Caroline Desgranges

List of Publications by Year
in descending order

80 papers	1,643 citations	293460 24 h-index	371746 37 g-index
80 all docs	80 docs citations	80 times ranked	1121 citing authors

#	Article	IF	Citations
1	Machine-Learned Free Energy Surfaces for Capillary Condensation and Evaporation in Mesopores. Entropy, 2022, 24, 97.	1.1	0
2	Entropy determination for mixtures in the adiabatic grand-isobaric ensemble. Journal of Chemical Physics, 2022, 156, 084113.	1.2	1
3	Designing, synthesizing, and modeling active fluids. Physics of Fluids, 2022, 34, .	1.6	6
4	Towards a machine learned thermodynamics: exploration of free energy landscapes in molecular fluids, biological systems and for gas storage and separation in metalâ€“organic frameworks. Molecular Systems Design and Engineering, 2021, 6, 52-65.	1.7	8
5	Entropy scaling close to criticality: From simple to metallic systems. Physical Review E, 2021, 103, 052102.	0.8	0
6	Ensemble Learning of Partition Functions for the Prediction of Thermodynamic Properties of Adsorption in Metalâ€“Organic and Covalent Organic Frameworks. Journal of Physical Chemistry C, 2020, 124, 1907-1917.	1.5	13
7	Entropy in Molecular Fluids: Interplay between Interaction Complexity and Criticality. Journal of Physical Chemistry B, 2020, 124, 11463-11471.	1.2	2
8	Unraveling liquid polymorphism in silicon driven out-of-equilibrium. Journal of Chemical Physics, 2020, 153, 054502.	1.2	5
9	The central role of entropy in adiabatic ensembles and its application to phase transitions in the grand-isobaric adiabatic ensemble. Journal of Chemical Physics, 2020, 153, 094114.	1.2	4
10	Entropy production in model colloidal suspensions under shear via the fluctuation theorem. Journal of Chemical Physics, 2020, 153, 224113.	1.2	2
11	Nucleation of Capillary Bridges and Bubbles in Nanoconfined CO2. Langmuir, 2019, 35, 15401-15409.	1.6	8
12	Can Ordered Precursors Promote the Nucleation of Solid Solutions?. Physical Review Letters, 2019, 123, 195701.	2.9	26
13	Stabilization of Nanobubbles under Hydrophobic Confinement. Journal of Physical Chemistry C, 2019, 123, 11707-11713.	1.5	6
14	Viscosity of a highly compressed methylated alkane via equilibrium and nonequilibrium molecular dynamics simulations. Chemical Physics Letters, 2019, 719, 103-109.	1.2	8
15	Determination of mixture properties via a combined Expanded Wang-Landau simulations-Machine Learning approach. Chemical Physics Letters, 2019, 715, 1-6.	1.2	5
16	Prediction of the boiling and critical points of polycyclic aromatic hydrocarbons via Wang-Landau simulations and machine learning. Fluid Phase Equilibria, 2019, 484, 225-231.	1.4	9
17	Modeling antigen-antibody nanoparticle bioconjugates and their polymorphs. Journal of Chemical Physics, 2018, 148, 124507.	1.2	2
18	Calculating free energy profiles using entropy as a reaction coordinate: Application to water nucleation. Chemical Physics Letters, 2018, 695, 194-199.	1.2	1

