Jerome Delhommelle

List of Publications by Year
in descending order

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132 papers	3,334 citations	147801 31 h-index	182427 51 g-index
136 all docs	136 docs citations	136 times ranked	2022 citing authors

#	Article	IF	Citations
1	Machine-Learned Free Energy Surfaces for Capillary Condensation and Evaporation in Mesopores. Entropy, 2022, 24, 97.	2.2	0
2	Machine Learning and Deep Learning Algorithms for Skin Cancer Classification from Dermoscopic Images. Bioengineering, 2022, 9, 97.	3.5	42
3	Entropy determination for mixtures in the adiabatic grand-isobaric ensemble. Journal of Chemical Physics, 2022, 156, 084113.	3.0	1
4	Designing, synthesizing, and modeling active fluids. Physics of Fluids, 2022, 34, .	4.0	6
5	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.	3.4	8
6	Free Energy Simulations III. Molecular Simulation, 2021, 47, 378-378.	2.0	0
7	Entropy scaling close to criticality: From simple to metallic systems. Physical Review E, 2021, 103, 052102.	2.1	0
8	Recent developments in molecular simulation. Molecular Simulation, 2021, 47, 785-785.	2.0	0
9	Folding Free-Energy Landscape of Î±-Synuclein (35â€“97) Via Replica Exchange Molecular Dynamics. Journal of Chemical Information and Modeling, 2021, 61, 432-443.	5.4	10
10	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.	3.1	13
11	Entropy in Molecular Fluids: Interplay between Interaction Complexity and Criticality. Journal of Physical Chemistry B, 2020, 124, 11463-11471.	2.6	2
12	Unraveling liquid polymorphism in silicon driven out-of-equilibrium. Journal of Chemical Physics, 2020, 153, 054502.	3.0	5
13	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.	3.0	4
14	Entropy production in model colloidal suspensions under shear via the fluctuation theorem. Journal of Chemical Physics, 2020, 153, 224113.	3.0	2
15	Nucleation of Capillary Bridges and Bubbles in Nanoconfined CO2. Langmuir, 2019, 35, 15401-15409.	3.5	8
16	Can Ordered Precursors Promote the Nucleation of Solid Solutions?. Physical Review Letters, 2019, 123, 195701.	7.8	26
17	Recent advances in molecular simulation. Molecular Simulation, 2019, 45, 1067-1068.	2.0	2
18	Stabilization of Nanobubbles under Hydrophobic Confinement. Journal of Physical Chemistry C, 2019, 123, 11707-11713.	3.1	6

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19	Viscosity of a highly compressed methylated alkane via equilibrium and nonequilibrium molecular dynamics simulations. Chemical Physics Letters, 2019, 719, 103-109.	2.6	8
20	Determination of mixture properties via a combined Expanded Wang-Landau simulations-Machine Learning approach. Chemical Physics Letters, 2019, 715, 1-6.	2.6	5
21	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	9
22	Modeling antigen-antibody nanoparticle bioconjugates and their polymorphs. Journal of Chemical Physics, 2018, 148, 124507.	3.0	2
23	Calculating free energy profiles using entropy as a reaction coordinate: Application to water nucleation. Chemical Physics Letters, 2018, 695, 194-199.	2.6	1
24	Unusual Crystallization Behavior Close to the Glass Transition. Physical Review Letters, 2018, 120, 115701.	7.8	32
25	Crystal nucleation along an entropic pathway: Teaching liquids how to transition. Physical Review E, 2018, 98, .	2.1	13
26	Communication: Existence and control of liquid polymorphism in methanol under shear. Journal of Chemical Physics, 2018, 149, 111101.	3.0	9
27	A new approach for the prediction of partition functions using machine learning techniques. Journal of Chemical Physics, 2018, 149, 044118.	3.0	19
28	Prediction of the phase equilibria for island-type asphaltenes via HMC-WL simulations. Journal of Chemical Physics, 2018, 149, 072307.	3.0	3
29	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
30	Ginzburg-Landau free energy for molecular fluids: Determination and coarse-graining. Chemical Physics Letters, 2017, 669, 218-223.	2.6	1
31	Surface Chemistry. Molecular Simulation, 2017, 43, 326-326.	2.0	1
32	Free energy calculations along entropic pathways. III. Nucleation of capillary bridges and bubbles. Journal of Chemical Physics, 2017, 146, 184104.	3.0	13
33	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
34	Benchmark Free Energies and Entropies for Saturated and Compressed Water. Journal of Chemical & Engineering Data, 2017, 62, 4032-4040.	1.9	6
35	Selectivity and Desorption Free Energies for Methaneâ€“Ethane Mixtures in Covalent Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 24692-24700.	3.1	11
36	Free Energy of Nucleation and Interplay between Size and Composition in CuNi Systems. Journal of Physical Chemistry B, 2017, 121, 8558-8563.	2.6	4

