

Caroline Desgranges

List of Publications by Year in descending order

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80
papers

1,643
citations

257450

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37
g-index

80
all docs

80
docs citations

80
times ranked

985
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Mechanism for the Cross-Nucleation between Polymorphs. Journal of the American Chemical Society, 2006, 128, 10368-10369.	13.7	115
2	Controlling Polymorphism during the Crystallization of an Atomic Fluid. Physical Review Letters, 2007, 98, 235502.	7.8	111
3	Insights into the Molecular Mechanism Underlying Polymorph Selection. Journal of the American Chemical Society, 2006, 128, 15104-15105.	13.7	86
4	Molecular Insight into the Pathway to Crystallization of Aluminum. Journal of the American Chemical Society, 2007, 129, 7012-7013.	13.7	64
5	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.	3.0	52
6	Polymorph selection during the crystallization of Yukawa systems. Journal of Chemical Physics, 2007, 126, 054501.	3.0	46
7	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.	3.0	46
8	Vapor-liquid equilibria of copper using hybrid Monte Carlo Wang-Landau simulations. Fluid Phase Equilibria, 2010, 287, 79-83.	2.5	43
9	Role of Liquid Polymorphism during the Crystallization of Silicon. Journal of the American Chemical Society, 2011, 133, 2872-2874.	13.7	43
10	Molecular simulation of the crystallization of aluminum from the supercooled liquid. Journal of Chemical Physics, 2007, 127, 144509.	3.0	41
11	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.	3.0	41
12	Crystallization mechanisms for supercooled liquid Xe at high pressure and temperature: Hybrid Monte Carlo molecular simulations. Physical Review B, 2008, 77, .	3.2	40
13	Molecular Simulation of the Nucleation and Growth of Gold Nanoparticles. Journal of Physical Chemistry C, 2009, 113, 3607-3611.	3.1	40
14	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.	3.0	35
15	Viscosity of liquid iron under high pressure and high temperature: Equilibrium and nonequilibrium molecular dynamics simulation studies. Physical Review B, 2007, 76, .	3.2	32
16	Unusual Crystallization Behavior Close to the Glass Transition. Physical Review Letters, 2018, 120, 115701.	7.8	32
17	Rheology of liquid fcc metals: Equilibrium and transient-time correlation-function nonequilibrium molecular dynamics simulations. Physical Review B, 2008, 78, .	3.2	30
18	Molecular Simulation of Cross-Nucleation between Polymorphs. Journal of Physical Chemistry B, 2007, 111, 1465-1469.	2.6	28

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19	Phase equilibria of polyaromatic hydrocarbons by hybrid Monte Carlo Wang-Landau simulations. <i>Molecular Physics</i> , 2010, 108, 151-158.	1.7	28
20	Scaling Laws and Critical Properties for fcc and hcp Metals. <i>Journal of Physical Chemistry B</i> , 2016, 120, 5255-5261.	2.6	28
21	Unraveling the Coupling between Demixing and Crystallization in Mixtures. <i>Journal of the American Chemical Society</i> , 2014, 136, 8145-8148.	13.7	26
22	Can Ordered Precursors Promote the Nucleation of Solid Solutions?. <i>Physical Review Letters</i> , 2019, 123, 195701.	7.8	26
23	Molecular simulation of transport in nanopores: Application of the transient-time correlation function formalism. <i>Physical Review E</i> , 2008, 77, 027701.	2.1	25
24	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.	3.1	25
25	Structural characterization of an Sb delta-doping layer in silicon. <i>Applied Physics Letters</i> , 1989, 55, 963-965.	3.3	24
26	Many-Body Effects on the Thermodynamics of Fluids, Mixtures, and Nanoconfined Fluids. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5401-5414.	5.3	24
27	Ideality contours and thermodynamic regularities in supercritical molecular fluids. <i>Chemical Physics Letters</i> , 2016, 658, 37-42.	2.6	24
28	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.	3.0	21
29	Wang-Landau configurational bias Monte Carlo simulations: vapour-liquid equilibria of alkenes. <i>Molecular Simulation</i> , 2012, 38, 653-658.	2.0	20
30	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.	3.0	20
31	Polymorph Selection during the Crystallization of Softly Repulsive Spheres: The Inverse Power Law Potential. <i>Journal of Physical Chemistry B</i> , 2007, 111, 12257-12262.	2.6	19
32	Numerical estimate for boiling points via Wang-Landau simulations. <i>Molecular Simulation</i> , 2012, 38, 1265-1270.	2.0	19
33	Adsorption and diffusion of the antiparkinsonian drug amantadine in carbon nanotubes. <i>Molecular Simulation</i> , 2014, 40, 656-663.	2.0	19
34	A new approach for the prediction of partition functions using machine learning techniques. <i>Journal of Chemical Physics</i> , 2018, 149, 044118.	3.0	19
35	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.	2.0	18
36	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

