waals interactions determine the unique properties of water. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 8368-73	11.5	230
145	Non-equilibrium simulations of thermally induced electric fields in water. *Journal of Chemical Physics*, **2016**, 144, 224102	3.9	16
144	New methods: general discussion. *Faraday Discussions*, **2016**, 195, 521-556	3.6	2
143	Nucleation and structural growth of cluster crystals. *Journal of Chemical Physics*, **2016**, 145, 074504	3.9	5
142	A Statistical Methodology to Reconstruct Nucleation Pathways in the Fe-Cu System. *Materials Science Forum*, **2016**, 879, 1529-1534	0.4	
141	Effect of entropy on the nucleation of cavitation bubbles in water under tension. *Journal of Chemical Physics*, **2016**, 145, 211918	3.9	10
140	Heterogeneous Crystallization on Pairs of Pre-Structured Seeds. *Journal of Physical Chemistry B*, **2016**, 120, 9230-9	3.4	2

139	A string reaction coordinate for the folding of a polymer chain. *Journal of Physics Condensed Matter*, **2015**, 27, 194126	1.8	3
138	Non-equilibrium steady state of a driven levitated particle with feedback cooling. *New Journal of Physics*, **2015**, 17, 045011	2.9	23
137	Entropy and kinetics of point defects in two-dimensional dipolar crystals. *Physical Review E*, **2015**, 91, 032304	2.4	3
136	Dynamical phases of attractive particles sliding on a structured surface. *Journal of Physics Condensed Matter*, **2015**, 27, 194122	1.8	0
135	Computing the crystal growth rate by the interface pinning method. *Journal of Chemical Physics*, **2015**, 142, 044104	3.9	9
134	Calculating thermal stability and attempt frequency of advanced recording structures without free parameters. *Journal of Applied Physics*, **2015**, 117, 163907	2.5	9
133	Caveats of mean first-passage time methods applied to the crystallization transition: Effects of non-Markovianity. *Journal of Chemical Physics*, **2015**, 142, 064103	3.9	7
132	On the reaction coordinate for seeded crystallisation. *Molecular Physics*, **2015**, 113, 2735-2741	1.7	5
131	An enhanced version of the heat exchange algorithm with excellent energy conservation properties. *Journal of Chemical Physics*, **2015**, 143, 124104	3.9	71
130	Practical and conceptual path sampling issues. *European Physical Journal: Special Topics*, **2015**, 224, 2409-2427	2.3	35
129	Self-assembly of DNA-functionalized colloids. *Condensed Matter Physics*, **2015**, 22801	1.3	17
128	Dynamic relaxation of a levitated nanoparticle from a non-equilibrium steady state. *Nature Nanotechnology*, **2014**, 9, 358-64	28.7	112
127	Frictional dynamics of stiff monolayers: from nucleation dynamics to thermal sliding. *Nanoscale*, **2014**, 6, 10161-8	7.7	10
126	Proton Ordering of Cubic Ice Ic: Spectroscopy and Computer Simulations. *Journal of Physical Chemistry C*, **2014**, 118, 10989-10997	3.8	31
125	Computing Equilibrium Free Energies Using Non-Equilibrium Molecular Dynamics. *Entropy*, **2014**, 16, 41-61	2.8	48
124	Detecting vapour bubbles in simulations of metastable water. *Journal of Chemical Physics*, **2014**, 141, 18C511	3.9	14
123	Folding mechanism of a polymer chain with short-range attractions. *Journal of Chemical Physics*, **2014**, 141, 134901	3.9	15
122	Computing Gibbs free energy differences by interface pinning. *Physical Review B*, **2013**, 88,	3.3	44

121	Neural networks for local structure detection in polymorphic systems. *Journal of Chemical Physics*, **2013**, 139, 164105	3.9	84
120	Simulating rare switching events of magnetic nanostructures with forward flux sampling. *Physical Review B*, **2013**, 88,	3.3	21
119	Self-organized defect strings in two-dimensional crystals. *Physical Review E*, **2013**, 88, 060402	2.4	12
118	Optimising reaction coordinates for crystallisation by tuning the crystallinity definition. *Molecular Physics*, **2013**, 111, 3527-3533	1.7	29
117	Dynamic phases of colloidal monolayers sliding on commensurate substrates. *Soft Matter*, **2013**, 9, 5867	3.6	27
