Christoph Dellago

List of Publications by Citations

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	Transition path sampling: throwing ropes over rough mountain passes, in the dark. *Annual Review of Physical Chemistry*, **2002**, 53, 291-318	15.7	1477
191	Transition path sampling and the calculation of rate constants. *Journal of Chemical Physics*, **1998**, 108, 1964-1977	3.9	819
190	Autoionization in liquid water. *Science*, **2001**, 291, 2121-4	33.3	594
189	Accurate determination of crystal structures based on averaged local bond order parameters. *Journal of Chemical Physics*, **2008**, 129, 114707	3.9	562
188	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
187	Proton transport through water-filled carbon nanotubes. *Physical Review Letters*, **2003**, 90, 105902	7.4	304
186	Efficient transition path sampling: Application to Lennard-Jones cluster rearrangements. *Journal of Chemical Physics*, **1998**, 108, 9236-9245	3.9	286
185	Kinetic Pathways of Ion Pair Dissociation in Water. *Journal of Physical Chemistry B*, **1999**, 103, 3706-3710	3.4	275
184	On the calculation of reaction rate constants in the transition path ensemble. *Journal of Chemical Physics*, **1999**, 110, 6617-6625	3.9	270
183	Sampling ensembles of deterministic transition pathways. *Faraday Discussions*, **1998**, 110, 421-436	3.6	262
182	Transition Path Sampling. *Advances in Chemical Physics*, **2003**, 1-78		259
181	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
180	Direct Measurement of Photon Recoil from a Levitated Nanoparticle. *Physical Review Letters*, **2016**, 116, 243601	7.4	176
179	Melting of icosahedral gold nanoclusters from molecular dynamics simulations. *Journal of Chemical Physics*, **2005**, 122, 214722	3.9	171
178	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
177	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
176	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

175	Lyapunov instability in a system of hard disks in equilibrium and nonequilibrium steady states. *Physical Review E*, **1996**, 53, 1485-1501	2.4	129
174	Dynamic relaxation of a levitated nanoparticle from a non-equilibrium steady state. *Nature Nanotechnology*, **2014**, 9, 358-64	28.7	112
173	Role of the prestructured surface cloud in crystal nucleation. *Physical Review Letters*, **2011**, 106, 085701	7.4	110
172	Mechanisms of the wurtzite to rocksalt transformation in CdSe nanocrystals. *Physical Review Letters*, **2006**, 96, 255701	7.4	95
171	Library-Based LAMMPS Implementation of High-Dimensional Neural Network Potentials. *Journal of Chemical Theory and Computation*, **2019**, 15, 1827-1840	6.4	94
170	Single-file water in nanopores. *Physical Chemistry Chemical Physics*, **2011**, 13, 15403-17	3.6	88
169	Neural networks for local structure detection in polymorphic systems. *Journal of Chemical Physics*, **2013**, 139, 164105	3.9	84
168	Kinetics and mechanism of proton transport across membrane nanopores. *Physical Review Letters*, **2006**, 97, 245901	7.4	79
167	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
166	CarÞarrinello molecular dynamics simulation of the calcium ion in liquid water. *Chemical Physics Letters*, **2003**, 369, 159-164	2.5	76
165	Largest Lyapunov Exponent for Many Particle Systems at Low Densities. *Physical Review Letters*, **1998**, 80, 2035-2038	7.4	73
164	An enhanced version of the heat exchange algorithm with excellent energy conservation properties. *Journal of Chemical Physics*, **2015**, 143, 124104	3.9	71
163	Direct measurement of Kramers turnover with a levitated nanoparticle. *Nature Nanotechnology*, **2017**, 12, 1130-1133	28.7	69
162	Melting and equilibrium shape of icosahedral gold nanoparticles. *Chemical Physics Letters*, **2004**, 394, 257-261	2.5	69
161	Surface-driven bulk reorganization of gold nanorods. *Nano Letters*, **2005**, 5, 2174-8	11.5	65
160	Equilibrium free energies from fast-switching trajectories with large time steps. *Journal of Chemical Physics*, **2006**, 124, 044113	3.9	62
159	Parallel Multistream Training of High-Dimensional Neural Network Potentials. *Journal of Chemical Theory and Computation*, **2019**, 15, 3075-3092	6.4	61
158	Transition Path Sampling Simulations of Biological Systems **2006**, 291-317		58