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37	Competition between crystalline and icosahedral order during crystal growth in bimetallic systems. Journal of Crystal Growth, 2017, 478, 22-27.	1.5	4
38	Coarse-Grained Model and Boiling Point Prediction for Asphaltene Model Compounds via HMC-WL Simulations. Energy & Fuels, 2017, 31, 10699-10705.	5.1	12
39	Energy applications. Molecular Simulation, 2017, 43, 729-729.	2.0	1
40	Similarity law and critical properties in ionic systems.. Chemical Physics Letters, 2017, 687, 9-13.	2.6	8
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. Journal of Chemical Physics, 2016, 145, 184504.	3.0	14
42	Free energy calculations along entropic pathways. I. Homogeneous vapor-liquid nucleation for atomic and molecular systems. Journal of Chemical Physics, 2016, 145, 204112.	3.0	17
43	Nonequilibrium Systems. Molecular Simulation, 2016, 42, 1299-1299.	2.0	1
44	Free energy calculations along entropic pathways. II. Droplet nucleation in binary mixtures. Journal of Chemical Physics, 2016, 145, 234505.	3.0	10
45	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.	3.0	20
46	Ideality contours and thermodynamic regularities in supercritical molecular fluids. Chemical Physics Letters, 2016, 658, 37-42.	2.6	24
47	Effect of the Composition on the Free Energy of Crystal Nucleation for CuPd Nanoalloys. Journal of Physical Chemistry C, 2016, 120, 27657-27664.	3.1	8
48	Impact of Friedel oscillations on vapor-liquid equilibria and supercritical properties in two and three dimensions. Physical Review E, 2016, 94, 012612.	2.1	7
49	Scaling Laws and Critical Properties for fcc and hcp Metals. Journal of Physical Chemistry B, 2016, 120, 5255-5261.	2.6	28
50	Many-Body Effects on the Thermodynamics of Fluids, Mixtures, and Nanoconfined Fluids. Journal of Chemical Theory and Computation, 2015, 11, 5401-5414.	5.3	24
51	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	10
52	Recent advances in the molecular simulation of chemical reactions. Molecular Simulation, 2015, 41, 1-2.	2.0	11
53	Recent advances in molecular biology. Molecular Simulation, 2014, 40, 731-731.	2.0	0
54	A festschrift for Professor A. H. Fuchs. Molecular Simulation, 2014, 40, 1-2.	2.0	10

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55	Adsorption and diffusion of the antiparkinsonian drug amantadine in carbon nanotubes. Molecular Simulation, 2014, 40, 656-663.	2.0	19
56	Adsorption of hydrogen in covalent organic frameworks using expanded Wangâ€“Landau simulations. Molecular Simulation, 2014, 40, 71-79.	2.0	15
57	Recent advances in the molecular simulation of adsorption. Molecular Simulation, 2014, 40, 515-515.	2.0	0
58	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
59	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.	2.6	14
60	Unraveling the Coupling between Demixing and Crystallization in Mixtures. Journal of the American Chemical Society, 2014, 136, 8145-8148.	13.7	26
61	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.	3.1	25
62	Wangâ€“Landau configurational bias Monte Carlo simulations: vapourâ€“liquid equilibria of alkenes. Molecular Simulation, 2012, 38, 653-658.	2.0	20
63	Numerical estimate for boiling points via Wangâ€“Landau simulations. Molecular Simulation, 2012, 38, 1265-1270.	2.0	19
64	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
65	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
66	Prediction of critical properties for Naphthacene, Triphenylene and Chrysene by Wangâ€“Landau simulations. Fluid Phase Equilibria, 2012, 322-323, 92-96.	2.5	18
67	Crystal nucleation and growth in Pdâ€“Ni alloys: a molecular simulation study. CrystEngComm, 2011, 13, 1132-1140.	2.6	14
68	Role of Liquid Polymorphism during the Crystallization of Silicon. Journal of the American Chemical Society, 2011, 133, 2872-2874.	13.7	43
69	Crystal nucleation and growth from supercooled melts. Molecular Simulation, 2011, 37, 613-620.	2.0	15
70	Polymorph selection during the crystallization of iron under the conditions of Earthâ€™s inner core. Chemical Physics Letters, 2011, 511, 57-61.	2.6	13
71	Vaporâ€“liquid equilibria of copper using hybrid Monte Carlo Wangâ€”Landau simulations. Fluid Phase Equilibria, 2010, 287, 79-83.	2.5	43
72	Phase equilibria of polyaromatic hydrocarbons by hybrid Monte Carlo Wangâ€“Landau simulations. Molecular Physics, 2010, 108, 151-158.	1.7	28

