Christoph Dellago

List of Publications by Year
in descending order

194 papers	12,666 citations	41344 49 h-index	25787 108 g-index
199 all docs	199 docs citations	199 times ranked	8974 citing authors

#	Article	IF	Citations
1	Improved description of atomic environments using low-cost polynomial functions with compact support. Machine Learning: Science and Technology, 2021, 2, 035026.	5.0	10
2	The microscopic mechanism of bulk melting of ice. Journal of Chemical Physics, 2021, 155, 124501.	3.0	5
3	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
4	Elastic forces drive nonequilibrium pattern formation in a model of nanocrystal ion exchange. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	3
5	Identification of Protein Functional Regions. ChemPhysChem, 2020, 21, 335-347.	2.1	1
6	Ab initio structure and thermodynamics of the RPBE-D3 water/vapor interface by neural-network molecular dynamics. Journal of Chemical Physics, 2020, 153, 144710.	3.0	24
7	Weak scaling of the contact distance between two fluctuating interfaces with system size. Physical Review E, 2020, 102, 062801.	2.1	3
8	Hierarchical self-assembly of patchy colloidal platelets. Soft Matter, 2020, 16, 2774-2785.	2.7	18
9	Protein design under competing conditions for the availability of amino acids. Scientific Reports, 2020, 10, 2684.	3.3	4
10	The generic unfolding of a biomimetic polymer during force spectroscopy. Soft Matter, 2020, 16, 3941-3951.	2.7	1
11	Enhancing transport by shaping barriers. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 2238-2240.	7.1	2
12	How patchiness controls the properties of chain-like assemblies of colloidal platelets. Journal of Physics Condensed Matter, 2020, 32, 204001.	1.8	3
13	Origin of mean-field behavior in an elastic Ising model. Physical Review B, 2020, 102, .	3.2	8
14	Catalytic Mechanism of Processive GlfT2: Transition Path Sampling Investigation of Substrate Translocation. ACS Omega, 2020, 5, 21374-21384.	3.5	3
15	General Methodology to Identify the Minimum Alphabet Size for Heteropolymer Design. Advanced Theory and Simulations, 2019, 2, 1900031.	2.8	8
16	Design of Patchy Rhombi: From Close-Packed Tilings to Open Lattices. Nano Letters, 2019, 19, 7806-7815.	9.1	17
17	A High Coordination of Cross-Links Is Beneficial for the Strength of Cross-Linked Fibers. Biomimetics, 2019, 4, 12.	3.3	13
18	Phase stability of the ice XVII-based CO2 chiral hydrate from molecular dynamics simulations. Journal of Chemical Physics, 2019, 151, 104502.	3.0	3

