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	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
2	Optimization of the anisotropic united atoms intermolecular potential forn-alkanes. Journal of Chemical Physics, 2000, 112, 5499-5510.	3.0	270
3	Molecular Mechanism for the Cross-Nucleation between Polymorphs. Journal of the American Chemical Society, 2006, 128, 10368-10369.	13.7	115
4	Controlling Polymorphism during the Crystallization of an Atomic Fluid. Physical Review Letters, 2007, 98, 235502.	7.8	111
5	Insights into the Molecular Mechanism Underlying Polymorph Selection. Journal of the American Chemical Society, 2006, 128, 15104-15105.	13.7	86
6	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
7	Molecular Insight into the Pathway to Crystallization of Aluminum. Journal of the American Chemical Society, 2007, 129, 7012-7013.	13.7	64
8	Comparison of thermostatting mechanisms in NVT and NPT simulations of decane under shear. Journal of Chemical Physics, 2001, 115, 43-49.	3.0	54
9	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
10	Reexamination of string phase and shear thickening in simple fluids. Physical Review E, 2003, 68, 031201.	2.1	50
11	Should â€œlane formationâ€•occur systematically in driven liquids and colloids?. Physical Review E, 2005, 71, 016705.	2.1	50
12	Polymorph selection during the crystallization of Yukawa systems. Journal of Chemical Physics, 2007, 126, 054501.	3.0	46
13	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
14	Vaporâ€“liquid equilibria of copper using hybrid Monte Carlo Wangâ€”Landau simulations. Fluid Phase Equilibria, 2010, 287, 79-83.	2.5	43
15	Role of Liquid Polymorphism during the Crystallization of Silicon. Journal of the American Chemical Society, 2011, 133, 2872-2874.	13.7	43
16	Machine Learning and Deep Learning Algorithms for Skin Cancer Classification from Dermoscopic Images. Bioengineering, 2022, 9, 97.	3.5	42
17	Configurational temperature profile in confined fluids. I. Atomic fluid. Journal of Chemical Physics, 2001, 114, 6229-6235.	3.0	41
18	Molecular simulation of the crystallization of aluminum from the supercooled liquid. Journal of Chemical Physics, 2007, 127, 144509.	3.0	41

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19	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
20	Configurational thermostats for molecular systems. Molecular Physics, 2002, 100, 2387-2395.	1.7	40
21	Crystallization mechanisms for supercooled liquid Xe at high pressure and temperature: Hybrid Monte Carlo molecular simulations. Physical Review B, 2008, 77, .	3.2	40
22	Molecular Simulation of the Nucleation and Growth of Gold Nanoparticles. Journal of Physical Chemistry C, 2009, 113, 3607-3611.	3.1	40
23	Atomistic simulation of the homogeneous nucleation and of the growth of N2 crystallites. Journal of Chemical Physics, 2005, 122, 104510.	3.0	36
24	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
25	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
26	Conductivity of molten sodium chloride and its supercritical vapor in strong dc electric fields. Journal of Chemical Physics, 2003, 118, 7477.	3.0	34
27	Simulations of shear-induced melting in two dimensions. Physical Review B, 2004, 69, .	3.2	32
28	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
29	Simulation of friction in nanoconfined fluids for an arbitrarily low shear rate. Physical Review B, 2005, 72, .	3.2	32
30	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
31	Unusual Crystallization Behavior Close to the Glass Transition. Physical Review Letters, 2018, 120, 115701.	7.8	32
32	On the effects of assuming flow profiles in nonequilibrium simulations. Journal of Chemical Physics, 2003, 119, 11005-11010.	3.0	31
33	Poiseuille flow of a micropolar fluid. Molecular Physics, 2002, 100, 2857-2865.	1.7	30
34	A molecular dynamics study of homogeneous crystal nucleation in liquid nitrogen. Chemical Physics Letters, 2003, 375, 612-618.	2.6	30
35	Rheology of liquid fcc metals: Equilibrium and transient-time correlation-function nonequilibrium molecular dynamics simulations. Physical Review B, 2008, 78, .	3.2	30
36	Configurational temperature profile in confined fluids. II. Molecular fluids. Journal of Chemical Physics, 2001, 114, 6236-6241.	3.0	29