116	Nanoparticle-based crystal growth via multistep self-assembly. *CrystEngComm*, **2013**, 15, 5114	3.3	21
115	Design and folding of colloidal patchy polymers. *Soft Matter*, **2013**, 9, 938-944	3.6	26
114	Sequence controlled self-knotting colloidal patchy polymers. *Physical Review Letters*, **2013**, 110, 075501	7.4	45
113	Crystallization on prestructured seeds. *Physical Review E*, **2013**, 87, 012305	2.4	18
112	A coarse-grained model for DNA-functionalized spherical colloids, revisited: effective pair potential from parallel replica simulations. *Journal of Chemical Physics*, **2013**, 138, 025101	3.9	19
111	Toward the mechanism of ionic dissociation in water. *Journal of Physical Chemistry B*, **2012**, 116, 13490-7	3.4	44
110	Phase transition and interpore correlations of water in nanopore membranes. *Physical Review Letters*, **2012**, 109, 020602	7.4	13
109	The configurational space of colloidal patchy polymers with heterogeneous sequences. *Journal of Physics Condensed Matter*, **2012**, 24, 284111	1.8	8
108	The Eighth Liquid Matter Conference. *Journal of Physics Condensed Matter*, **2012**, 24, 280401	1.8	1
107	Optimizing transition interface sampling simulations. *Journal of Chemical Physics*, **2011**, 134, 244118	3.9	13
106	Crystallization of a binary Lennard-Jones mixture. *Journal of Chemical Physics*, **2011**, 134, 104501	3.9	49
105	Single-file water in nanopores. *Physical Chemistry Chemical Physics*, **2011**, 13, 15403-17	3.6	88
104	Heterogeneous crystallization on tiny clusters. *Europhysics Letters*, **2011**, 96, 56006	1.6	18

103	Vibrational spectroscopy of water in narrow nanopores. *Journal of Physical Chemistry B*, **2011**, 115, 5268-77	3.4	9
102	Role of the prestructured surface cloud in crystal nucleation. *Physical Review Letters*, **2011**, 106, 085701	7.4	110
101	Reaction coordinates for the crystal nucleation of colloidal suspensions extracted from the reweighted path ensemble. *Journal of Chemical Physics*, **2011**, 135, 154110	3.9	35
100	Optimum protocol for fast-switching free-energy calculations. *Physical Review E*, **2010**, 81, 021127	2.4	24
99	Microscopic properties of nanopore water from its time-dependent dielectric response. *Physical Review B*, **2010**, 82,	3.3	8
98	Overcoming barriers in trajectory space: mechanism and kinetics of rare events via Wang-Landau enhanced transition path sampling. *Journal of Chemical Physics*, **2010**, 133, 134112	3.9	15
97	Single-file water as a one-dimensional Ising model. *New Journal of Physics*, **2010**, 12,	2.9	15
96	Demixing of a binary symmetric mixture studied with transition path sampling. *Journal of Chemical Physics*, **2010**, 133, 104505	3.9	7
95	Time-reversal symmetry and covariant Lyapunov vectors for simple particle models in and out of thermal equilibrium. *Physical Review E*, **2010**, 82, 046218	2.4	15
94	The Fourier Monte Carlo Approach to Lattice Spin Models. *Physics Procedia*, **2010**, 6, 106-116		5
93	Identifying rare chaotic and regular trajectories in dynamical systems with Lyapunov weighted path sampling. *Chemical Physics*, **2010**, 375, 309-315	2.3	17
92	Transition Path Sampling Studies of Solid-Solid Transformations in Nanocrystals under Pressure. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 61-84	0.7	2
91	Orientational dynamics and dielectric response of nanopore water. *Physical Review Letters*, **2009**, 103, 080601	7.4	25
90	Mechanism of alkane dehydrogenation catalyzed by acidic zeolites: Ab initio transition path sampling. *Journal of Chemical Physics*, **2009**, 131, 214508	3.9	50
89	Transition Path Sampling and Other Advanced Simulation Techniques for Rare Events **2009**, 167-233		53
88	Transition state analysis of solid-solid transformations in nanocrystals. *Journal of Chemical Physics*, **2009**, 131, 164116	3.9	19
87	Efficient extraction of free energy profiles from nonequilibrium experiments. *Journal of Computational Chemistry*, **2009**, 30, 1726-36	3.5	15