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19	Consequences of Lattice Mismatch for Phase Equilibrium in Heterostructured Solids. Physical Review Letters, 2019, 123, 135701.	7.8	13
20	Library-Based LAMMPS Implementation of High-Dimensional Neural Network Potentials. Journal of Chemical Theory and Computation, 2019, 15, 1827-1840.	5.3	175
21	Parallel Multistream Training of High-Dimensional Neural Network Potentials. Journal of Chemical Theory and Computation, 2019, 15, 3075-3092.	5.3	124
22	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.	3.0	2
23	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.	7.1	201
24	Design of Proteinâ€“Protein Binding Sites Suggests a Rationale for Naturally Occurring Contact Areas. Journal of Chemical Theory and Computation, 2019, 15, 1383-1392.	5.3	4
25	Calibration and energy measurement of optically levitated nanoparticle sensors. Review of Scientific Instruments, 2018, 89, 033111.	1.3	54
26	Theoretical prediction of the homogeneous ice nucleation rate: disentangling thermodynamics and kinetics. Physical Chemistry Chemical Physics, 2018, 20, 28732-28740.	2.8	25
27	Melting Si: Beyond Density Functional Theory. Physical Review Letters, 2018, 121, 195701.	7.8	46
28	State-dependent diffusion coefficients and free energies for nucleation processes from Bayesian trajectory analysis. Molecular Physics, 2018, 116, 2987-2997.	1.7	5
29	Heteropolymer Design and Folding of Arbitrary Topologies Reveals an Unexpected Role of Alphabet Size on the Knot Population. Macromolecules, 2018, 51, 8346-8356.	4.8	9
30	Density anomaly of water at negative pressures from first principles. Journal of Physics Condensed Matter, 2018, 30, 254005.	1.8	10
31	Theoretical Prediction of Thermal Polarization. Physical Review Letters, 2018, 120, 226001.	7.8	6
32	A Shapeâ€Induced Orientation Phase within 3D Nanocrystal Solids. Advanced Materials, 2018, 30, e1802078.	21.0	7
33	Nanocrystals: A Shape-Induced Orientation Phase within 3D Nanocrystal Solids (Adv. Mater. 32/2018). Advanced Materials, 2018, 30, 1870235.	21.0	0
34	Rigid-lattice Monte Carlo study of nucleation kinetics in dilute bcc Fe-Cu alloys using statistical sampling techniques. Acta Materialia, 2018, 159, 429-438.	7.9	6
35	Long-Range Dispersion Effects on the Water/Vapor Interface Simulated Using the Most Common Models. Journal of Physical Chemistry B, 2017, 121, 3798-3803.	2.6	40
36	Numerical evidence for thermally induced monopoles. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 4911-4914.	7.1	11

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37	Crystallization and flow in active patch systems. Soft Matter, 2017, 13, 930-936.	2.7	7
38	Direct measurement of Kramers turnover with a levitated nanoparticle. Nature Nanotechnology, 2017, 12, 1130-1133.	31.5	102
39	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.	3.0	12
40	The role of directional interactions in the designability of generalized heteropolymers. Scientific Reports, 2017, 7, 4986.	3.3	18
41	Role of Water in the Selection of Stable Proteins at Ambient and Extreme Thermodynamic Conditions. Physical Review X, 2017, 7, .	8.9	18
42	Perspectives on the Future of Ice Nucleation Research: Research Needs and Unanswered Questions Identified from Two International Workshops. Atmosphere, 2017, 8, 138.	2.3	56
43	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, 8368-8373.	7.1	312
44	Non-equilibrium simulations of thermally induced electric fields in water. Journal of Chemical Physics, 2016, 144, 224102.	3.0	17
45	New methods: general discussion. Faraday Discussions, 2016, 195, 521-556.	3.2	2
46	Nucleation and structural growth of cluster crystals. Journal of Chemical Physics, 2016, 145, 074504.	3.0	6
47	A Statistical Methodology to Reconstruct Nucleation Pathways in the Fe-Cu System. Materials Science Forum, 2016, 879, 1529-1534.	0.3	0
48	Effect of entropy on the nucleation of cavitation bubbles in water under tension. Journal of Chemical Physics, 2016, 145, 211918.	3.0	14
49	Heterogeneous Crystallization on Pairs of Pre-Structured Seeds. Journal of Physical Chemistry B, 2016, 120, 9230-9239.	2.6	3
50	Pathways to self-organization: Crystallization via nucleation and growth. European Physical Journal E, 2016, 39, 77.	1.6	36
51	Direct Measurement of Photon Recoil from a Levitated Nanoparticle. Physical Review Letters, 2016, 116, 243601.	7.8	239
52	Avoiding traps in trajectory space: Metadynamics enhanced transition path sampling. European Physical Journal: Special Topics, 2016, 225, 1609-1620.	2.6	7
53	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.	7.1	110
54	S-shooting: a Bennettâ€“Chandler-like method for the computation of rate constants from committor trajectories. Faraday Discussions, 2016, 195, 345-364.	3.2	10