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37	Configurational temperature thermostat for fluids undergoing shear flow: application to liquid chlorine. Molecular Physics, 2001, 99, 1825-1829.	1.7	29
38	Correspondence between configurational temperature and molecular kinetic temperature thermostats. Journal of Chemical Physics, 2002, 117, 6016-6021.	3.0	29
39	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
40	Shear viscosity of molten sodium chloride. Journal of Chemical Physics, 2003, 118, 2783.	3.0	28
41	Molecular Simulation of Cross-Nucleation between Polymorphs. Journal of Physical Chemistry B, 2007, 111, 1465-1469.	2.6	28
42	Phase equilibria of polyaromatic hydrocarbons by hybrid Monte Carlo Wangâ€“Landau simulations. Molecular Physics, 2010, 108, 151-158.	1.7	28
43	Scaling Laws and Critical Properties for fcc and hcp Metals. Journal of Physical Chemistry B, 2016, 120, 5255-5261.	2.6	28
44	Molecular simulation of the homogeneous crystal nucleation of carbon dioxide. Journal of Chemical Physics, 2005, 122, 184518.	3.0	27
45	Unraveling the Coupling between Demixing and Crystallization in Mixtures. Journal of the American Chemical Society, 2014, 136, 8145-8148.	13.7	26
46	Can Ordered Precursors Promote the Nucleation of Solid Solutions?. Physical Review Letters, 2019, 123, 195701.	7.8	26
47	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
48	Non-Newtonian behavior in simple fluids. Journal of Chemical Physics, 2004, 120, 6117-6123.	3.0	25
49	Conductivity of molten sodium chloride in an arbitrarily weak dc electric field. Journal of Chemical Physics, 2005, 123, 114505.	3.0	25
50	Molecular simulation of transport in nanopores: Application of the transient-time correlation function formalism. Physical Review E, 2008, 77, 027701.	2.1	25
51	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
52	Structural characterization of an Sb deltaâ€doping layer in silicon. Applied Physics Letters, 1989, 55, 963-965.	3.3	24
53	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
54	Ideality contours and thermodynamic regularities in supercritical molecular fluids. Chemical Physics Letters, 2016, 658, 37-42.	2.6	24

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55	Shear thickening in a model colloidal suspension. Journal of Chemical Physics, 2005, 123, 074707.	3.0	22
56	Hydrogen bonding in ethanol under shear. Journal of Chemical Physics, 2005, 122, 234509.	3.0	22
57	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
58	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
59	Wangâ€“Landau configurational bias Monte Carlo simulations: vapourâ€“liquid equilibria of alkenes. Molecular Simulation, 2012, 38, 653-658.	2.0	20
60	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
61	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
62	Numerical estimate for boiling points via Wangâ€“Landau simulations. Molecular Simulation, 2012, 38, 1265-1270.	2.0	19
63	Adsorption and diffusion of the antiparkinsonian drug amantadine in carbon nanotubes. Molecular Simulation, 2014, 40, 656-663.	2.0	19
64	A new approach for the prediction of partition functions using machine learning techniques. Journal of Chemical Physics, 2018, 149, 044118.	3.0	19
65	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
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	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
68	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
69	Monte Carlo simulations of squalane in the Gibbs ensemble. Fluid Phase Equilibria, 1999, 155, 167-176.	2.5	16
70	Crystal nucleation and growth from supercooled melts. Molecular Simulation, 2011, 37, 613-620.	2.0	15
71	Adsorption of hydrogen in covalent organic frameworks using expanded Wangâ€“Landau simulations. Molecular Simulation, 2014, 40, 71-79.	2.0	15
72	Crystal nucleation and growth in Pdâ€“Ni alloys: a molecular simulation study. CrystEngComm, 2011, 13, 1132-1140.	2.6	14

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73	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
74	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
75	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
76	Conductivity of molten sodium chloride in an alternating electric field. Journal of Chemical Physics, 2003, 119, 8511-8518.	3.0	13
77	Onset of shear thickening in a simple fluid. European Physical Journal E, 2004, 15, 65-69.	1.6	13
78	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
79	Free energy calculations along entropic pathways. III. Nucleation of capillary bridges and bubbles. Journal of Chemical Physics, 2017, 146, 184104.	3.0	13
80	Crystal nucleation along an entropic pathway: Teaching liquids how to transition. Physical Review E, 2018, 98, .	2.1	13
81	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
82	Coarse-Grained Model and Boiling Point Prediction for Asphaltene Model Compounds via HMC-WL Simulations. Energy & Fuels, 2017, 31, 10699-10705.	5.1	12
83	Recent advances in the molecular simulation of chemical reactions. Molecular Simulation, 2015, 41, 1-2.	2.0	11
84	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
85	A festschrift for Professor A. H. Fuchs. Molecular Simulation, 2014, 40, 1-2.	2.0	10
86	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
87	Free energy calculations along entropic pathways. II. Droplet nucleation in binary mixtures. Journal of Chemical Physics, 2016, 145, 234505.	3.0	10
88	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
89	Communication: Existence and control of liquid polymorphism in methanol under shear. Journal of Chemical Physics, 2018, 149, 111101.	3.0	9
90	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

