# Jerome Delhommelle

## List of Publications by Year in Descending Order



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| 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 | Machine Learning and Deep Learning Algorithms for Skin Cancer Classification from Dermoscopic Images.. *Bioengineering*, **2022**, 9, | 5.3 | 2 |
| 123 | Entropy determination for mixtures in the adiabatic grand-isobaric ensemble.. *Journal of Chemical Physics*, **2022**, 156, 084113 | 3.9 | |
| 122 | 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 |
| 121 | Entropy scaling close to criticality: From simple to metallic systems. *Physical Review E*, **2021**, 103, 052102 | 2.4 | |
| 120 | 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 |
| 119 | Entropy production in model colloidal suspensions under shear via the fluctuation theorem. *Journal of Chemical Physics*, **2020**, 153, 224113 | 3.9 | 0 |
| 118 | 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 |
| 117 | Entropy in Molecular Fluids: Interplay between Interaction Complexity and Criticality. *Journal of Physical Chemistry B*, **2020**, 124, 11463-11471 | 3.4 | 0 |
| 116 | Unraveling liquid polymorphism in silicon driven out-of-equilibrium. *Journal of Chemical Physics*, **2020**, 153, 054502 | 3.9 | 4 |
| 115 | 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 |
| 114 | Stabilization of Nanobubbles under Hydrophobic Confinement. *Journal of Physical Chemistry C*, **2019**, 123, 11707-11713 | 3.8 | 3 |
| 113 | Nucleation of Capillary Bridges and Bubbles in Nanoconfined CO. *Langmuir*, **2019**, 35, 15401-15409 | 4 | 5 |
| 112 | Can Ordered Precursors Promote the Nucleation of Solid Solutions?. *Physical Review Letters*, **2019**, 123, 195701 | 7.4 | 15 |
| 111 | Viscosity of a highly compressed methylated alkane via equilibrium and nonequilibrium molecular dynamics simulations. *Chemical Physics Letters*, **2019**, 719, 103-109 | 2.5 | 5 |
| 110 | Determination of mixture properties via a combined Expanded Wang-Landau simulations-Machine Learning approach. *Chemical Physics Letters*, **2019**, 715, 1-6 | 2.5 | 3 |
| 109 | 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 |
| 108 | Modeling antigen-antibody nanoparticle bioconjugates and their polymorphs. *Journal of Chemical Physics*, **2018**, 148, 124507 | 3.9 | 2 |

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| 107 | Calculating free energy profiles using entropy as a reaction coordinate: Application to water nucleation. *Chemical Physics Letters*, **2018**, 695, 194-199 | 2.5 | 1 |
| 106 | Unusual Crystallization Behavior Close to the Glass Transition. *Physical Review Letters*, **2018**, 120, 115701 | 7.4 | 25 |
| 105 | A new approach for the prediction of partition functions using machine learning techniques. *Journal of Chemical Physics*, **2018**, 149, 044118 | 3.9 | 15 |
| 104 | Prediction of the phase equilibria for island-type asphaltenes via HMC-WL simulations. *Journal of Chemical Physics*, **2018**, 149, 072307 | 3.9 | 2 |
| 103 | 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 |
| 102 | Crystal nucleation along an entropic pathway: Teaching liquids how to transition. *Physical Review E*, **2018**, 98, | 2.4 | 12 |
| 101 | Communication: Existence and control of liquid polymorphism in methanol under shear. *Journal of Chemical Physics*, **2018**, 149, 111101 | 3.9 | 8 |
| 100 | Ginzburg-Landau free energy for molecular fluids: Determination and coarse-graining. *Chemical Physics Letters*, **2017**, 669, 218-223 | 2.5 | 1 |
| 99 | Free energy calculations along entropic pathways. III. Nucleation of capillary bridges and bubbles. *Journal of Chemical Physics*, **2017**, 146, 184104 | 3.9 | 11 |
| 98 | 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 |
| 97 | Benchmark Free Energies and Entropies for Saturated and Compressed Water. *Journal of Chemical & Engineering Data*, **2017**, 62, 4032-4040 | 2.8 | 6 |
| 96 | 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 |
| 95 | 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 |
| 94 | Competition between crystalline and icosahedral order during crystal growth in bimetallic systems. *Journal of Crystal Growth*, **2017**, 478, 22-27 | 1.6 | 4 |
| 93 | Coarse-Grained Model and Boiling Point Prediction for Asphaltene Model Compounds via HMC-WL Simulations. *Energy & Fuels*, **2017**, 31, 10699-10705 | 4.1 | 7 |
| 92 | Energy applications. *Molecular Simulation*, **2017**, 43, 729-729 | 2 | 1 |
| 91 | Similarity law and critical properties in ionic systems.. *Chemical Physics Letters*, **2017**, 687, 9-13 | 2.5 | 4 |
| 90 | 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 |