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55	On the reaction coordinate for seeded crystallisation. Molecular Physics, 2015, 113, 2735-2741.	1.7	6
56	An enhanced version of the heat exchange algorithm with excellent energy conservation properties. Journal of Chemical Physics, 2015, 143, 124104.	3.0	108
57	Practical and conceptual path sampling issues. European Physical Journal: Special Topics, 2015, 224, 2409-2427.	2.6	48
58	A string reaction coordinate for the folding of a polymer chain. Journal of Physics Condensed Matter, 2015, 27, 194126.	1.8	5
59	Non-equilibrium steady state of a driven levitated particle with feedback cooling. New Journal of Physics, 2015, 17, 045011.	2.9	29
60	Entropy and kinetics of point defects in two-dimensional dipolar crystals. Physical Review E, 2015, 91, 032304.	2.1	3
61	Dynamical phases of attractive particles sliding on a structured surface. Journal of Physics Condensed Matter, 2015, 27, 194122.	1.8	1
62	Computing the crystal growth rate by the interface pinning method. Journal of Chemical Physics, 2015, 142, 044104.	3.0	15
63	Calculating thermal stability and attempt frequency of advanced recording structures without free parameters. Journal of Applied Physics, 2015, 117, 163907.	2.5	12
64	Caveats of mean first-passage time methods applied to the crystallization transition: Effects of non-Markovianity. Journal of Chemical Physics, 2015, 142, 064103.	3.0	7
65	Self-assembly of DNA-functionalized colloids. Condensed Matter Physics, 2015, , 22801.	0.7	21
66	Computing Equilibrium Free Energies Using Non-Equilibrium Molecular Dynamics. Entropy, 2014, 16, 41-61.	2.2	60
67	Detecting vapour bubbles in simulations of metastable water. Journal of Chemical Physics, 2014, 141, 18C511.	3.0	19
68	Folding mechanism of a polymer chain with short-range attractions. Journal of Chemical Physics, 2014, 141, 134901.	3.0	19
69	Dynamic relaxation of a levitated nanoparticle from a non-equilibrium steady state. Nature Nanotechnology, 2014, 9, 358-364.	31.5	151
70	Frictional dynamics of stiff monolayers: from nucleation dynamics to thermal sliding. Nanoscale, 2014, 6, 10161-10168.	5.6	12
71	Proton Ordering of Cubic Ice Ic: Spectroscopy and Computer Simulations. Journal of Physical Chemistry C, 2014, 118, 10989-10997.	3.1	35
72	Computing Gibbs free energy differences by interface pinning. Physical Review B, 2013, 88, .	3.2	64

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73	Neural networks for local structure detection in polymorphic systems. Journal of Chemical Physics, 2013, 139, 164105.	3.0	115
74	Simulating rare switching events of magnetic nanostructures with forward flux sampling. Physical Review B, 2013, 88, .	3.2	24
75	Self-organized defect strings in two-dimensional crystals. Physical Review E, 2013, 88, 060402.	2.1	15
76	Optimising reaction coordinates for crystallisation by tuning the crystallinity definition. Molecular Physics, 2013, 111, 3527-3533.	1.7	33
77	Dynamic phases of colloidal monolayers sliding on commensurate substrates. Soft Matter, 2013, 9, 5867.	2.7	31
78	Nanoparticle-based crystal growth via multistep self-assembly. CrystEngComm, 2013, 15, 5114.	2.6	25
79	Design and folding of colloidal patchy polymers. Soft Matter, 2013, 9, 938-944.	2.7	28
80	Sequence Controlled Self-Knotting Colloidal Patchy Polymers. Physical Review Letters, 2013, 110, 075501.	7.8	55
81	Crystallization on prestructured seeds. Physical Review E, 2013, 87, 012305.	2.1	21
82	A coarse-grained model for DNA-functionalized spherical colloids, revisited: Effective pair potential from parallel replica simulations. Journal of Chemical Physics, 2013, 138, 025101.	3.0	20
83	The configurational space of colloidal patchy polymers with heterogeneous sequences. Journal of Physics Condensed Matter, 2012, 24, 284111.	1.8	8
84	The Eighth Liquid Matter Conference. Journal of Physics Condensed Matter, 2012, 24, 280301.	1.8	0
85	The Eighth Liquid Matter Conference. Journal of Physics Condensed Matter, 2012, 24, 280401.	1.8	1
86	Toward the Mechanism of Ionic Dissociation in Water. Journal of Physical Chemistry B, 2012, 116, 13490-13497.	2.6	54
87	Wired-up water. Nature Chemistry, 2012, 4, 245-247.	13.6	7
88	Phase Transition and Interpore Correlations of Water in Nanopore Membranes. Physical Review Letters, 2012, 109, 020602.	7.8	15
89	Vibrational Spectroscopy of Water in Narrow Nanopores. Journal of Physical Chemistry B, 2011, 115, 5268-5277.	2.6	9
90	Optimizing transition interface sampling simulations. Journal of Chemical Physics, 2011, 134, 244118.	3.0	14