86	Defect interactions in two-dimensional colloidal crystals: vacancy and interstitial strings. *Soft Matter*, **2009**, 5, 2752	3.6	22

85	A one-dimensional dipole lattice model for water in narrow nanopores. *Journal of Chemical Physics*, **2009**, 130, 154110	3.9	21
84	The statistics of electric field fluctuations in liquid water. *Molecular Physics*, **2009**, 107, 495-502	1.7	30
83	Point defects in two-dimensional colloidal crystals: simulation vs. elasticity theory. *Soft Matter*, **2009**, 5, 646-659	3.6	20
82	Nucleation and growth in structural transformations of nanocrystals. *Nano Letters*, **2009**, 9, 2099-102	11.5	48
81	Accurate determination of crystal structures based on averaged local bond order parameters. *Journal of Chemical Physics*, **2008**, 129, 114707	3.9	562
80	Biasing the center of charge in molecular dynamics simulations with empirical valence bond models: free energetics of an excess proton in a water droplet. *Journal of Physical Chemistry B*, **2008**, 112, 2349-56	3.4	20
79	Displacement fields of point defects in two-dimensional colloidal crystals. *Journal of Physics Condensed Matter*, **2008**, 20, 404202	1.8	7
78	Macroscopically ordered water in nanopores. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 13218-22	11.5	129
77	Precision shooting: Sampling long transition pathways. *Journal of Chemical Physics*, **2008**, 129, 194101	3.9	33
76	Gas-phase formation of large neutral alkaline-earth metal tryptophan complexes. *Journal of the American Society for Mass Spectrometry*, **2008**, 19, 1021-6	3.5	20
75	Optimum bias for fast-switching free energy calculations. *Computer Physics Communications*, **2008**, 179, 41-45	4.2	18
74	Large time-step, fast-switching free energy calculations with non-symplectic integrators. *Israel Journal of Chemistry*, **2007**, 47, 215-223	3.4	3
73	An efficient transition path sampling algorithm for nanoparticles under pressure. *Journal of Chemical Physics*, **2007**, 127, 154718	3.9	24
72	Coarse Graining the ϕ^4 Model: Landau-Ginzburg Potentials from Computer Simulations. *Ferroelectrics*, **2007**, 354, 225-237	0.6	12
71	On the efficiency of path sampling methods for the calculation of free energies from non-equilibrium simulations. *Journal of Statistical Mechanics: Theory and Experiment*, **2007**, 2007, P04001-P04001	1.9	29
70	Single molecule pulling with large time steps. *Physical Review E*, **2007**, 75, 061106	2.4	22
69	Effect of Surface Structure on Shape Transformations of Gold Nanorods. *Journal of Computational and Theoretical Nanoscience*, **2007**, 4, 282-290	0.3	10
68	Transition Path Sampling and the Calculation of Free Energies. *Springer Series in Chemical Physics*, **2007**, 249-276	0.3	5

67	Equilibrium free energies from fast-switching trajectories with large time steps. *Journal of Chemical Physics*, **2006**, 124, 044113	3.9	62
66	A proof of Jarzynski? nonequilibrium work theorem for dynamical systems that conserve the canonical distribution. *Journal of Chemical Physics*, **2006**, 125, 054105	3.9	37
65	Mechanisms of the wurtzite to rocksalt transformation in CdSe nanocrystals. *Physical Review Letters*, **2006**, 96, 255701	7.4	95
64	Kinetics and mechanism of proton transport across membrane nanopores. *Physical Review Letters*, **2006**, 97, 245901	7.4	79
63	Transition Path Sampling Methods **2006**, 349-391		19
62	Ideal gas pressure bath: a method for applying hydrostatic pressure in the computer simulation of nanoparticles. *Molecular Physics*, **2006**, 104, 3709-3715	1.7	21
61	Transition Path Sampling Simulations of Biological Systems **2006**, 291-317		58
60	Biased sampling of nonequilibrium trajectories: can fast switching simulations outperform conventional free energy calculation methods?. *Journal of Physical Chemistry B*, **2005**, 109, 6902-15	3.4	132
59	Melting of icosahedral gold nanoclusters from molecular dynamics simulations. *Journal of Chemical Physics*, **2005**, 122, 214722	3.9	171