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| 89 | 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 |
| 88 | Scaling Laws and Critical Properties for fcc and hcp Metals. *Journal of Physical Chemistry B*, **2016**, 120, 5255-61 | 3.4 | 20 |
| 87 | 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 |
| 86 | 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 |
| 85 | Nonequilibrium Systems. *Molecular Simulation*, **2016**, 42, 1299-1299 | 2 | 1 |
| 84 | Free energy calculations along entropic pathways. II. Droplet nucleation in binary mixtures. *Journal of Chemical Physics*, **2016**, 145, 234505 | 3.9 | 9 |
| 83 | 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 |
| 82 | Ideality contours and thermodynamic regularities in supercritical molecular fluids. *Chemical Physics Letters*, **2016**, 658, 37-42 | 2.5 | 18 |
| 81 | 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 |
| 80 | Recent advances in the molecular simulation of chemical reactions. *Molecular Simulation*, **2015**, 41, 1-2 | 2 | 11 |
| 79 | 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 |
| 78 | Recent advances in the molecular simulation of adsorption. *Molecular Simulation*, **2014**, 40, 515-515 | 2 | |
| 77 | 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 |
| 76 | 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 |
| 75 | Unraveling the coupling between demixing and crystallization in mixtures. *Journal of the American Chemical Society*, **2014**, 136, 8145-8 | 16.4 | 23 |
| 74 | Recent advances in molecular biology. *Molecular Simulation*, **2014**, 40, 731-731 | 2 | |
| 73 | A festschrift for Professor A. H. Fuchs. *Molecular Simulation*, **2014**, 40, 1-2 | 2 | 8 |
| 72 | Adsorption and diffusion of the antiparkinsonian drug amantadine in carbon nanotubes. *Molecular Simulation*, **2014**, 40, 656-663 | 2 | 17 |

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| 71 | Adsorption of hydrogen in covalent organic frameworks using expanded Wang–Landau simulations. *Molecular Simulation*, **2014**, 40, 71-79 | 2 | 15 |
| 70 | 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 | 4.8 | 23 |
| 69 | Wang–Landau configurational bias Monte Carlo simulations: vapour–liquid equilibria of alkenes. *Molecular Simulation*, **2012**, 38, 653-658 | 2 | 20 |
| 68 | Numerical estimate for boiling points via Wang–Landau simulations. *Molecular Simulation*, **2012**, 38, 1265-1270 | 2 | 17 |
| 67 | 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 |
| 66 | 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 |
| 65 | Prediction of critical properties for Naphthacene, Triphenylene and Chrysene by Wang–Landau simulations. *Fluid Phase Equilibria*, **2012**, 322-323, 92-96 | 2.5 | 18 |
| 64 | Crystal nucleation and growth from supercooled melts. *Molecular Simulation*, **2011**, 37, 613-620 | 2 | 14 |
| 63 | Crystal nucleation and growth in Pd–Ni alloys: a molecular simulation study. *CrystEngComm*, **2011**, 13, 1132-1140 | 3.3 | 14 |
| 62 | Role of liquid polymorphism during the crystallization of silicon. *Journal of the American Chemical Society*, **2011**, 133, 2872-4 | 16.4 | 42 |
| 61 | 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 |
| 60 | Phase equilibria of polyaromatic hydrocarbons by hybrid Monte Carlo Wang–Landau simulations. *Molecular Physics*, **2010**, 108, 151-158 | 1.7 | 28 |
| 59 | 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 |
| 58 | Vapor–liquid equilibria of copper using hybrid Monte Carlo Wang–Landau simulations. *Fluid Phase Equilibria*, **2010**, 287, 79-83 | 2.5 | 42 |
| 57 | Universal scaling law for energy and pressure in a shearing fluid. *Physical Review E*, **2009**, 79, 052201 | 2.4 | 3 |
| 56 | 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 |
| 55 | 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 |
| 54 | 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 |

