Jerome Delhommelle

List of Publications by Citations

124 papers	2,939 citations	29 h-index	47 g-index
136 ext. papers	3,123 ext. citations	3.7 avg, IF	5.68 L-index

#	Paper	IF	Citations
124	Optimization of the anisotropic united atoms intermolecular potential for n-alkanes. *Journal of Chemical Physics*, **2000**, 112, 5499-5510	3.9	252
123	Inadequacy of the Lorentz-Berthelot combining rules for accurate predictions of equilibrium properties by molecular simulation. *Molecular Physics*, **2001**, 99, 619-625	1.7	236
122	Molecular mechanism for the cross-nucleation between polymorphs. *Journal of the American Chemical Society*, **2006**, 128, 10368-9	16.4	108
121	Controlling polymorphism during the crystallization of an atomic fluid. *Physical Review Letters*, **2007**, 98, 235502	7.4	101
120	Insights into the molecular mechanism underlying polymorph selection. *Journal of the American Chemical Society*, **2006**, 128, 15104-5	16.4	81
119	Molecular insight into the pathway to crystallization of aluminum. *Journal of the American Chemical Society*, **2007**, 129, 7012-3	16.4	61
118	Derivation of an Optimized Potential Model for Phase Equilibria (OPPE) for Sulfides and Thiols. *Journal of Physical Chemistry B*, **2000**, 104, 4745-4753	3.4	60
117	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
116	Comparison of thermostatting mechanisms in NVT and NPT simulations of decane under shear. *Journal of Chemical Physics*, **2001**, 115, 43-49	3.9	50
115	Reexamination of string phase and shear thickening in simple fluids. *Physical Review E*, **2003**, 68, 031201	2.4	47
114	Should "lane formation" occur systematically in driven liquids and colloids?. *Physical Review E*, **2005**, 71, 016705	2.4	46
113	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
112	Role of liquid polymorphism during the crystallization of silicon. *Journal of the American Chemical Society*, **2011**, 133, 2872-4	16.4	42
111	Vapor□liquid equilibria of copper using hybrid Monte Carlo Wang□landau simulations. *Fluid Phase Equilibria*, **2010**, 287, 79-83	2.5	42
110	Polymorph selection during the crystallization of Yukawa systems. *Journal of Chemical Physics*, **2007**, 126, 054501	3.9	41
109	Configurational temperature profile in confined fluids. I. Atomic fluid. *Journal of Chemical Physics*, **2001**, 114, 6229-6235	3.9	41
108	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

107	Molecular simulation of the crystallization of aluminum from the supercooled liquid. *Journal of Chemical Physics*, **2007**, 127, 144509	3.9	39
106	Configurational thermostats for molecular systems. *Molecular Physics*, **2002**, 100, 2387-2395	1.7	39
105	Molecular Simulation of the Nucleation and Growth of Gold Nanoparticles. *Journal of Physical Chemistry C*, **2009**, 113, 3607-3611	3.8	38
104	Crystallization mechanisms for supercooled liquid Xe at high pressure and temperature: Hybrid Monte Carlo molecular simulations. *Physical Review B*, **2008**, 77,	3.3	36
103	Atomistic simulation of the homogeneous nucleation and of the growth of N2 crystallites. *Journal of Chemical Physics*, **2005**, 122, 104510	3.9	35
102	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
101	Simulations of shear-induced melting in two dimensions. *Physical Review B*, **2004**, 69,	3.3	31
100	Reorganization and growth of metastable alpha-N2 critical nuclei into stable beta-N2 crystals. *Journal of the American Chemical Society*, **2004**, 126, 12286-7	16.4	31
99	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	31
98	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
97	Conductivity of molten sodium chloride and its supercritical vapor in strong dc electric fields. *Journal of Chemical Physics*, **2003**, 118, 7477	3.9	30
96	A molecular dynamics study of homogeneous crystal nucleation in liquid nitrogen. *Chemical Physics Letters*, **2003**, 375, 612-618	2.5	29
95	Simulation of friction in nanoconfined fluids for an arbitrarily low shear rate. *Physical Review B*, **2005**, 72,	3.3	29
94	Phase equilibria of polyaromatic hydrocarbons by hybrid Monte Carlo Wang□andau simulations. *Molecular Physics*, **2010**, 108, 151-158	1.7	28
93	Shear viscosity of molten sodium chloride. *Journal of Chemical Physics*, **2003**, 118, 2783	3.9	28
92	On the effects of assuming flow profiles in nonequilibrium simulations. *Journal of Chemical Physics*, **2003**, 119, 11005-11010	3.9	28
91	Configurational temperature thermostat for fluids undergoing shear flow: application to liquid chlorine. *Molecular Physics*, **2001**, 99, 1825-1829	1.7	28
90	Correspondence between configurational temperature and molecular kinetic temperature thermostats. *Journal of Chemical Physics*, **2002**, 117, 6016-6021	3.9	28