58	Dipole moment of water molecules in narrow pores. *Computer Physics Communications*, **2005**, 169, 36-39	4.2	15
57	Free energies of the ?4 model from Wang-Landau simulations. *Physical Review B*, **2005**, 72,	3.3	35
56	Surface-driven bulk reorganization of gold nanorods. *Nano Letters*, **2005**, 5, 2174-8	11.5	65
55	Wang-Landau sampling with self-adaptive range. *Physical Review E*, **2005**, 71, 066705	2.4	47
54	Transition Path Sampling **2005**, 1585-1596		5
53	Transition Path Sampling **2005**, 1585-1596		
52	Activation Energies from Transition Path Sampling Simulations. *Molecular Simulation*, **2004**, 30, 795-799	2	31
51	Melting and equilibrium shape of icosahedral gold nanoparticles. *Chemical Physics Letters*, **2004**, 394, 257-261	2.5	69
50	Equilibrium Time Correlation Functions from Irreversible Transformations in Trajectory Space *Journal of Physical Chemistry B*, **2004**, 108, 6667-6672	3.4	24

49	Dissociation of Hydrogen Chloride and Proton Transfer in Liquid Glycerol: An Ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2004**, 108, 19647-19656	3.4	15
48	Transition Path Sampling. *Advances in Chemical Physics*, **2003**, 1-78		259
47	Monte Carlo Sampling in Path Space: Calculating Time Correlation Functions by Transforming Ensembles of Trajectories. *AIP Conference Proceedings*, **2003**,	0	2
46	CarParrinello molecular dynamics simulation of the calcium ion in liquid water. *Chemical Physics Letters*, **2003**, 369, 159-164	2.5	76
45	Structural and Morphological Transitions in Gold Nanorods: A Computer Simulation Study. *Journal of Physical Chemistry B*, **2003**, 107, 9214-9219	3.4	57
44	Proton transport through water-filled carbon nanotubes. *Physical Review Letters*, **2003**, 90, 105902	7.4	304
43	Simulation algorithms for multidimensional nonlinear response of classical many-body systems. *Journal of Chemical Physics*, **2003**, 119, 9344-9354	3.9	25
42	Simulation strategies and signatures of chaos in classical nonlinear response. *Physical Review E*, **2003**, 67, 035205	2.4	27
41	Nonlinear Response of Classical Dynamical Systems to Short Pulses. *Bulletin of the Korean Chemical Society*, **2003**, 24, 1107-1110	1.2	3
40	Transition path sampling: throwing ropes over rough mountain passes, in the dark. *Annual Review of Physical Chemistry*, **2002**, 53, 291-318	15.7	1477
39	Lyapunov Modes of Two-Dimensional Many-Body Systems; Soft Disks, Hard Disks, and Rotors. *Journal of Statistical Physics*, **2002**, 109, 765-776	1.5	28
38	Comment on "Dissociation of water under pressure". *Physical Review Letters*, **2002**, 89, 199601; author reply 199602	7.4	8
37	Fluctuations, convergence times, correlation functions, and power laws from many-body Lyapunov spectra for soft and hard disks and spheres. *Physical Review E*, **2002**, 65, 056216	2.4	8
36	Bridging the Time Scale Gap with Transition Path Sampling. *Lecture Notes in Physics*, **2002**, 321-333	0.8	6
35	Field-dependent collision frequency of the two-dimensional driven random Lorentz gas. *Physical Review E*, **2001**, 64, 036217	2.4	1
34	Dynamical Aspects of Isomerization and Melting Transitions in [H2O]8. *Journal of Physical Chemistry A*, **2001**, 105, 2646-2651	2.8	35
33	Autoionization in liquid water. *Science*, **2001**, 291, 2121-4	33.3	594
32	Ab initio analysis of proton transfer dynamics in (H2O)3H+. *Chemical Physics Letters*, **2000**, 321, 225-230	2.5	50

31	Are local Lyapunov exponents continuous in phase space?. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2000**, 268, 330-334	2.3	7
30	Potential energy landscape for proton transfer in (H2O)3H+: comparison of density functional theory and wavefunction-based methods. *Chemical Physics Letters*, **2000**, 324, 149-155	2.5	19
29	Density-Dependent Diffusion in the Periodic Lorentz Gas. *Journal of Statistical Physics*, **2000**, 101, 145-159	1.5	33
28	Transition path sampling: throwing ropes over mountains in the dark. *Journal of Physics Condensed Matter*, **2000**, 12, A147-A152	1.8	45