157	Chemical dynamics of the protonated water trimer analyzed by transition path sampling. *Physical Chemistry Chemical Physics*, **1999**, 1, 1317-1322	3.6	58
156	Structural and Morphological Transitions in Gold Nanorods: A Computer Simulation Study. *Journal of Physical Chemistry B*, **2003**, 107, 9214-9219	3.4	57
155	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
154	Kolmogorov-Sinai entropy for dilute gases in equilibrium. *Physical Review E*, **1997**, 56, 5272-5277	2.4	54
153	Transition Path Sampling and Other Advanced Simulation Techniques for Rare Events **2009**, 167-233		53
152	Mechanism of alkane dehydrogenation catalyzed by acidic zeolites: Ab initio transition path sampling. *Journal of Chemical Physics*, **2009**, 131, 214508	3.9	50
151	Ab initio analysis of proton transfer dynamics in (H2O)3H+. *Chemical Physics Letters*, **2000**, 321, 225-230	2.5	50
150	Crystallization of a binary Lennard-Jones mixture. *Journal of Chemical Physics*, **2011**, 134, 104501	3.9	49
149	Computing Equilibrium Free Energies Using Non-Equilibrium Molecular Dynamics. *Entropy*, **2014**, 16, 41-61	2.8	48
148	Nucleation and growth in structural transformations of nanocrystals. *Nano Letters*, **2009**, 9, 2099-102	11.5	48
147	Wang-Landau sampling with self-adaptive range. *Physical Review E*, **2005**, 71, 066705	2.4	47
146	Sequence controlled self-knotting colloidal patchy polymers. *Physical Review Letters*, **2013**, 110, 075501	7.4	45
145	Transition path sampling: throwing ropes over mountains in the dark. *Journal of Physics Condensed Matter*, **2000**, 12, A147-A152	1.8	45
144	Diffusion of isobutane in silicalite studied by transition path sampling. *Journal of Chemical Physics*, **2000**, 113, 8791-8799	3.9	45
143	Computing Gibbs free energy differences by interface pinning. *Physical Review B*, **2013**, 88,	3.3	44
142	Toward the mechanism of ionic dissociation in water. *Journal of Physical Chemistry B*, **2012**, 116, 13490-7	3.4	44
141	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
140	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

139	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
138	Practical and conceptual path sampling issues. *European Physical Journal: Special Topics*, **2015**, 224, 2409-2427	2.5	35
137	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
136	Free energies of the ?4 model from Wang-Landau simulations. *Physical Review B*, **2005**, 72,	3.3	35
135	Dynamical Aspects of Isomerization and Melting Transitions in [H2O]8. *Journal of Physical Chemistry A*, **2001**, 105, 2646-2651	2.8	35
134	Lyapunov exponents of systems with elastic hard collisions. *Physical Review E*, **1995**, 52, 2401-2406	2.4	34
133	Precision shooting: Sampling long transition pathways. *Journal of Chemical Physics*, **2008**, 129, 194101	3.9	33
132	Density-Dependent Diffusion in the Periodic Lorentz Gas. *Journal of Statistical Physics*, **2000**, 101, 145-158	1.5	33
131	Melting Si: Beyond Density Functional Theory. *Physical Review Letters*, **2018**, 121, 195701	7.4	33
130	Lyapunov Exponents from Kinetic Theory for a Dilute, Field-Driven Lorentz Gas. *Physical Review Letters*, **1996**, 77, 1974-1977	7.4	32
129	Proton Ordering of Cubic Ice Ic: Spectroscopy and Computer Simulations. *Journal of Physical Chemistry C*, **2014**, 118, 10989-10997	3.8	31
128	Activation Energies from Transition Path Sampling Simulations. *Molecular Simulation*, **2004**, 30, 795-799	2	31
127	The statistics of electric field fluctuations in liquid water. *Molecular Physics*, **2009**, 107, 495-502	1.7	30
126	On the accuracy of the size distribution information obtained from light extinction and scattering measurements. Basic considerations and models. *Journal of Aerosol Science*, **1993**, 24, 129-141	4.3	30
125	Calibration and energy measurement of optically levitated nanoparticle sensors. *Review of Scientific Instruments*, **2018**, 89, 033111	1.7	29
124	Pathways to self-organization: Crystallization via nucleation and growth. *European Physical Journal E*, **2016**, 39, 77	1.5	29
123	Optimising reaction coordinates for crystallisation by tuning the crystallinity definition. *Molecular Physics*, **2013**, 111, 3527-3533	1.7	29
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	1.9	29