89	Rheology of liquid fcc metals: Equilibrium and transient-time correlation-function nonequilibrium molecular dynamics simulations. *Physical Review B*, **2008**, 78,	3.3	27
88	Molecular simulation of cross-nucleation between polymorphs. *Journal of Physical Chemistry B*, **2007**, 111, 1465-9	3.4	27
87	Configurational temperature profile in confined fluids. II. Molecular fluids. *Journal of Chemical Physics*, **2001**, 114, 6236-6241	3.9	27
86	Poiseuille flow of a micropolar fluid. *Molecular Physics*, **2002**, 100, 2857-2865	1.7	26
85	Molecular Simulation of Vapour-Liquid Coexistence Curves for Hydrogen Sulfide-Alkane and Carbon Dioxide-Alkane Mixtures. *Molecular Simulation*, **1999**, 22, 351-368	2	26
84	Unusual Crystallization Behavior Close to the Glass Transition. *Physical Review Letters*, **2018**, 120, 115701	7.4	25
83	Molecular simulation of the homogeneous crystal nucleation of carbon dioxide. *Journal of Chemical Physics*, **2005**, 122, 184518	3.9	25
82	Non-Newtonian behavior in simple fluids. *Journal of Chemical Physics*, **2004**, 120, 6117-23	3.9	24
81	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	24
80	A new approach for the prediction of partition functions using machine learning techniques. *Applied Physics Letters*, **1989**, 55, 963-965	3.4	24
79	Unraveling the coupling between demixing and crystallization in mixtures. *Journal of the American Chemical Society*, **2014**, 136, 8145-8	16.4	23
78	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
77	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
76	Molecular simulation of transport in nanopores: application of the transient-time correlation function formalism. *Physical Review E*, **2008**, 77, 027701	2.4	22
75	Shear thickening in a model colloidal suspension. *Journal of Chemical Physics*, **2005**, 123, 074707	3.9	22
74	Conductivity of molten sodium chloride in an arbitrarily weak dc electric field. *Journal of Chemical Physics*, **2005**, 123, 114505	3.9	22
73	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	3.9	21
72	Scaling Laws and Critical Properties for fcc and hcp Metals. *Journal of Physical Chemistry B*, **2016**, 120, 5255-61	3.4	20

71	Wang–Landau configurational bias Monte Carlo simulations: vapour–liquid equilibria of alkenes. *Molecular Simulation*, **2012**, 38, 653-658	2	20
70	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
69	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
68	Hydrogen bonding in ethanol under shear. *Journal of Chemical Physics*, **2005**, 122, 234509	3.9	19
67	Prediction of critical properties for Naphthacene, Triphenylene and Chrysene by Wang–Landau simulations. *Fluid Phase Equilibria*, **2012**, 322-323, 92-96	2.5	18
66	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
65	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
64	Ideality contours and thermodynamic regularities in supercritical molecular fluids. *Chemical Physics Letters*, **2016**, 658, 37-42	2.5	18
63	Adsorption and diffusion of the antiparkinsonian drug amantadine in carbon nanotubes. *Molecular Simulation*, **2014**, 40, 656-663	2	17
62	Numerical estimate for boiling points via Wang–Landau simulations. *Molecular Simulation*, **2012**, 38, 1265-1270		17
61	Influence of temperature, pressure and internal degrees of freedom on hydrogen bonding and diffusion in liquid ethanol. *Chemical Physics*, **2003**, 286, 303-314	2.3	17
60	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
59	A new approach for the prediction of partition functions using machine learning techniques. *Journal of Chemical Physics*, **2018**, 149, 044118	3.9	15
58	Can Ordered Precursors Promote the Nucleation of Solid Solutions?. *Physical Review Letters*, **2019**, 123, 195701	7.4	15
57	Adsorption of hydrogen in covalent organic frameworks using expanded Wang–Landau simulations. *Molecular Simulation*, **2014**, 40, 71-79	2	15
56	Monte Carlo simulations of squalane in the Gibbs ensemble. *Fluid Phase Equilibria*, **1999**, 155, 167-176	2.5	15
55	Crystal nucleation and growth from supercooled melts. *Molecular Simulation*, **2011**, 37, 613-620	2	14
54	Crystal nucleation and growth in Pd–Ni alloys: a molecular simulation study. *CrystEngComm*, **2011**, 13, 1132-1140	3.3	14

53	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
52	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
51	Onset of shear thickening in a simple fluid. *European Physical Journal E*, **2004**, 15, 65-9	1.5	12
50	A new method for deriving atomic charges and dipoles for n, -alkanes: investigation of transferability and geometry dependence. *Molecular Physics*, **1999**, 97, 1117-1128	1.7	12
49	Crystal nucleation along an entropic pathway: Teaching liquids how to transition. *Physical Review E*, **2018**, 98,	2.4	12
48	Free energy calculations along entropic pathways. III. Nucleation of capillary bridges and bubbles. *Journal of Chemical Physics*, **2017**, 146, 184104	3.9	11
47	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
46	Recent advances in the molecular simulation of chemical reactions. *Molecular Simulation*, **2015**, 41, 1-2	2	11
45	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
44	Conductivity of molten sodium chloride in an alternating electric field. *Journal of Chemical Physics*, **2003**, 119, 8511-8518	3.9	11
43	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
42	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
41	Free energy calculations along entropic pathways. II. Droplet nucleation in binary mixtures. *Journal of Chemical Physics*, **2016**, 145, 234505	3.9	9
40	A festschrift for Professor A. H. Fuchs. *Molecular Simulation*, **2014**, 40, 1-2	2	8
39	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
38	Communication: Existence and control of liquid polymorphism in methanol under shear. *Journal of Chemical Physics*, **2018**, 149, 111101	3.9	8
37	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
36	Coarse-Grained Model and Boiling Point Prediction for Asphaltene Model Compounds via HMC-WL Simulations. *Energy & Fuels*, **2017**, 31, 10699-10705	4.1	7

