Caroline Desgranges

List of Publications by Year in Descending Order

78 papers	1,471 citations	22 h-index	34 g-index
80 ext. papers	1,564 ext. citations	4.1 avg, IF	5.29 L-index

#	Paper	IF	Citations
78	Entropy determination for mixtures in the adiabatic grand-isobaric ensemble.. *Journal of Chemical Physics*, **2022**, 156, 084113	3.9	
77	Entropy scaling close to criticality: From simple to metallic systems. *Physical Review E*, **2021**, 103, 052102	2.4	
76	Towards a machine learned thermodynamics: exploration of free energy landscapes in molecular fluids, biological systems and for gas storage and separation in metal Organic frameworks. *Molecular Systems Design and Engineering*, **2021**, 6, 52-65	4.6	4
75	Entropy production in model colloidal suspensions under shear via the fluctuation theorem. *Journal of Chemical Physics*, **2020**, 153, 224113	3.9	0
74	Ensemble Learning of Partition Functions for the Prediction of Thermodynamic Properties of Adsorption in Metal Organic and Covalent Organic Frameworks. *Journal of Physical Chemistry C*, **2020**, 124, 1907-1917	3.8	10
73	Entropy in Molecular Fluids: Interplay between Interaction Complexity and Criticality. *Journal of Physical Chemistry B*, **2020**, 124, 11463-11471	3.4	0
72	Unraveling liquid polymorphism in silicon driven out-of-equilibrium. *Journal of Chemical Physics*, **2020**, 153, 054502	3.9	4
71	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	3.9	3
70	Stabilization of Nanobubbles under Hydrophobic Confinement. *Journal of Physical Chemistry C*, **2019**, 123, 11707-11713	3.8	3
69	Nucleation of Capillary Bridges and Bubbles in Nanoconfined CO. *Langmuir*, **2019**, 35, 15401-15409	4	5
68	Can Ordered Precursors Promote the Nucleation of Solid Solutions?. *Physical Review Letters*, **2019**, 123, 195701	7.4	15
67	Viscosity of a highly compressed methylated alkane via equilibrium and nonequilibrium molecular dynamics simulations. *Chemical Physics Letters*, **2019**, 719, 103-109	2.5	5
66	Determination of mixture properties via a combined Expanded Wang-Landau simulations-Machine Learning approach. *Chemical Physics Letters*, **2019**, 715, 1-6	2.5	3
65	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	2.5	7
64	Modeling antigen-antibody nanoparticle bioconjugates and their polymorphs. *Journal of Chemical Physics*, **2018**, 148, 124507	3.9	2
63	Calculating free energy profiles using entropy as a reaction coordinate: Application to water nucleation. *Chemical Physics Letters*, **2018**, 695, 194-199	2.5	1
62	Unusual Crystallization Behavior Close to the Glass Transition. *Physical Review Letters*, **2018**, 120, 115701	7.4	25