121	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
120	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
119	Dynamic phases of colloidal monolayers sliding on commensurate substrates. *Soft Matter*, **2013**, 9, 5867	3.6	27
118	Mixing, Lyapunov instability, and the approach to equilibrium in a hard-sphere gas. *Physical Review E*, **1997**, 55, R9-R12	2.4	27
117	Simulation strategies and signatures of chaos in classical nonlinear response. *Physical Review E*, **2003**, 67, 035205	2.4	27
116	Design and folding of colloidal patchy polymers. *Soft Matter*, **2013**, 9, 938-944	3.6	26
115	Orientational dynamics and dielectric response of nanopore water. *Physical Review Letters*, **2009**, 103, 080601	7.4	25
114	Simulation algorithms for multidimensional nonlinear response of classical many-body systems. *Journal of Chemical Physics*, **2003**, 119, 9344-9354	3.9	25
113	Optimum protocol for fast-switching free-energy calculations. *Physical Review E*, **2010**, 81, 021127	2.4	24
112	An efficient transition path sampling algorithm for nanoparticles under pressure. *Journal of Chemical Physics*, **2007**, 127, 154718	3.9	24
111	Equilibrium Time Correlation Functions from Irreversible Transformations in Trajectory Space *Journal of Physical Chemistry B*, **2004**, 108, 6667-6672	3.4	24
110	Non-equilibrium steady state of a driven levitated particle with feedback cooling. *New Journal of Physics*, **2015**, 17, 045011	2.9	23
109	Lyapunov spectrum of the driven Lorentz gas. *Physical Review E*, **1995**, 52, 4817-4826	2.4	23
108	Defect interactions in two-dimensional colloidal crystals: vacancy and interstitial strings. *Soft Matter*, **2009**, 5, 2752	3.6	22
107	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
106	Single molecule pulling with large time steps. *Physical Review E*, **2007**, 75, 061106	2.4	22
105	Simulating rare switching events of magnetic nanostructures with forward flux sampling. *Physical Review B*, **2013**, 88,	3.3	21
104	Nanoparticle-based crystal growth via multistep self-assembly. *CrystEngComm*, **2013**, 15, 5114	3.3	21

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100	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
99	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
98	Theoretical prediction of the homogeneous ice nucleation rate: disentangling thermodynamics and kinetics. *Physical Chemistry Chemical Physics*, **2018**, 20, 28732-28740	3.6	20
97	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
96	Transition state analysis of solid-solid transformations in nanocrystals. *Journal of Chemical Physics*, **2009**, 131, 164116	3.9	19
95	Transition Path Sampling Methods **2006**, 349-391		19
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87	Self-assembly of DNA-functionalized colloids. *Condensed Matter Physics*, **2015**, 22801	1.3	17
86	Non-equilibrium simulations of thermally induced electric fields in water. *Journal of Chemical Physics*, **2016**, 144, 224102	3.9	16