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73	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.	2.0	18
74	Universal scaling law for energy and pressure in a shearing fluid. Physical Review E, 2009, 79, 052201.	2.1	5
75	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.	2.0	5
76	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.	3.0	8
77	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.	3.0	52
78	Molecular Simulation of the Nucleation and Growth of Gold Nanoparticles. Journal of Physical Chemistry C, 2009, 113, 3607-3611.	3.1	40
79	Estimating the conductivity of a nanoconfined liquid subjected to an experimentally accessible external field. Molecular Simulation, 2008, 34, 177-181.	2.0	8
80	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.	3.0	21
81	Molecular simulation of transport in nanopores: Application of the transient-time correlation function formalism. Physical Review E, 2008, 77, 027701.	2.1	25
82	Rheology of liquid fcc metals: Equilibrium and transient-time correlation-function nonequilibrium molecular dynamics simulations. Physical Review B, 2008, 78, .	3.2	30
83	Crystallization mechanisms for supercooled liquid Xe at high pressure and temperature: Hybrid Monte Carlo molecular simulations. Physical Review B, 2008, 77, .	3.2	40
84	Hit and miss of classical nucleation theory as revealed by a molecular simulation study of crystal nucleation in supercooled sulfur hexafluoride. Journal of Chemical Physics, 2007, 127, 044504.	3.0	21
85	Controlling Polymorphism during the Crystallization of an Atomic Fluid. Physical Review Letters, 2007, 98, 235502.	7.8	111
86	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
87	Structure and thermodynamics of the expanded liquid mercury by Monte Carlo simulation: a first attempt. Journal of Non-Crystalline Solids, 2007, 353, 3454-3458.	3.1	5
88	Polymorph selection during the crystallization of Yukawa systems. Journal of Chemical Physics, 2007, 126, 054501.	3.0	46
89	Molecular Simulation of Cross-Nucleation between Polymorphs. Journal of Physical Chemistry B, 2007, 111, 1465-1469.	2.6	28
90	Guest editorial: Recent developments in molecular simulation. Molecular Simulation, 2007, 33, 711-712.	2.0	0

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91	Polymorph Selection during the Crystallization of Softly Repulsive Spheres:â€‰ The Inverse Power Law Potential. Journal of Physical Chemistry B, 2007, 111, 12257-12262.	2.6	19
92	Molecular Insight into the Pathway to Crystallization of Aluminum. Journal of the American Chemical Society, 2007, 129, 7012-7013.	13.7	64
93	Molecular simulation of the crystallization of aluminum from the supercooled liquid. Journal of Chemical Physics, 2007, 127, 144509.	3.0	41
94	Molecular Mechanism for the Cross-Nucleation between Polymorphs. Journal of the American Chemical Society, 2006, 128, 10368-10369.	13.7	115
95	Insights into the Molecular Mechanism Underlying Polymorph Selection. Journal of the American Chemical Society, 2006, 128, 15104-15105.	13.7	86
96	Guest Editorial: Frontiers of Molecular Simulation. Molecular Simulation, 2006, 32, 173-174.	2.0	1
97	Conductivity of molten sodium chloride in an arbitrarily weak dc electric field. Journal of Chemical Physics, 2005, 123, 114505.	3.0	25
98	Atomistic simulation of the homogeneous nucleation and of the growth of N2 crystallites. Journal of Chemical Physics, 2005, 122, 104510.	3.0	36
99	Should â€œlane formationâ€•occur systematically in driven liquids and colloids?. Physical Review E, 2005, 71, 016705.	2.1	50
100	Simulation of friction in nanoconfined fluids for an arbitrarily low shear rate. Physical Review B, 2005, 72, .	3.2	32
101	Molecular simulation of the homogeneous crystal nucleation of carbon dioxide. Journal of Chemical Physics, 2005, 122, 184518.	3.0	27
102	Shear thickening in a model colloidal suspension. Journal of Chemical Physics, 2005, 123, 074707.	3.0	22
103	Hydrogen bonding in ethanol under shear. Journal of Chemical Physics, 2005, 122, 234509.	3.0	22
104	Non-Newtonian behavior in simple fluids. Journal of Chemical Physics, 2004, 120, 6117-6123.	3.0	25
105	Simulations of shear-induced melting in two dimensions. Physical Review B, 2004, 69, .	3.2	32
106	Onset of shear thickening in a simple fluid. European Physical Journal E, 2004, 15, 65-69.	1.6	13
107	Nonequilibrium Molecular Dynamics Simulations of Molten Sodium Chloride. International Journal of Thermophysics, 2004, 25, 1375-1393.	2.1	7
108	Reorganization and Growth of Metastable Î±-N2Critical Nuclei into Stable Î²-N2Crystals. Journal of the American Chemical Society, 2004, 126, 12286-12287.	13.7	32