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91	Crystallization of a binary Lennard-Jones mixture. Journal of Chemical Physics, 2011, 134, 104501.	3.0	50
92	Single-file water in nanopores. Physical Chemistry Chemical Physics, 2011, 13, 15403.	2.8	99
93	Heterogeneous crystallization on tiny clusters. Europhysics Letters, 2011, 96, 56006.	2.0	21
94	Role of the Prestructured Surface Cloud in Crystal Nucleation. Physical Review Letters, 2011, 106, 085701.	7.8	122
95	Reaction coordinates for the crystal nucleation of colloidal suspensions extracted from the reweighted path ensemble. Journal of Chemical Physics, 2011, 135, 154110.	3.0	40
96	The Fourier Monte Carlo Approach to Lattice Spin Models. Physics Procedia, 2010, 6, 106-116.	1.2	5
97	Identifying rare chaotic and regular trajectories in dynamical systems with Lyapunov weighted path sampling. Chemical Physics, 2010, 375, 309-315.	1.9	19
98	Optimum protocol for fast-switching free-energy calculations. Physical Review E, 2010, 81, 021127.	2.1	36
99	Microscopic properties of nanopore water from its time-dependent dielectric response. Physical Review B, 2010, 82, .	3.2	9
100	Overcoming barriers in trajectory space: Mechanism and kinetics of rare events via Wangâ€“Landau enhanced transition path sampling. Journal of Chemical Physics, 2010, 133, 134112.	3.0	16
101	Single-file water as a one-dimensional Ising model. New Journal of Physics, 2010, 12, 093044.	2.9	20
102	Demixing of a binary symmetric mixture studied with transition path sampling. Journal of Chemical Physics, 2010, 133, 104505.	3.0	7
103	Time-reversal symmetry and covariant Lyapunov vectors for simple particle models in and out of thermal equilibrium. Physical Review E, 2010, 82, 046218.	2.1	16
104	Transition Path Sampling Studies of Solid-Solid Transformations in Nanocrystals under Pressure. Challenges and Advances in Computational Chemistry and Physics, 2010, , 61-84.	0.6	2
105	Orientational Dynamics and Dielectric Response of Nanopore Water. Physical Review Letters, 2009, 103, 080601.	7.8	27
106	Mechanism of alkane dehydrogenation catalyzed by acidic zeolites: Ab initio transition path sampling. Journal of Chemical Physics, 2009, 131, 214508.	3.0	55
107	Transition Path Sampling and Other Advanced Simulation Techniques for Rare Events. , 2009, , 167-233.		69
108	Transition state analysis of solid-solid transformations in nanocrystals. Journal of Chemical Physics, 2009, 131, 164116.	3.0	20