61	A new approach for the prediction of partition functions using machine learning techniques. *Journal of Chemical Physics*, **2018**, 149, 044118	3.9	15
60	Prediction of the phase equilibria for island-type asphaltenes via HMC-WL simulations. *Journal of Chemical Physics*, **2018**, 149, 072307	3.9	2
59	Non-monotonic variations of the nucleation free energy in a glass-forming ultra-soft particles fluid. *Soft Matter*, **2018**, 14, 5977-5985	3.6	1
58	Crystal nucleation along an entropic pathway: Teaching liquids how to transition. *Physical Review E*, **2018**, 98,	2.4	12
57	Communication: Existence and control of liquid polymorphism in methanol under shear. *Journal of Chemical Physics*, **2018**, 149, 111101	3.9	8
56	Ginzburg-Landau free energy for molecular fluids: Determination and coarse-graining. *Chemical Physics Letters*, **2017**, 669, 218-223	2.5	1
55	Free energy calculations along entropic pathways. III. Nucleation of capillary bridges and bubbles. *Journal of Chemical Physics*, **2017**, 146, 184104	3.9	11
54	Classical and quantum many-body effects on the critical properties and thermodynamic regularities of silicon. *Journal of Physics Condensed Matter*, **2017**, 29, 045401	1.8	2
53	Benchmark Free Energies and Entropies for Saturated and Compressed Water. *Journal of Chemical & Engineering Data*, **2017**, 62, 4032-4040	2.8	6
52	Selectivity and Desorption Free Energies for Methane–Ethane Mixtures in Covalent Organic Frameworks. *Journal of Physical Chemistry C*, **2017**, 121, 24692-24700	3.8	11
51	Free Energy of Nucleation and Interplay between Size and Composition in CuNi Systems. *Journal of Physical Chemistry B*, **2017**, 121, 8558-8563	3.4	2
50	Competition between crystalline and icosahedral order during crystal growth in bimetallic systems. *Journal of Crystal Growth*, **2017**, 478, 22-27	1.6	4
49	Coarse-Grained Model and Boiling Point Prediction for Asphaltene Model Compounds via HMC-WL Simulations. *Energy & Fuels*, **2017**, 31, 10699-10705	4.1	7
48	Similarity law and critical properties in ionic systems.. *Chemical Physics Letters*, **2017**, 687, 9-13	2.5	4
47	Effect of the Composition on the Free Energy of Crystal Nucleation for CuPd Nanoalloys. *Journal of Physical Chemistry C*, **2016**, 120, 27657-27664	3.8	7
46	Impact of Friedel oscillations on vapor-liquid equilibria and supercritical properties in two and three dimensions. *Physical Review E*, **2016**, 94, 012612	2.4	5
45	Scaling Laws and Critical Properties for fcc and hcp Metals. *Journal of Physical Chemistry B*, **2016**, 120, 5255-61	3.4	20
44	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	3.9	13

43	Free energy calculations along entropic pathways. I. Homogeneous vapor-liquid nucleation for atomic and molecular systems. *Journal of Chemical Physics*, **2016**, 145, 204112	3.9	16
42	Free energy calculations along entropic pathways. II. Droplet nucleation in binary mixtures. *Journal of Chemical Physics*, **2016**, 145, 234505	3.9	9
41	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	3.9	20
40	Ideality contours and thermodynamic regularities in supercritical molecular fluids. *Chemical Physics Letters*, **2016**, 658, 37-42	2.5	18
39	A new force field for H2S and its binary and ternary mixtures with CO2 and CH4. *Fluid Phase Equilibria*, **2015**, 402, 69-77	2.5	9
38	Many-Body Effects on the Thermodynamics of Fluids, Mixtures, and Nanoconfined Fluids. *Journal of Chemical Theory and Computation*, **2015**, 11, 5401-14	6.4	22
37	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	3.9	30
36	Thermodynamics of phase coexistence and metal-nonmetal transition in mercury: assessment of effective potentials via expanded Wang-Landau simulations. *Journal of Physical Chemistry B*, **2014**, 118, 3175-82	3.4	13
35	Unraveling the coupling between demixing and crystallization in mixtures. *Journal of the American Chemical Society*, **2014**, 136, 8145-8	16.4	23
34	Adsorption and diffusion of the antiparkinsonian drug amantadine in carbon nanotubes. *Molecular Simulation*, **2014**, 40, 656-663	2	17
33	Adsorption of hydrogen in covalent organic frameworks using expanded Wang□andau simulations. *Molecular Simulation*, **2014**, 40, 71-79	2	15
32	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	3.8	23
31	Wang□andau configurational bias Monte Carlo simulations: vapour□quid equilibria of alkenes. *Molecular Simulation*, **2012**, 38, 653-658	2	20
30	Numerical estimate for boiling points via Wang□andau simulations. *Molecular Simulation*, **2012**, 38, 1265-1270	2	17
29	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	3.9	43
28	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	3.9	39
27	Prediction of critical properties for Naphthacene, Triphenylene and Chrysene by Wang□andau simulations. *Fluid Phase Equilibria*, **2012**, 322-323, 92-96	2.5	18
26	Crystal nucleation and growth in Pd□Ni alloys: a molecular simulation study. *CrystEngComm*, **2011**, 13, 1132-1140	3.3	14

