

Caroline Desgranges

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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	Molecular mechanism for the cross-nucleation between polymorphs. <i>Journal of the American Chemical Society</i> , 2006 , 128, 10368-9	16.4	108
77	Controlling polymorphism during the crystallization of an atomic fluid. <i>Physical Review Letters</i> , 2007 , 98, 235502	7.4	101
76	Insights into the molecular mechanism underlying polymorph selection. <i>Journal of the American Chemical Society</i> , 2006 , 128, 15104-5	16.4	81
75	Molecular insight into the pathway to crystallization of aluminum. <i>Journal of the American Chemical Society</i> , 2007 , 129, 7012-3	16.4	61
74	Phase equilibria of molecular fluids via hybrid Monte Carlo Wang-Landau simulations: applications to benzene and n-alkanes. <i>Journal of Chemical Physics</i> , 2009 , 130, 244109	3.9	50
73	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. <i>Journal of Chemical Physics</i> , 2012 , 136, 184107	3.9	43
72	Role of liquid polymorphism during the crystallization of silicon. <i>Journal of the American Chemical Society</i> , 2011 , 133, 2872-4	16.4	42
71	Vapor-liquid equilibria of copper using hybrid Monte Carlo Wang-Landau simulations. <i>Fluid Phase Equilibria</i> , 2010 , 287, 79-83	2.5	42
70	Polymorph selection during the crystallization of Yukawa systems. <i>Journal of Chemical Physics</i> , 2007 , 126, 054501	3.9	41
69	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. II. Adsorption of atomic and molecular fluids in a porous material. <i>Journal of Chemical Physics</i> , 2012 , 136, 184108	3.9	39
68	Molecular simulation of the crystallization of aluminum from the supercooled liquid. <i>Journal of Chemical Physics</i> , 2007 , 127, 144509	3.9	39
67	Molecular Simulation of the Nucleation and Growth of Gold Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 3607-3611	3.8	38
66	Crystallization mechanisms for supercooled liquid Xe at high pressure and temperature: Hybrid Monte Carlo molecular simulations. <i>Physical Review B</i> , 2008 , 77,	3.3	36
65	Viscosity of liquid iron under high pressure and high temperature: Equilibrium and nonequilibrium molecular dynamics simulation studies. <i>Physical Review B</i> , 2007 , 76,	3.3	31
64	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. III. Impact of combining rules on mixtures properties. <i>Journal of Chemical Physics</i> , 2014 , 140, 104109	3.9	30
63	Phase equilibria of polyaromatic hydrocarbons by hybrid Monte Carlo Wang-Landau simulations. <i>Molecular Physics</i> , 2010 , 108, 151-158	1.7	28
62	Rheology of liquid fcc metals: Equilibrium and transient-time correlation-function nonequilibrium molecular dynamics simulations. <i>Physical Review B</i> , 2008 , 78,	3.3	27