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37	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.	3.0	17
38	Adsorption of hydrogen in covalent organic frameworks using expanded Wang-Landau simulations. <i>Molecular Simulation</i> , 2014, 40, 71-79.	2.0	15
39	Crystal nucleation and growth in Pd-Ni alloys: a molecular simulation study. <i>CrystEngComm</i> , 2011, 13, 1132-1140.	2.6	14
40	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, 3175-3182.	2.6	14
41	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.	3.0	14
42	Polymorph selection during the crystallization of iron under the conditions of Earth's inner core. <i>Chemical Physics Letters</i> , 2011, 511, 57-61.	2.6	13
43	Free energy calculations along entropic pathways. III. Nucleation of capillary bridges and bubbles. <i>Journal of Chemical Physics</i> , 2017, 146, 184104.	3.0	13
44	Crystal nucleation along an entropic pathway: Teaching liquids how to transition. <i>Physical Review E</i> , 2018, 98, .	2.1	13
45	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.	3.1	13
46	Coarse-Grained Model and Boiling Point Prediction for Asphaltene Model Compounds via HMC-WL Simulations. <i>Energy & Fuels</i> , 2017, 31, 10699-10705.	5.1	12
47	Selectivity and Desorption Free Energies for Methane-Ethane Mixtures in Covalent Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24692-24700.	3.1	11
48	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	10
49	Free energy calculations along entropic pathways. II. Droplet nucleation in binary mixtures. <i>Journal of Chemical Physics</i> , 2016, 145, 234505.	3.0	10
50	Communication: Existence and control of liquid polymorphism in methanol under shear. <i>Journal of Chemical Physics</i> , 2018, 149, 111101.	3.0	9
51	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	9
52	Estimating the conductivity of a nanoconfined liquid subjected to an experimentally accessible external field. <i>Molecular Simulation</i> , 2008, 34, 177-181.	2.0	8
53	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.	3.0	8
54	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.	3.1	8

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55	Nucleation of Capillary Bridges and Bubbles in Nanoconfined CO ₂ . <i>Langmuir</i> , 2019, 35, 15401-15409.	3.5	8
56	Viscosity of a highly compressed methylated alkane via equilibrium and nonequilibrium molecular dynamics simulations. <i>Chemical Physics Letters</i> , 2019, 719, 103-109.	2.6	8
57	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.	3.4	8
58	Similarity law and critical properties in ionic systems.. <i>Chemical Physics Letters</i> , 2017, 687, 9-13.	2.6	8
59	Impact of Friedel oscillations on vapor-liquid equilibria and supercritical properties in two and three dimensions. <i>Physical Review E</i> , 2016, 94, 012612.	2.1	7
60	Benchmark Free Energies and Entropies for Saturated and Compressed Water. <i>Journal of Chemical & Engineering Data</i> , 2017, 62, 4032-4040.	1.9	6
61	Stabilization of Nanobubbles under Hydrophobic Confinement. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11707-11713.	3.1	6
62	Designing, synthesizing, and modeling active fluids. <i>Physics of Fluids</i> , 2022, 34, .	4.0	6
63	Universal scaling law for energy and pressure in a shearing fluid. <i>Physical Review E</i> , 2009, 79, 052201.	2.1	5
64	Accurate determination of normal stress differences via transient-time correlation function $\hat{\alpha}$ non-equilibrium molecular dynamics (TTCF-NEMD) simulations. <i>Molecular Simulation</i> , 2009, 35, 405-408.	2.0	5
65	Determination of mixture properties via a combined Expanded Wang-Landau simulations-Machine Learning approach. <i>Chemical Physics Letters</i> , 2019, 715, 1-6.	2.6	5
66	Unraveling liquid polymorphism in silicon driven out-of-equilibrium. <i>Journal of Chemical Physics</i> , 2020, 153, 054502.	3.0	5
67	Free Energy of Nucleation and Interplay between Size and Composition in CuNi Systems. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8558-8563.	2.6	4
68	Competition between crystalline and icosahedral order during crystal growth in bimetallic systems. <i>Journal of Crystal Growth</i> , 2017, 478, 22-27.	1.5	4
69	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.	3.0	4
70	Prediction of the phase equilibria for island-type asphaltenes via HMC-WL simulations. <i>Journal of Chemical Physics</i> , 2018, 149, 072307.	3.0	3
71	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
72	Modeling antigen-antibody nanoparticle bioconjugates and their polymorphs. <i>Journal of Chemical Physics</i> , 2018, 148, 124507.	3.0	2

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73	Entropy in Molecular Fluids: Interplay between Interaction Complexity and Criticality. Journal of Physical Chemistry B, 2020, 124, 11463-11471.	2.6	2
74	Entropy production in model colloidal suspensions under shear via the fluctuation theorem. Journal of Chemical Physics, 2020, 153, 224113.	3.0	2
75	Ginzburg-Landau free energy for molecular fluids: Determination and coarse-graining. Chemical Physics Letters, 2017, 669, 218-223.	2.6	1
76	Calculating free energy profiles using entropy as a reaction coordinate: Application to water nucleation. Chemical Physics Letters, 2018, 695, 194-199.	2.6	1
77	Non-monotonic variations of the nucleation free energy in a glass-forming ultra-soft particles fluid. Soft Matter, 2018, 14, 5977-5985.	2.7	1
78	Entropy determination for mixtures in the adiabatic grand-isobaric ensemble. Journal of Chemical Physics, 2022, 156, 084113.	3.0	1
79	Entropy scaling close to criticality: From simple to metallic systems. Physical Review E, 2021, 103, 052102.	2.1	0
80	Machine-Learned Free Energy Surfaces for Capillary Condensation and Evaporation in Mesopores. Entropy, 2022, 24, 97.	2.2	0