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19	Unusual Crystallization Behavior Close to the Glass Transition. Physical Review Letters, 2018, 120, 115701.	2.9	32
20	Crystal nucleation along an entropic pathway: Teaching liquids how to transition. Physical Review E, 2018, 98, .	0.8	13
21	Communication: Existence and control of liquid polymorphism in methanol under shear. Journal of Chemical Physics, 2018, 149, 111101.	1.2	9
22	A new approach for the prediction of partition functions using machine learning techniques. Journal of Chemical Physics, 2018, 149, 044118.	1.2	19
23	Prediction of the phase equilibria for island-type asphaltenes via HMC-WL simulations. Journal of Chemical Physics, 2018, 149, 072307.	1.2	3
24	Non-monotonic variations of the nucleation free energy in a glass-forming ultra-soft particles fluid. Soft Matter, 2018, 14, 5977-5985.	1.2	1
25	Ginzburg-Landau free energy for molecular fluids: Determination and coarse-graining. Chemical Physics Letters, 2017, 669, 218-223.	1.2	1
26	Free energy calculations along entropic pathways. III. Nucleation of capillary bridges and bubbles. Journal of Chemical Physics, 2017, 146, 184104.	1.2	13
27	Classical and quantum many-body effects on the critical properties and thermodynamic regularities of silicon. Journal of Physics Condensed Matter, 2017, 29, 045401.	0.7	2
28	Benchmark Free Energies and Entropies for Saturated and Compressed Water. Journal of Chemical & Engineering Data, 2017, 62, 4032-4040.	1.0	6
29	Selectivity and Desorption Free Energies for Methaneâ€“Ethane Mixtures in Covalent Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 24692-24700.	1.5	11
30	Free Energy of Nucleation and Interplay between Size and Composition in CuNi Systems. Journal of Physical Chemistry B, 2017, 121, 8558-8563.	1.2	4
31	Competition between crystalline and icosahedral order during crystal growth in bimetallic systems. Journal of Crystal Growth, 2017, 478, 22-27.	0.7	4
32	Coarse-Grained Model and Boiling Point Prediction for Asphaltene Model Compounds via HMC-WL Simulations. Energy & Fuels, 2017, 31, 10699-10705.	2.5	12
33	Similarity law and critical properties in ionic systems.. Chemical Physics Letters, 2017, 687, 9-13.	1.2	8
34	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. V. Impact of an electric field on the thermodynamic properties and ideality contours of water. Journal of Chemical Physics, 2016, 145, 184504.	1.2	14
35	Free energy calculations along entropic pathways. I. Homogeneous vapor-liquid nucleation for atomic and molecular systems. Journal of Chemical Physics, 2016, 145, 204112.	1.2	17
36	Free energy calculations along entropic pathways. II. Droplet nucleation in binary mixtures. Journal of Chemical Physics, 2016, 145, 234505.	1.2	10

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37	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. IV. Performance of many-body force fields and tight-binding schemes for the fluid phases of silicon. Journal of Chemical Physics, 2016, 144, 124510.	1.2	20
38	Ideality contours and thermodynamic regularities in supercritical molecular fluids. Chemical Physics Letters, 2016, 658, 37-42.	1.2	24
39	Effect of the Composition on the Free Energy of Crystal Nucleation for CuPd Nanoalloys. Journal of Physical Chemistry C, 2016, 120, 27657-27664.	1.5	8
40	Impact of Friedel oscillations on vapor-liquid equilibria and supercritical properties in two and three dimensions. Physical Review E, 2016, 94, 012612.	0.8	7
41	Scaling Laws and Critical Properties for fcc and hcp Metals. Journal of Physical Chemistry B, 2016, 120, 5255-5261.	1.2	28
42	Many-Body Effects on the Thermodynamics of Fluids, Mixtures, and Nanoconfined Fluids. Journal of Chemical Theory and Computation, 2015, 11, 5401-5414.	2.3	24
43	A new force field for H2S and its binary and ternary mixtures with CO2 and CH4. Fluid Phase Equilibria, 2015, 402, 69-77.	1.4	10
44	Adsorption and diffusion of the antiparkinsonian drug amantadine in carbon nanotubes. Molecular Simulation, 2014, 40, 656-663.	0.9	19
45	Adsorption of hydrogen in covalent organic frameworks using expanded Wangâ€“Landau simulations. Molecular Simulation, 2014, 40, 71-79.	0.9	15
46	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. III. Impact of combining rules on mixtures properties. Journal of Chemical Physics, 2014, 140, 104109.	1.2	35
47	Thermodynamics of Phase Coexistence and Metalâ€“Nonmetal Transition in Mercury: Assessment of Effective Potentials via Expanded Wangâ€“Landau Simulations. Journal of Physical Chemistry B, 2014, 118, 3175-3182.	1.2	14
48	Unraveling the Coupling between Demixing and Crystallization in Mixtures. Journal of the American Chemical Society, 2014, 136, 8145-8148.	6.6	26
49	Characterization and Comparison of the Performance of IRMOF-1, IRMOF-8, and IRMOF-10 for CO₂ Adsorption in the Subcritical and Supercritical Regimes. Journal of Physical Chemistry C, 2012, 116, 22938-22946.	1.5	25
50	Wangâ€“Landau configurational bias Monte Carlo simulations: vapourâ€“liquid equilibria of alkenes. Molecular Simulation, 2012, 38, 653-658.	0.9	20
51	Numerical estimate for boiling points via Wangâ€“Landau simulations. Molecular Simulation, 2012, 38, 1265-1270.	0.9	19
52	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. I. Thermodynamic properties in the bulk and at the liquid-vapor phase boundary. Journal of Chemical Physics, 2012, 136, 184107.	1.2	46
53	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. II. Adsorption of atomic and molecular fluids in a porous material. Journal of Chemical Physics, 2012, 136, 184108.	1.2	41
54	Prediction of critical properties for Naphthacene, Triphenylene and Chrysene by Wangâ€“Landau simulations. Fluid Phase Equilibria, 2012, 322-323, 92-96.	1.4	18