27	Finite-precision stationary states at and away from equilibrium. *Physical Review E*, **2000**, 62, 6275-81	2.4	14
26	Reaction coordinates of biomolecular isomerization. *Proceedings of the National Academy of Sciences of the United States of America*, **2000**, 97, 5877-82	11.5	330
25	Diffusion of isobutane in silicalite studied by transition path sampling. *Journal of Chemical Physics*, **2000**, 113, 8791-8799	3.9	45
24	On the calculation of reaction rate constants in the transition path ensemble. *Journal of Chemical Physics*, **1999**, 110, 6617-6625	3.9	270
23	Kinetic Pathways of Ion Pair Dissociation in Water. *Journal of Physical Chemistry B*, **1999**, 103, 3706-3710	3.4	275
22	Chemical dynamics of the protonated water trimer analyzed by transition path sampling. *Physical Chemistry Chemical Physics*, **1999**, 1, 1317-1322	3.6	58
21	Field and density dependence of the Lyapunov spectrum for the driven random Lorentz gas. *Physica D: Nonlinear Phenomena*, **1998**, 112, 241-249	3.3	2
20	Sampling ensembles of deterministic transition pathways. *Faraday Discussions*, **1998**, 110, 421-436	3.6	262
19	Transition path sampling and the calculation of rate constants. *Journal of Chemical Physics*, **1998**, 108, 1964-1977	3.9	819
18	Efficient transition path sampling: Application to Lennard-Jones cluster rearrangements. *Journal of Chemical Physics*, **1998**, 108, 9236-9245	3.9	286
17	Isomorphic multifractal shear flows for hard disks via adiabatic and isokinetic nonequilibrium molecular dynamics. *Physical Review E*, **1998**, 57, 4969-4975	2.4	5
16	Largest Lyapunov Exponent for Many Particle Systems at Low Densities. *Physical Review Letters*, **1998**, 80, 2035-2038	7.4	73
15	Kolmogorov-Sinai entropy for dilute gases in equilibrium. *Physical Review E*, **1997**, 56, 5272-5277	2.4	54
14	Lyapunov Spectrum and the Conjugate Pairing Rule for a Thermostatted Random Lorentz Gas: Numerical Simulations. *Physical Review Letters*, **1997**, 78, 211-214	7.4	22

13	Mixing, Lyapunov instability, and the approach to equilibrium in a hard-sphere gas. *Physical Review E*, **1997**, 55, R9-R12	2.4	27
12	Kolmogorov-Sinai entropy and Lyapunov spectra of a hard-sphere gas. *Physica A: Statistical Mechanics and Its Applications*, **1997**, 240, 68-83	3.3	56
11	Lyapunov instability in the extended XY-model: Equilibrium and nonequilibrium molecular dynamics simulations. *Physica A: Statistical Mechanics and Its Applications*, **1997**, 237, 95-112	3.3	18
10	Lyapunov instability in a system of hard disks in equilibrium and nonequilibrium steady states. *Physical Review E*, **1996**, 53, 1485-1501	2.4	129
9	Lyapunov instability, local curvature, and the fluid-solid phase transition in two-dimensional particle systems. *Physica A: Statistical Mechanics and Its Applications*, **1996**, 230, 364-387	3.3	38
8	Lyapunov Exponents from Kinetic Theory for a Dilute, Field-Driven Lorentz Gas. *Physical Review Letters*, **1996**, 77, 1974-1977	7.4	32
7	Lyapunov spectrum of the driven Lorentz gas. *Physical Review E*, **1995**, 52, 4817-4826	2.4	23
6	Lyapunov exponents of systems with elastic hard collisions. *Physical Review E*, **1995**, 52, 2401-2406	2.4	34
5	On the accuracy of the size distribution information obtained from light extinction and scattering measurements I. Basic considerations and models. *Journal of Aerosol Science*, **1993**, 24, 129-141	4.3	30
4	On the accuracy of the size distribution information obtained from light extinction and scattering measurements II. Case studies. *Journal of Aerosol Science*, **1993**, 24, 143-154	4.3	17
3	A surface with variable reflectivity. *Review of Scientific Instruments*, **1990**, 61, 1993-1994	1.7	1
2	On the accuracy of the size distribution information obtained from spectral extinction/scattering measurements. *Journal of Aerosol Science*, **1990**, 21, S155-S158	4.3	4
1	Trajectory-Based Rare Event Simulations. *Reviews in Computational Chemistry*,111-210		16