85	Trajectory-Based Rare Event Simulations. *Reviews in Computational Chemistry*,111-210		16
84	Folding mechanism of a polymer chain with short-range attractions. *Journal of Chemical Physics*, **2014**, 141, 134901	3.9	15
83	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
82	Single-file water as a one-dimensional Ising model. *New Journal of Physics*, **2010**, 12,	2.9	15
81	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
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77	The role of directional interactions in the designability of generalized heteropolymers. *Scientific Reports*, **2017**, 7, 4986	4.9	14
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75	Finite-precision stationary states at and away from equilibrium. *Physical Review E*, **2000**, 62, 6275-81	2.4	14
74	Design of Patchy Rhombi: From Close-Packed Tilings to Open Lattices. *Nano Letters*, **2019**, 19, 7806-7815	11.5	13
73	Phase transition and interpore correlations of water in nanopore membranes. *Physical Review Letters*, **2012**, 109, 020602	7.4	13
72	Optimizing transition interface sampling simulations. *Journal of Chemical Physics*, **2011**, 134, 244118	3.9	13
71	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
70	Hierarchical self-assembly of patchy colloidal platelets. *Soft Matter*, **2020**, 16, 2774-2785	3.6	12
69	Self-organized defect strings in two-dimensional crystals. *Physical Review E*, **2013**, 88, 060402	2.4	12
68	Role of Water in the Selection of Stable Proteins at Ambient and Extreme Thermodynamic Conditions. *Physical Review X*, **2017**, 7,	9.1	12

67	Coarse Graining the Φ4 Model: Landau-Ginzburg Potentials from Computer Simulations. *Ferroelectrics*, **2007**, 354, 225-237	0.6	12
66	A High Coordination of Cross-Links Is Beneficial for the Strength of Cross-Linked Fibers. *Biomimetics*, **2019**, 4,	3.7	11
65	Frictional dynamics of stiff monolayers: from nucleation dynamics to thermal sliding. *Nanoscale*, **2014**, 6, 10161-8	7.7	10
64	Effect of Surface Structure on Shape Transformations of Gold Nanorods. *Journal of Computational and Theoretical Nanoscience*, **2007**, 4, 282-290	0.3	10
63	Effect of entropy on the nucleation of cavitation bubbles in water under tension. *Journal of Chemical Physics*, **2016**, 145, 211918	3.9	10
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61	Calculating thermal stability and attempt frequency of advanced recording structures without free parameters. *Journal of Applied Physics*, **2015**, 117, 163907	2.5	9
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59	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
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49	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
48	Density anomaly of water at negative pressures from first principles. *Journal of Physics Condensed Matter*, **2018**, 30, 254005	1.8	7
47	Crystallization and flow in active patch systems. *Soft Matter*, **2017**, 13, 930-936	3.6	6
46	Consequences of Lattice Mismatch for Phase Equilibrium in Heterostructured Solids. *Physical Review Letters*, **2019**, 123, 135701	7.4	6
45	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
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41	The Fourier Monte Carlo Approach to Lattice Spin Models. *Physics Procedia*, **2010**, 6, 106-116		5
40	Isomorphic multifractal shear flows for hard disks via adiabatic and isokinetic nonequilibrium molecular dynamics. *Physical Review E*, **1998**, 57, 4969-4975	2.4	5
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38	Nucleation and structural growth of cluster crystals. *Journal of Chemical Physics*, **2016**, 145, 074504	3.9	5
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36	Transition Path Sampling **2005**, 1585-1596		5
35	Avoiding traps in trajectory space: Metadynamics enhanced transition path sampling. *European Physical Journal: Special Topics*, **2016**, 225, 1609-1620	2.3	4
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20	Monte Carlo Sampling in Path Space: Calculating Time Correlation Functions by Transforming Ensembles of Trajectories. *AIP Conference Proceedings*, **2003**,	0	2
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9	A surface with variable reflectivity. *Review of Scientific Instruments*, **1990**, 61, 1993-1994	1.7	1
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6	Dynamical phases of attractive particles sliding on a structured surface. *Journal of Physics Condensed Matter*, **2015**, 27, 194122	1.8	0
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3	Nanocrystals: A Shape-Induced Orientation Phase within 3D Nanocrystal Solids (Adv. Mater. 32/2018). *Advanced Materials*, **2018**, 30, 1870235	24	
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1	Transition Path Sampling **2005**, 1585-1596		