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91	Estimating the conductivity of a nanoconfined liquid subjected to an experimentally accessible external field. Molecular Simulation, 2008, 34, 177-181.	2.0	8
92	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
93	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
94	Nucleation of Capillary Bridges and Bubbles in Nanoconfined CO2. Langmuir, 2019, 35, 15401-15409.	3.5	8
95	Viscosity of a highly compressed methylated alkane via equilibrium and nonequilibrium molecular dynamics simulations. Chemical Physics Letters, 2019, 719, 103-109.	2.6	8
96	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
97	Similarity law and critical properties in ionic systems.. Chemical Physics Letters, 2017, 687, 9-13.	2.6	8
98	Rotational viscosity of uniaxial molecules. Molecular Physics, 2002, 100, 3479-3482.	1.7	7
99	Nonequilibrium Molecular Dynamics Simulations of Molten Sodium Chloride. International Journal of Thermophysics, 2004, 25, 1375-1393.	2.1	7
100	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
101	Benchmark Free Energies and Entropies for Saturated and Compressed Water. Journal of Chemical & Engineering Data, 2017, 62, 4032-4040.	1.9	6
102	Stabilization of Nanobubbles under Hydrophobic Confinement. Journal of Physical Chemistry C, 2019, 123, 11707-11713.	3.1	6
103	Designing, synthesizing, and modeling active fluids. Physics of Fluids, 2022, 34, .	4.0	6
104	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
105	Universal scaling law for energy and pressure in a shearing fluid. Physical Review E, 2009, 79, 052201.	2.1	5
106	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
107	Determination of mixture properties via a combined Expanded Wang-Landau simulations-Machine Learning approach. Chemical Physics Letters, 2019, 715, 1-6.	2.6	5
108	Unraveling liquid polymorphism in silicon driven out-of-equilibrium. Journal of Chemical Physics, 2020, 153, 054502.	3.0	5

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109	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
110	Competition between crystalline and icosahedral order during crystal growth in bimetallic systems. Journal of Crystal Growth, 2017, 478, 22-27.	1.5	4
111	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
112	Prediction of the phase equilibria for island-type asphaltenes via HMC-WL simulations. Journal of Chemical Physics, 2018, 149, 072307.	3.0	3
113	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
114	Modeling antigen-antibody nanoparticle bioconjugates and their polymorphs. Journal of Chemical Physics, 2018, 148, 124507.	3.0	2
115	Recent advances in molecular simulation. Molecular Simulation, 2019, 45, 1067-1068.	2.0	2
116	Entropy in Molecular Fluids: Interplay between Interaction Complexity and Criticality. Journal of Physical Chemistry B, 2020, 124, 11463-11471.	2.6	2
117	Entropy production in model colloidal suspensions under shear via the fluctuation theorem. Journal of Chemical Physics, 2020, 153, 224113.	3.0	2
118	Guest Editorial: Frontiers of Molecular Simulation. Molecular Simulation, 2006, 32, 173-174.	2.0	1
119	Nonequilibrium Systems. Molecular Simulation, 2016, 42, 1299-1299.	2.0	1
120	Ginzburg-Landau free energy for molecular fluids: Determination and coarse-graining. Chemical Physics Letters, 2017, 669, 218-223.	2.6	1
121	Surface Chemistry. Molecular Simulation, 2017, 43, 326-326.	2.0	1
122	Energy applications. Molecular Simulation, 2017, 43, 729-729.	2.0	1
123	Calculating free energy profiles using entropy as a reaction coordinate: Application to water nucleation. Chemical Physics Letters, 2018, 695, 194-199.	2.6	1
124	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
125	Entropy determination for mixtures in the adiabatic grand-isobaric ensemble. Journal of Chemical Physics, 2022, 156, 084113.	3.0	1
126	Guest editorial: Recent developments in molecular simulation. Molecular Simulation, 2007, 33, 711-712.	2.0	0

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127	Recent advances in molecular biology. Molecular Simulation, 2014, 40, 731-731.	2.0	0
128	Recent advances in the molecular simulation of adsorption. Molecular Simulation, 2014, 40, 515-515.	2.0	0
129	Free Energy Simulations III. Molecular Simulation, 2021, 47, 378-378.	2.0	0
130	Entropy scaling close to criticality: From simple to metallic systems. Physical Review E, 2021, 103, 052102.	2.1	0
131	Recent developments in molecular simulation. Molecular Simulation, 2021, 47, 785-785.	2.0	0
132	Machine-Learned Free Energy Surfaces for Capillary Condensation and Evaporation in Mesopores. Entropy, 2022, 24, 97.	2.2	0