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109	Efficient extraction of free energy profiles from nonequilibrium experiments. Journal of Computational Chemistry, 2009, 30, 1726-1736.	3.3	16
110	Defect interactions in two-dimensional colloidal crystals: vacancy and interstitial strings. Soft Matter, 2009, 5, 2752.	2.7	25
111	A one-dimensional dipole lattice model for water in narrow nanopores. Journal of Chemical Physics, 2009, 130, 154110.	3.0	24
112	The statistics of electric field fluctuations in liquid water. Molecular Physics, 2009, 107, 495-502.	1.7	39
113	Point defects in two-dimensional colloidal crystals: simulation vs. elasticity theory. Soft Matter, 2009, 5, 646-659.	2.7	21
114	Nucleation and Growth in Structural Transformations of Nanocrystals. Nano Letters, 2009, 9, 2099-2102.	9.1	49
115	Gas-phase formation of large neutral alkaline-earth metal tryptophan complexes. Journal of the American Society for Mass Spectrometry, 2008, 19, 1021-1026.	2.8	22
116	Optimum bias for fast-switching free energy calculations. Computer Physics Communications, 2008, 179, 41-45.	7.5	18
117	Accurate determination of crystal structures based on averaged local bond order parameters. Journal of Chemical Physics, 2008, 129, 114707.	3.0	707
118	Biasing the Center of Charge in Molecular Dynamics Simulations with Empirical Valence Bond Models:â€‰ Free Energetics of an Excess Proton in a Water Droplet. Journal of Physical Chemistry B, 2008, 112, 2349-2356.	2.6	23
119	Displacement fields of point defects in two-dimensional colloidal crystals. Journal of Physics Condensed Matter, 2008, 20, 404202.	1.8	8
120	Macroscopically ordered water in nanopores. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 13218-13222.	7.1	145
121	Precision shooting: Sampling long transition pathways. Journal of Chemical Physics, 2008, 129, 194101.	3.0	37
122	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.	2.3	32
123	Single molecule pulling with large time steps. Physical Review E, 2007, 75, 061106.	2.1	23
124	Effect of Surface Structure on Shape Transformations of Gold Nanorods. Journal of Computational and Theoretical Nanoscience, 2007, 4, 282-290.	0.4	10
125	Large timeâ€step, fastâ€switching free energy calculations with nonâ€symplectic integrators. Israel Journal of Chemistry, 2007, 47, 215-223.	2.3	4
126	An efficient transition path sampling algorithm for nanoparticles under pressure. Journal of Chemical Physics, 2007, 127, 154718.	3.0	26

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127	Coarse Graining the Ï†⁴Model: Landau-Ginzburg Potentials from Computer Simulations. Ferroelectrics, 2007, 354, 225-237.	0.6	12
128	Transition Path Sampling and the Calculation of Free Energies. Springer Series in Chemical Physics, 2007, , 249-276.	0.2	5
129	Equilibrium free energies from fast-switching trajectories with large time steps. Journal of Chemical Physics, 2006, 124, 044113.	3.0	66
130	A proof of Jarzynskiâ€™s nonequilibrium work theorem for dynamical systems that conserve the canonical distribution. Journal of Chemical Physics, 2006, 125, 054105.	3.0	37
131	Mechanisms of the Wurtzite to Rocksalt Transformation in CdSe Nanocrystals. Physical Review Letters, 2006, 96, 255701.	7.8	98
132	Kinetics and Mechanism of Proton Transport across Membrane Nanopores. Physical Review Letters, 2006, 97, 245901.	7.8	84
133	Transition Path Sampling Methods. , 2006, , 349-391.		23
134	Ideal gas pressure bath: a method for applying hydrostatic pressure in the computer simulation of nanoparticles. Molecular Physics, 2006, 104, 3709-3715.	1.7	22
135	Transition Path Sampling Simulations of Biological Systems. , 2006, , 291-317.		64
136	Dipole moment of water molecules in narrow pores. Computer Physics Communications, 2005, 169, 36-39.	7.5	21
137	Free energies of theÏ•4model from Wang-Landau simulations. Physical Review B, 2005, 72, .	3.2	37
138	Surface-Driven Bulk Reorganization of Gold Nanorods. Nano Letters, 2005, 5, 2174-2178.	9.1	69
139	Wang-Landau sampling with self-adaptive range. Physical Review E, 2005, 71, 066705.	2.1	52
140	Biased Sampling of Nonequilibrium Trajectories:Â Can Fast Switching Simulations Outperform Conventional Free Energy Calculation Methods?â€. Journal of Physical Chemistry B, 2005, 109, 6902-6915.	2.6	151
141	Melting of icosahedral gold nanoclusters from molecular dynamics simulations. Journal of Chemical Physics, 2005, 122, 214722.	3.0	194
142	Transition Path Sampling. , 2005, , 1585-1596.		18
143	Transition Path Sampling. , 2005, , 1585-1596.		0
144	Activation Energies from Transition Path Sampling Simulations. Molecular Simulation, 2004, 30, 795-799.	2.0	33