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109	A molecular dynamics study of homogeneous crystal nucleation in liquid nitrogen. Chemical Physics Letters, 2003, 375, 612-618.	2.6	30
110	Influence of temperature, pressure and internal degrees of freedom on hydrogen bonding and diffusion in liquid ethanol. Chemical Physics, 2003, 286, 303-314.	1.9	17
111	Reexamination of string phase and shear thickening in simple fluids. Physical Review E, 2003, 68, 031201.	2.1	50
112	Shear viscosity of molten sodium chloride. Journal of Chemical Physics, 2003, 118, 2783.	3.0	28
113	Conductivity of molten sodium chloride in an alternating electric field. Journal of Chemical Physics, 2003, 119, 8511-8518.	3.0	13
114	On the effects of assuming flow profiles in nonequilibrium simulations. Journal of Chemical Physics, 2003, 119, 11005-11010.	3.0	31
115	Conductivity of molten sodium chloride and its supercritical vapor in strong dc electric fields. Journal of Chemical Physics, 2003, 118, 7477.	3.0	34
116	Rotational viscosity of uniaxial molecules. Molecular Physics, 2002, 100, 3479-3482.	1.7	7
117	Correspondence between configurational temperature and molecular kinetic temperature thermostats. Journal of Chemical Physics, 2002, 117, 6016-6021.	3.0	29
118	Configurational thermostats for molecular systems. Molecular Physics, 2002, 100, 2387-2395.	1.7	40
119	Poiseuille flow of a micropolar fluid. Molecular Physics, 2002, 100, 2857-2865.	1.7	30
120	Inadequacy of the Lorentz-Berthelot combining rules for accurate predictions of equilibrium properties by molecular simulation. Molecular Physics, 2001, 99, 619-625.	1.7	332
121	Configurational temperature profile in confined fluids. II. Molecular fluids. Journal of Chemical Physics, 2001, 114, 6236-6241.	3.0	29
122	Configurational temperature profile in confined fluids. I. Atomic fluid. Journal of Chemical Physics, 2001, 114, 6229-6235.	3.0	41
123	Configurational temperature thermostat for fluids undergoing shear flow: application to liquid chlorine. Molecular Physics, 2001, 99, 1825-1829.	1.7	29
124	Comparison of thermostatting mechanisms in NVT and NPT simulations of decane under shear. Journal of Chemical Physics, 2001, 115, 43-49.	3.0	54
125	Optimization of the anisotropic united atoms intermolecular potential forn-alkanes. Journal of Chemical Physics, 2000, 112, 5499-5510.	3.0	270
126	On the role of the definition of potential models in Gibbs ensemble phase equilibria simulations of the H₂S-pentane mixture. Molecular Physics, 2000, 98, 1895-1905.	1.7	25

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127	Derivation of an Optimized Potential Model for Phase Equilibria (OPPE) for Sulfides and Thiols. Journal of Physical Chemistry B, 2000, 104, 4745-4753.	2.6	64
128	Molecular Simulation of Vapour-Liquid Coexistence Curves for Hydrogen Sulfide-Alkane and Carbon Dioxide-Alkane Mixtures. Molecular Simulation, 1999, 22, 351-368.	2.0	28
129	Vapour-liquid coexistence curves of the united-atom and anisotropic united-atom force fields for alkane mixtures. Molecular Physics, 1999, 96, 1517-1524.	1.7	34
130	Monte Carlo simulations of squalane in the Gibbs ensemble. Fluid Phase Equilibria, 1999, 155, 167-176.	2.5	16
131	A new method for deriving atomic charges and dipoles forn, -alkanes: investigation of transferability and geometry dependence. Molecular Physics, 1999, 97, 1117-1128.	1.7	13
132	Structural characterization of an Sb deltaâ€doping layer in silicon. Applied Physics Letters, 1989, 55, 963-965.	3.3	24