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| 53 | Molecular Simulation of the Nucleation and Growth of Gold Nanoparticles. *Journal of Physical Chemistry C*, **2009**, 113, 3607-3611 | 3.8 | 38 |
| 52 | Estimating the conductivity of a nanoconfined liquid subjected to an experimentally accessible external field. *Molecular Simulation*, **2008**, 34, 177-181 | 2 | 7 |
| 51 | 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 |
| 50 | Molecular simulation of transport in nanopores: application of the transient-time correlation function formalism. *Physical Review E*, **2008**, 77, 027701 | 2.4 | 22 |
| 49 | Rheology of liquid fcc metals: Equilibrium and transient-time correlation-function nonequilibrium molecular dynamics simulations. *Physical Review B*, **2008**, 78, | 3.3 | 27 |
| 48 | Crystallization mechanisms for supercooled liquid Xe at high pressure and temperature: Hybrid Monte Carlo molecular simulations. *Physical Review B*, **2008**, 77, | 3.3 | 36 |
| 47 | Molecular simulation of cross-nucleation between polymorphs. *Journal of Physical Chemistry B*, **2007**, 111, 1465-9 | 3.4 | 27 |
| 46 | 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 |
| 45 | Molecular insight into the pathway to crystallization of aluminum. *Journal of the American Chemical Society*, **2007**, 129, 7012-3 | 16.4 | 61 |
| 44 | Molecular simulation of the crystallization of aluminum from the supercooled liquid. *Journal of Chemical Physics*, **2007**, 127, 144509 | 3.9 | 39 |
| 43 | 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 |
| 42 | Controlling polymorphism during the crystallization of an atomic fluid. *Physical Review Letters*, **2007**, 98, 235502 | 7.4 | 101 |
| 41 | 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 |
| 40 | 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 |
| 39 | Polymorph selection during the crystallization of Yukawa systems. *Journal of Chemical Physics*, **2007** , 126, 054501 | 3.9 | 41 |
| 38 | Molecular mechanism for the cross-nucleation between polymorphs. *Journal of the American Chemical Society*, **2006**, 128, 10368-9 | 16.4 | 108 |
| 37 | Insights into the molecular mechanism underlying polymorph selection. *Journal of the American Chemical Society*, **2006**, 128, 15104-5 | 16.4 | 81 |
| 36 | Shear thickening in a model colloidal suspension. *Journal of Chemical Physics*, **2005**, 123, 074707 | 3.9 | 22 |