25	Role of liquid polymorphism during the crystallization of silicon. *Journal of the American Chemical Society*, **2011**, 133, 2872-4	16.4	42
24	Polymorph selection during the crystallization of iron under the conditions of Earth's inner core. *Chemical Physics Letters*, **2011**, 511, 57-61	2.5	11
23	Phase equilibria of polyaromatic hydrocarbons by hybrid Monte Carlo Wang–Landau simulations. *Molecular Physics*, **2010**, 108, 151-158	1.7	28
22	Optimisation of multiple time-step hybrid Monte Carlo Wang–Landau simulations in the isobaric–isothermal ensemble for the determination of phase equilibria. *Molecular Simulation*, **2010**, 36, 544-551	2	18
21	Vapor–liquid equilibria of copper using hybrid Monte Carlo Wang–Landau simulations. *Fluid Phase Equilibria*, **2010**, 287, 79-83	2.5	42
20	Universal scaling law for energy and pressure in a shearing fluid. *Physical Review E*, **2009**, 79, 052201	2.4	3
19	Accurate determination of normal stress differences via transient-time correlation function – non-equilibrium molecular dynamics (TTCF–NEMD) simulations. *Molecular Simulation*, **2009**, 35, 405-408	2	4
18	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	3.9	8
17	Phase equilibria of molecular fluids via hybrid Monte Carlo Wang-Landau simulations: applications to benzene and n-alkanes. *Journal of Chemical Physics*, **2009**, 130, 244109	3.9	50
16	Molecular Simulation of the Nucleation and Growth of Gold Nanoparticles. *Journal of Physical Chemistry C*, **2009**, 113, 3607-3611	3.8	38
15	Estimating the conductivity of a nanoconfined liquid subjected to an experimentally accessible external field. *Molecular Simulation*, **2008**, 34, 177-181	2	7
14	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	3.9	18
13	Molecular simulation of transport in nanopores: application of the transient-time correlation function formalism. *Physical Review E*, **2008**, 77, 027701	2.4	22
12	Rheology of liquid fcc metals: Equilibrium and transient-time correlation-function nonequilibrium molecular dynamics simulations. *Physical Review B*, **2008**, 78,	3.3	27
11	Crystallization mechanisms for supercooled liquid Xe at high pressure and temperature: Hybrid Monte Carlo molecular simulations. *Physical Review B*, **2008**, 77,	3.3	36
10	Molecular simulation of cross-nucleation between polymorphs. *Journal of Physical Chemistry B*, **2007**, 111, 1465-9	3.4	27
9	Polymorph selection during the crystallization of softly repulsive spheres: the inverse power law potential. *Journal of Physical Chemistry B*, **2007**, 111, 12257-62	3.4	19
8	Molecular insight into the pathway to crystallization of aluminum. *Journal of the American Chemical Society*, **2007**, 129, 7012-3	16.4	61

7	Molecular simulation of the crystallization of aluminum from the supercooled liquid. *Journal of Chemical Physics*, **2007**, 127, 144509	3.9	39
6	Controlling polymorphism during the crystallization of an atomic fluid. *Physical Review Letters*, **2007**, 98, 235502	7.4	101
5	Viscosity of liquid iron under high pressure and high temperature: Equilibrium and nonequilibrium molecular dynamics simulation studies. *Physical Review B*, **2007**, 76,	3.3	31
4	Polymorph selection during the crystallization of Yukawa systems. *Journal of Chemical Physics*, **2007** , 126, 054501	3.9	41
3	Molecular mechanism for the cross-nucleation between polymorphs. *Journal of the American Chemical Society*, **2006**, 128, 10368-9	16.4	108
2	Insights into the molecular mechanism underlying polymorph selection. *Journal of the American Chemical Society*, **2006**, 128, 15104-5	16.4	81
1	A new approach for the prediction of partition functions using machine learning techniques. *Applied Physics Letters*, **1989**, 55, 963-965	3.4	24