61	Molecular simulation of cross-nucleation between polymorphs. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 1465-9	3.4	27
60	Unusual Crystallization Behavior Close to the Glass Transition. <i>Physical Review Letters</i> , 2018 , 120, 115701	7.4	25
59	A new approach for the prediction of partition functions using machine learning techniques. <i>Applied Physics Letters</i> , 1989 , 55, 963-965	3.4	24
58	Unraveling the coupling between demixing and crystallization in mixtures. <i>Journal of the American Chemical Society</i> , 2014 , 136, 8145-8	16.4	23
57	Characterization and Comparison of the Performance of IRMOF-1, IRMOF-8, and IRMOF-10 for CO ₂ Adsorption in the Subcritical and Supercritical Regimes. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 22938-22946	3.8	23
56	Many-Body Effects on the Thermodynamics of Fluids, Mixtures, and Nanoconfined Fluids. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5401-14	6.4	22
55	Molecular simulation of transport in nanopores: application of the transient-time correlation function formalism. <i>Physical Review E</i> , 2008 , 77, 027701	2.4	22
54	Scaling Laws and Critical Properties for fcc and hcp Metals. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 5255-61	3.4	20
53	Wang-Landau configurational bias Monte Carlo simulations: vapour-liquid equilibria of alkenes. <i>Molecular Simulation</i> , 2012 , 38, 653-658	2	20
52	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. <i>Journal of Chemical Physics</i> , 2016 , 144, 124510	3.9	20
51	Polymorph selection during the crystallization of softly repulsive spheres: the inverse power law potential. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 12257-62	3.4	19
50	Prediction of critical properties for Naphthacene, Triphenylene and Chrysene by Wang-Landau simulations. <i>Fluid Phase Equilibria</i> , 2012 , 322-323, 92-96	2.5	18
49	Optimisation of multiple time-step hybrid Monte Carlo Wang-Landau simulations in the isobaric-isothermal ensemble for the determination of phase equilibria. <i>Molecular Simulation</i> , 2010 , 36, 544-551	2	18
48	Shear viscosity of liquid copper at experimentally accessible shear rates: application of the transient-time correlation function formalism. <i>Journal of Chemical Physics</i> , 2008 , 128, 084506	3.9	18
47	Ideality contours and thermodynamic regularities in supercritical molecular fluids. <i>Chemical Physics Letters</i> , 2016 , 658, 37-42	2.5	18
46	Adsorption and diffusion of the antiparkinsonian drug amantadine in carbon nanotubes. <i>Molecular Simulation</i> , 2014 , 40, 656-663	2	17
45	Numerical estimate for boiling points via Wang-Landau simulations. <i>Molecular Simulation</i> , 2012 , 38, 1265-1270	2	17
44	Free energy calculations along entropic pathways. I. Homogeneous vapor-liquid nucleation for atomic and molecular systems. <i>Journal of Chemical Physics</i> , 2016 , 145, 204112	3.9	16

43	A new approach for the prediction of partition functions using machine learning techniques. <i>Journal of Chemical Physics</i> , 2018 , 149, 044118	3.9	15
42	Can Ordered Precursors Promote the Nucleation of Solid Solutions?. <i>Physical Review Letters</i> , 2019 , 123, 195701	7.4	15
41	Adsorption of hydrogen in covalent organic frameworks using expanded Wang-Landau simulations. <i>Molecular Simulation</i> , 2014 , 40, 71-79	2	15
40	Crystal nucleation and growth in PdNi alloys: a molecular simulation study. <i>CrystEngComm</i> , 2011 , 13, 1132-1140	3.3	14
39	Thermodynamics of phase coexistence and metal-nonmetal transition in mercury: assessment of effective potentials via expanded Wang-Landau simulations. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 3175-82	3.4	13
38	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. <i>Journal of Chemical Physics</i> , 2016 , 145, 184504	3.9	13
37	Crystal nucleation along an entropic pathway: Teaching liquids how to transition. <i>Physical Review E</i> , 2018 , 98,	2.4	12
36	Free energy calculations along entropic pathways. III. Nucleation of capillary bridges and bubbles. <i>Journal of Chemical Physics</i> , 2017 , 146, 184104	3.9	11
35	Selectivity and Desorption Free Energies for Methane-Ethane Mixtures in Covalent Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 24692-24700	3.8	11
34	Polymorph selection during the crystallization of iron under the conditions of Earth's inner core. <i>Chemical Physics Letters</i> , 2011 , 511, 57-61	2.5	11
33	Ensemble Learning of Partition Functions for the Prediction of Thermodynamic Properties of Adsorption in Metal-Organic and Covalent Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 1907-1917	3.8	10
32	A new force field for H ₂ S and its binary and ternary mixtures with CO ₂ and CH ₄ . <i>Fluid Phase Equilibria</i> , 2015 , 402, 69-77	2.5	9
31	Free energy calculations along entropic pathways. II. Droplet nucleation in binary mixtures. <i>Journal of Chemical Physics</i> , 2016 , 145, 234505	3.9	9
30	Nucleation and growth of C ₆₀ nanoparticles from the supersaturated vapor and from the undercooled liquid: a molecular simulation study. <i>Journal of Chemical Physics</i> , 2009 , 131, 244515	3.9	8
29	Communication: Existence and control of liquid polymorphism in methanol under shear. <i>Journal of Chemical Physics</i> , 2018 , 149, 111101	3.9	8
28	Effect of the Composition on the Free Energy of Crystal Nucleation for CuPd Nanoalloys. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 27657-27664	3.8	7
27	Coarse-Grained Model and Boiling Point Prediction for Asphaltene Model Compounds via HMC-WL Simulations. <i>Energy & Fuels</i> , 2017 , 31, 10699-10705	4.1	7
26	Estimating the conductivity of a nanoconfined liquid subjected to an experimentally accessible external field. <i>Molecular Simulation</i> , 2008 , 34, 177-181	2	7