35	Estimating the conductivity of a nanoconfined liquid subjected to an experimentally accessible external field. *Molecular Simulation*, **2008**, 34, 177-181	2	7
34	Nonequilibrium Molecular Dynamics Simulations of Molten Sodium Chloride. *International Journal of Thermophysics*, **2004**, 25, 1375-1393	2.1	7
33	Rotational viscosity of uniaxial molecules. *Molecular Physics*, **2002**, 100, 3479-3482	1.7	7
32	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
31	Benchmark Free Energies and Entropies for Saturated and Compressed Water. *Journal of Chemical & Engineering Data*, **2017**, 62, 4032-4040	2.8	6
30	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
29	Nucleation of Capillary Bridges and Bubbles in Nanoconfined CO. *Langmuir*, **2019**, 35, 15401-15409	4	5
28	Structure and thermodynamics of the expanded liquid mercury by Monte Carlo simulation: a first attempt. *Journal of Non-Crystalline Solids*, **2007**, 353, 3454-3458	3.9	5
27	Folding Free-Energy Landscape of Synuclein (35-97) Via Replica Exchange Molecular Dynamics. *Journal of Chemical Information and Modeling*, **2021**, 61, 432-443	6.1	5
26	Viscosity of a highly compressed methylated alkane via equilibrium and nonequilibrium molecular dynamics simulations. *Chemical Physics Letters*, **2019**, 719, 103-109	2.5	5
25	Competition between crystalline and icosahedral order during crystal growth in bimetallic systems. *Journal of Crystal Growth*, **2017**, 478, 22-27	1.6	4
24	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
23	Similarity law and critical properties in ionic systems.. *Chemical Physics Letters*, **2017**, 687, 9-13	2.5	4
22	Unraveling liquid polymorphism in silicon driven out-of-equilibrium. *Journal of Chemical Physics*, **2020**, 153, 054502	3.9	4
21	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
20	Stabilization of Nanobubbles under Hydrophobic Confinement. *Journal of Physical Chemistry C*, **2019**, 123, 11707-11713	3.8	3
19	Universal scaling law for energy and pressure in a shearing fluid. *Physical Review E*, **2009**, 79, 052201	2.4	3
18	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

17	Determination of mixture properties via a combined Expanded Wang-Landau simulations-Machine Learning approach. *Chemical Physics Letters*, **2019**, 715, 1-6	2.5	3
16	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
15	Modeling antigen-antibody nanoparticle bioconjugates and their polymorphs. *Journal of Chemical Physics*, **2018**, 148, 124507	3.9	2
14	Prediction of the phase equilibria for island-type asphaltenes via HMC-WL simulations. *Journal of Chemical Physics*, **2018**, 149, 072307	3.9	2
13	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
12	Machine Learning and Deep Learning Algorithms for Skin Cancer Classification from Dermoscopic Images.. *Bioengineering*, **2022**, 9,	5.3	2
11	Ginzburg-Landau free energy for molecular fluids: Determination and coarse-graining. *Chemical Physics Letters*, **2017**, 669, 218-223	2.5	1
10	Calculating free energy profiles using entropy as a reaction coordinate: Application to water nucleation. *Chemical Physics Letters*, **2018**, 695, 194-199	2.5	1
9	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
8	Energy applications. *Molecular Simulation*, **2017**, 43, 729-729	2	1
7	Nonequilibrium Systems. *Molecular Simulation*, **2016**, 42, 1299-1299	2	1
6	Entropy production in model colloidal suspensions under shear via the fluctuation theorem. *Journal of Chemical Physics*, **2020**, 153, 224113	3.9	0
5	Entropy in Molecular Fluids: Interplay between Interaction Complexity and Criticality. *Journal of Physical Chemistry B*, **2020**, 124, 11463-11471	3.4	0
4	Recent advances in the molecular simulation of adsorption. *Molecular Simulation*, **2014**, 40, 515-515	2	
3	Recent advances in molecular biology. *Molecular Simulation*, **2014**, 40, 731-731	2	
2	Entropy scaling close to criticality: From simple to metallic systems. *Physical Review E*, **2021**, 103, 052102	2.4	
1	Entropy determination for mixtures in the adiabatic grand-isobaric ensemble.. *Journal of Chemical Physics*, **2022**, 156, 084113	3.9	