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55	Crystal nucleation and growth in Pdâ€“Ni alloys: a molecular simulation study. CrystEngComm, 2011, 13, 1132-1140.	1.3	14
56	Role of Liquid Polymorphism during the Crystallization of Silicon. Journal of the American Chemical Society, 2011, 133, 2872-2874.	6.6	43
57	Polymorph selection during the crystallization of iron under the conditions of Earthâ€™s inner core. Chemical Physics Letters, 2011, 511, 57-61.	1.2	13
58	Vaporâ€“liquid equilibria of copper using hybrid Monte Carlo Wangâ€”Landau simulations. Fluid Phase Equilibria, 2010, 287, 79-83.	1.4	43
59	Phase equilibria of polyaromatic hydrocarbons by hybrid Monte Carlo Wangâ€“Landau simulations. Molecular Physics, 2010, 108, 151-158.	0.8	28
60	Optimisation of multiple time-step hybrid Monte Carlo Wangâ€“Landau simulations in the isobaricâ€“isothermal ensemble for the determination of phase equilibria. Molecular Simulation, 2010, 36, 544-551.	0.9	18
61	Universal scaling law for energy and pressure in a shearing fluid. Physical Review E, 2009, 79, 052201.	0.8	5
62	Accurate determination of normal stress differences via transient-time correlation function â€“ non-equilibrium molecular dynamics (TTCFâ€“NEMD) simulations. Molecular Simulation, 2009, 35, 405-408.	0.9	5
63	Nucleation and growth of C60 nanoparticles from the supersaturated vapor and from the undercooled liquid: A molecular simulation study. Journal of Chemical Physics, 2009, 131, 244515.	1.2	8
64	Phase equilibria of molecular fluids via hybrid Monte Carlo Wangâ€“Landau simulations: Applications to benzene and n-alkanes. Journal of Chemical Physics, 2009, 130, 244109.	1.2	52
65	Molecular Simulation of the Nucleation and Growth of Gold Nanoparticles. Journal of Physical Chemistry C, 2009, 113, 3607-3611.	1.5	40
66	Estimating the conductivity of a nanoconfined liquid subjected to an experimentally accessible external field. Molecular Simulation, 2008, 34, 177-181.	0.9	8
67	Shear viscosity of liquid copper at experimentally accessible shear rates: Application of the transient-time correlation function formalism. Journal of Chemical Physics, 2008, 128, 084506.	1.2	21
68	Molecular simulation of transport in nanopores: Application of the transient-time correlation function formalism. Physical Review E, 2008, 77, 027701.	0.8	25
69	Rheology of liquid fcc metals: Equilibrium and transient-time correlation-function nonequilibrium molecular dynamics simulations. Physical Review B, 2008, 78, .	1.1	30
70	Crystallization mechanisms for supercooled liquid Xe at high pressure and temperature: Hybrid Monte Carlo molecular simulations. Physical Review B, 2008, 77, .	1.1	40
71	Controlling Polymorphism during the Crystallization of an Atomic Fluid. Physical Review Letters, 2007, 98, 235502.	2.9	111
72	Viscosity of liquid iron under high pressure and high temperature: Equilibrium and nonequilibrium molecular dynamics simulation studies. Physical Review B, 2007, 76, .	1.1	32

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73	Polymorph selection during the crystallization of Yukawa systems. Journal of Chemical Physics, 2007, 126, 054501.	1.2	46
74	Molecular Simulation of Cross-Nucleation between Polymorphs. Journal of Physical Chemistry B, 2007, 111, 1465-1469.	1.2	28
75	Polymorph Selection during the Crystallization of Softly Repulsive Spheres:â€‰ The Inverse Power Law Potential. Journal of Physical Chemistry B, 2007, 111, 12257-12262.	1.2	19
76	Molecular Insight into the Pathway to Crystallization of Aluminum. Journal of the American Chemical Society, 2007, 129, 7012-7013.	6.6	64
77	Molecular simulation of the crystallization of aluminum from the supercooled liquid. Journal of Chemical Physics, 2007, 127, 144509.	1.2	41
78	Molecular Mechanism for the Cross-Nucleation between Polymorphs. Journal of the American Chemical Society, 2006, 128, 10368-10369.	6.6	115
79	Insights into the Molecular Mechanism Underlying Polymorph Selection. Journal of the American Chemical Society, 2006, 128, 15104-15105.	6.6	86
80	Structural characterization of an Sb deltaâ€doping layer in silicon. Applied Physics Letters, 1989, 55, 963-965.	1.5	24