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| 35 | Hydrogen bonding in ethanol under shear. *Journal of Chemical Physics*, **2005**, 122, 234509 | 3.9 | 19 |
| 34 | Conductivity of molten sodium chloride in an arbitrarily weak dc electric field. *Journal of Chemical Physics*, **2005**, 123, 114505 | 3.9 | 22 |
| 33 | Atomistic simulation of the homogeneous nucleation and of the growth of N2 crystallites. *Journal of Chemical Physics*, **2005**, 122, 104510 | 3.9 | 35 |
| 32 | Should "lane formation" occur systematically in driven liquids and colloids?. *Physical Review E*, **2005**, 71, 016705 | 2.4 | 46 |
| 31 | Simulation of friction in nanoconfined fluids for an arbitrarily low shear rate. *Physical Review B*, **2005**, 72, | 3.3 | 29 |
| 30 | Molecular simulation of the homogeneous crystal nucleation of carbon dioxide. *Journal of Chemical Physics*, **2005**, 122, 184518 | 3.9 | 25 |
| 29 | Non-Newtonian behavior in simple fluids. *Journal of Chemical Physics*, **2004**, 120, 6117-23 | 3.9 | 24 |
| 28 | Simulations of shear-induced melting in two dimensions. *Physical Review B*, **2004**, 69, | 3.3 | 31 |
| 27 | Onset of shear thickening in a simple fluid. *European Physical Journal E*, **2004**, 15, 65-9 | 1.5 | 12 |
| 26 | Nonequilibrium Molecular Dynamics Simulations of Molten Sodium Chloride. *International Journal of Thermophysics*, **2004**, 25, 1375-1393 | 2.1 | 7 |
| 25 | 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 |
| 24 | Conductivity of molten sodium chloride and its supercritical vapor in strong dc electric fields. *Journal of Chemical Physics*, **2003**, 118, 7477 | 3.9 | 30 |
| 23 | A molecular dynamics study of homogeneous crystal nucleation in liquid nitrogen. *Chemical Physics Letters*, **2003**, 375, 612-618 | 2.5 | 29 |
| 22 | 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 |
| 21 | Reexamination of string phase and shear thickening in simple fluids. *Physical Review E*, **2003**, 68, 031201 | 2.4 | 47 |
| 20 | Shear viscosity of molten sodium chloride. *Journal of Chemical Physics*, **2003**, 118, 2783 | 3.9 | 28 |
| 19 | Conductivity of molten sodium chloride in an alternating electric field. *Journal of Chemical Physics*, **2003**, 119, 8511-8518 | 3.9 | 11 |
| 18 | On the effects of assuming flow profiles in nonequilibrium simulations. *Journal of Chemical Physics*, **2003**, 119, 11005-11010 | 3.9 | 28 |

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| 17 | Poiseuille flow of a micropolar fluid. *Molecular Physics*, **2002**, 100, 2857-2865 | 1.7 | 26 |
| 16 | Rotational viscosity of uniaxial molecules. *Molecular Physics*, **2002**, 100, 3479-3482 | 1.7 | 7 |
| 15 | Correspondence between configurational temperature and molecular kinetic temperature thermostats. *Journal of Chemical Physics*, **2002**, 117, 6016-6021 | 3.9 | 28 |
| 14 | Configurational thermostats for molecular systems. *Molecular Physics*, **2002**, 100, 2387-2395 | 1.7 | 39 |
| 13 | Configurational temperature thermostat for fluids undergoing shear flow: application to liquid chlorine. *Molecular Physics*, **2001**, 99, 1825-1829 | 1.7 | 28 |
| 12 | Comparison of thermostatting mechanisms in NVT and NPT simulations of decane under shear. *Journal of Chemical Physics*, **2001**, 115, 43-49 | 3.9 | 50 |
| 11 | 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 |
| 10 | Configurational temperature profile in confined fluids. II. Molecular fluids. *Journal of Chemical Physics*, **2001**, 114, 6236-6241 | 3.9 | 27 |
| 9 | Configurational temperature profile in confined fluids. I. Atomic fluid. *Journal of Chemical Physics*, **2001**, 114, 6229-6235 | 3.9 | 41 |
| 8 | Optimization of the anisotropic united atoms intermolecular potential for n-alkanes. *Journal of Chemical Physics*, **2000**, 112, 5499-5510 | 3.9 | 252 |
| 7 | 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 |
| 6 | 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 |
| 5 | Molecular Simulation of Vapour-Liquid Coexistence Curves for Hydrogen Sulfide-Alkane and Carbon Dioxide-Alkane Mixtures. *Molecular Simulation*, **1999**, 22, 351-368 | 2 | 26 |
| 4 | 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 |
| 3 | Monte Carlo simulations of squalane in the Gibbs ensemble. *Fluid Phase Equilibria*, **1999**, 155, 167-176 | 2.5 | 15 |
| 2 | 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 |
| 1 | A new approach for the prediction of partition functions using machine learning techniques. *Applied Physics Letters*, **1989**, 55, 963-965 | 3.4 | 24 |