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145	Melting and equilibrium shape of icosahedral gold nanoparticles. Chemical Physics Letters, 2004, 394, 257-261.	2.6	73
146	Equilibrium Time Correlation Functions from Irreversible Transformations in Trajectory Space. Journal of Physical Chemistry B, 2004, 108, 6667-6672.	2.6	26
147	Dissociation of Hydrogen Chloride and Proton Transfer in Liquid Glycerol:Â An Ab Initio Molecular Dynamics Studyâ€. Journal of Physical Chemistry B, 2004, 108, 19647-19656.	2.6	16
148	Carâ€“Parrinello molecular dynamics simulation of the calcium ion in liquid water. Chemical Physics Letters, 2003, 369, 159-164.	2.6	85
149	Structural and Morphological Transitions in Gold Nanorods:Â A Computer Simulation Study. Journal of Physical Chemistry B, 2003, 107, 9214-9219.	2.6	62
150	Proton Transport through Water-Filled Carbon Nanotubes. Physical Review Letters, 2003, 90, 105902.	7.8	339
151	Simulation algorithms for multidimensional nonlinear response of classical many-body systems. Journal of Chemical Physics, 2003, 119, 9344-9354.	3.0	27
152	Simulation strategies and signatures of chaos in classical nonlinear response. Physical Review E, 2003, 67, 035205.	2.1	29
153	Transition Path Sampling. Advances in Chemical Physics, 2003, , 1-78.	0.3	310
154	Monte Carlo Sampling in Path Space: Calculating Time Correlation Functions by Transforming Ensembles of Trajectories. AIP Conference Proceedings, 2003, , .	0.4	2
155	Nonlinear Response of Classical Dynamical Systems to Short Pulses. Bulletin of the Korean Chemical Society, 2003, 24, 1107-1110.	1.9	3
156	Comment on â€œDissociation of Water under Pressureâ€• Physical Review Letters, 2002, 89, 199601; author reply 199602.	7.8	9
157	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.	2.1	8
158	TRANSITIONPATHSAMPLING: Throwing Ropes Over Rough Mountain Passes, in the Dark. Annual Review of Physical Chemistry, 2002, 53, 291-318.	10.8	1,704
159	Lyapunov Modes of Two-Dimensional Many-Body Systems; Soft Disks, Hard Disks, and Rotors. Journal of Statistical Physics, 2002, 109, 765-776.	1.2	28
160	Bridging the Time Scale Gap with Transition Path Sampling. Lecture Notes in Physics, 2002, , 321-333.	0.7	6
161	Dynamical Aspects of Isomerization and Melting Transitions in [H2O]8â€. Journal of Physical Chemistry A, 2001, 105, 2646-2651.	2.5	36
162	Autoionization in Liquid Water. Science, 2001, 291, 2121-2124.	12.6	672