25	Prediction of the boiling and critical points of polycyclic aromatic hydrocarbons via Wang-Landau simulations and machine learning. <i>Fluid Phase Equilibria</i> , 2019 , 484, 225-231	2.5	7
24	Benchmark Free Energies and Entropies for Saturated and Compressed Water. <i>Journal of Chemical & Engineering Data</i> , 2017 , 62, 4032-4040	2.8	6
23	Impact of Friedel oscillations on vapor-liquid equilibria and supercritical properties in two and three dimensions. <i>Physical Review E</i> , 2016 , 94, 012612	2.4	5
22	Nucleation of Capillary Bridges and Bubbles in Nanoconfined CO. <i>Langmuir</i> , 2019 , 35, 15401-15409	4	5
21	Viscosity of a highly compressed methylated alkane via equilibrium and nonequilibrium molecular dynamics simulations. <i>Chemical Physics Letters</i> , 2019 , 719, 103-109	2.5	5
20	Competition between crystalline and icosahedral order during crystal growth in bimetallic systems. <i>Journal of Crystal Growth</i> , 2017 , 478, 22-27	1.6	4
19	Accurate determination of normal stress differences via transient-time correlation function Π non-equilibrium molecular dynamics (TTCF-EMD) simulations. <i>Molecular Simulation</i> , 2009 , 35, 405-408	2	4
18	Similarity law and critical properties in ionic systems.. <i>Chemical Physics Letters</i> , 2017 , 687, 9-13	2.5	4
17	Unraveling liquid polymorphism in silicon driven out-of-equilibrium. <i>Journal of Chemical Physics</i> , 2020 , 153, 054502	3.9	4
16	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. <i>Molecular Systems Design and Engineering</i> , 2021 , 6, 52-65	4.6	4
15	Stabilization of Nanobubbles under Hydrophobic Confinement. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 11707-11713	3.8	3
14	Universal scaling law for energy and pressure in a shearing fluid. <i>Physical Review E</i> , 2009 , 79, 052201	2.4	3
13	The central role of entropy in adiabatic ensembles and its application to phase transitions in the grand-isobaric adiabatic ensemble. <i>Journal of Chemical Physics</i> , 2020 , 153, 094114	3.9	3
12	Determination of mixture properties via a combined Expanded Wang-Landau simulations-Machine Learning approach. <i>Chemical Physics Letters</i> , 2019 , 715, 1-6	2.5	3
11	Classical and quantum many-body effects on the critical properties and thermodynamic regularities of silicon. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 045401	1.8	2
10	Modeling antigen-antibody nanoparticle bioconjugates and their polymorphs. <i>Journal of Chemical Physics</i> , 2018 , 148, 124507	3.9	2
9	Prediction of the phase equilibria for island-type asphaltenes via HMC-WL simulations. <i>Journal of Chemical Physics</i> , 2018 , 149, 072307	3.9	2
8	Free Energy of Nucleation and Interplay between Size and Composition in CuNi Systems. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 8558-8563	3.4	2

7	Ginzburg-Landau free energy for molecular fluids: Determination and coarse-graining. <i>Chemical Physics Letters</i> , 2017 , 669, 218-223	2.5	1
6	Calculating free energy profiles using entropy as a reaction coordinate: Application to water nucleation. <i>Chemical Physics Letters</i> , 2018 , 695, 194-199	2.5	1
5	Non-monotonic variations of the nucleation free energy in a glass-forming ultra-soft particles fluid. <i>Soft Matter</i> , 2018 , 14, 5977-5985	3.6	1
4	Entropy production in model colloidal suspensions under shear via the fluctuation theorem. <i>Journal of Chemical Physics</i> , 2020 , 153, 224113	3.9	0
3	Entropy in Molecular Fluids: Interplay between Interaction Complexity and Criticality. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 11463-11471	3.4	0
2	Entropy scaling close to criticality: From simple to metallic systems. <i>Physical Review E</i> , 2021 , 103, 052102.	2.4	
1	Entropy determination for mixtures in the adiabatic grand-isobaric ensemble.. <i>Journal of Chemical Physics</i> , 2022 , 156, 084113	3.9	