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163	Field-dependent collision frequency of the two-dimensional driven random Lorentz gas. Physical Review E, 2001, 64, 036217.	2.1	2
164	Ab initio analysis of proton transfer dynamics in (H2O)3H+. Chemical Physics Letters, 2000, 321, 225-230.	2.6	54
165	Are local Lyapunov exponents continuous in phase space?. Physics Letters, Section A: General, Atomic and Solid State Physics, 2000, 268, 330-334.	2.1	9
166	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.	2.6	23
167	Density-Dependent Diffusion in the Periodic Lorentz Gas. Journal of Statistical Physics, 2000, 101, 145-159.	1.2	35
168	Transition path sampling: throwing ropes over mountains in the dark. Journal of Physics Condensed Matter, 2000, 12, A147-A152.	1.8	52
169	Finite-precision stationary states at and away from equilibrium. Physical Review E, 2000, 62, 6275-6281.	2.1	17
170	Reaction coordinates of biomolecular isomerization. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 5877-5882.	7.1	370
171	Diffusion of isobutane in silicalite studied by transition path sampling. Journal of Chemical Physics, 2000, 113, 8791-8799.	3.0	51
172	On the calculation of reaction rate constants in the transition path ensemble. Journal of Chemical Physics, 1999, 110, 6617-6625.	3.0	292
173	Kinetic Pathways of Ion Pair Dissociation in Water. Journal of Physical Chemistry B, 1999, 103, 3706-3710.	2.6	310
174	Chemical dynamics of the protonated water trimer analyzed by transition path sampling. Physical Chemistry Chemical Physics, 1999, 1, 1317-1322.	2.8	61
175	Field and density dependence of the Lyapunov spectrum for the driven random Lorentz gas. Physica D: Nonlinear Phenomena, 1998, 112, 241-249.	2.8	3
176	Sampling ensembles of deterministic transition pathways. Faraday Discussions, 1998, 110, 421-436.	3.2	282
177	Transition path sampling and the calculation of rate constants. Journal of Chemical Physics, 1998, 108, 1964-1977.	3.0	925
178	Efficient transition path sampling: Application to Lennard-Jones cluster rearrangements. Journal of Chemical Physics, 1998, 108, 9236-9245.	3.0	313
179	Isomorphic multifractal shear flows for hard disks via adiabatic and isokinetic nonequilibrium molecular dynamics. Physical Review E, 1998, 57, 4969-4975.	2.1	6
180	Largest Lyapunov Exponent for Many Particle Systems at Low Densities. Physical Review Letters, 1998, 80, 2035-2038.	7.8	81

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181	Kolmogorov-Sinai entropy for dilute gases in equilibrium. Physical Review E, 1997, 56, 5272-5277.	2.1	61
182	Lyapunov Spectrum and the Conjugate Pairing Rule for a Thermostatted Random Lorentz Gas: Numerical Simulations. Physical Review Letters, 1997, 78, 211-214.	7.8	26
183	Mixing, Lyapunov instability, and the approach to equilibrium in a hard-sphere gas. Physical Review E, 1997, 55, R9-R12.	2.1	28
184	Kolmogorov-Sinai entropy and Lyapunov spectra of a hard-sphere gas. Physica A: Statistical Mechanics and Its Applications, 1997, 240, 68-83.	2.6	59
185	Lyapunov instability in the extended XY-model: Equilibrium and nonequilibrium molecular dynamics simulations. Physica A: Statistical Mechanics and Its Applications, 1997, 237, 95-112.	2.6	22
186	Lyapunov instability in a system of hard disks in equilibrium and nonequilibrium steady states. Physical Review E, 1996, 53, 1485-1501.	2.1	143
187	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.	2.6	41
188	Lyapunov Exponents from Kinetic Theory for a Dilute, Field-Driven Lorentz Gas. Physical Review Letters, 1996, 77, 1974-1977.	7.8	35
189	Lyapunov spectrum of the driven Lorentz gas. Physical Review E, 1995, 52, 4817-4826.	2.1	31
190	Lyapunov exponents of systems with elastic hard collisions. Physical Review E, 1995, 52, 2401-2406.	2.1	39
191	On the accuracy of the size distribution information obtained from light extinction and scattering measurementsâ€"I. Basic considerations and models. Journal of Aerosol Science, 1993, 24, 129-141.	3.8	31
192	On the accuracy of the size distribution information obtained from light extinction and scattering measurementsâ€"II. Case studies. Journal of Aerosol Science, 1993, 24, 143-154.	3.8	23
193	A surface with variable reflectivity. Review of Scientific Instruments, 1990, 61, 1993-1994.	1.3	1
194	On the accuracy of the size distribution information obtained from spectral extinction/scattering measurements. Journal of Aerosol Science, 1990, 21, S155-S158.	3.8	4