List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/705518/publications.pdf Version: 2024-02-01



| #  | Article  | IF                             | CITATIONS |
|----|--|--------------------------------|-----------|
| 1  | Phase diagram of the NaCl–water system from computer simulations. Journal of Chemical Physics, 2022, 156, 064505.  | 3.0                            | 8         |
| 2  | Parasitic crystallization of colloidal electrolytes: growing a metastable crystal from the nucleus of a stable phase. Soft Matter, 2021, 17, 489-505.  | 2.7                            | 11        |
| 3  | Fcc <i>vs.</i> hcp competition in colloidal hard-sphere nucleation: on their relative stability,<br>interfacial free energy and nucleation rate. Physical Chemistry Chemical Physics, 2021, 23, 19611-19626.   | 2.8                            | 18        |
| 4  | Anomalous Behavior in the Nucleation of Ice at Negative Pressures. Physical Review Letters, 2021, 126, 015704.   | 7.8                            | 24        |
| 5  | Homogeneous nucleation of NaCl in supersaturated solutions. Physical Chemistry Chemical Physics, 2021, 23, 26843-26852.  | 2.8                            | 20        |
| 6  | The Young–Laplace equation for a solid–liquid interface. Journal of Chemical Physics, 2020, 153,<br>191102.  | 3.0                            | 35        |
| 7  | Interfacial Free Energy and Tolman Length of Curved Liquid–Solid Interfaces from Equilibrium<br>Studies. Journal of Physical Chemistry C, 2020, 124, 8795-8805.  | 3.1                            | 24        |
| 8  | Seeding approach to nucleation in the <mml:math<br>xmlns:mml="http://www.w3.org/1998/Math/MathML"&gt;<mml:mrow><mml:mi>N</mml:mi><mml:mi>Vensemble: The case of bubble cavitation in overstretched Lennard Jones fluids. Physical Review E, 2020,<br/>101, 022611.</mml:mi></mml:mrow></mml:math<br> | ni> <mml:mi<br>2.1</mml:mi<br> | >T        |
| 9  | Equivalence between condensation and boiling in a Lennard-Jones fluid. Physical Review E, 2020, 102, 062609.   | 2.1                            | 14        |
| 10 | lce growth rate: Temperature dependence and effect of heat dissipation. Journal of Chemical Physics, 2019, 151, 044509.  | 3.0                            | 20        |
| 11 | Interfacial free energy of a liquid-solid interface: Its change with curvature. Journal of Chemical Physics, 2019, 151, 144501.  | 3.0                            | 28        |
| 12 | Structure and fluctuations of the premelted liquid film of ice at the triple point. Molecular Physics, 2019, 117, 2846-2864.   | 1.7                            | 11        |
| 13 | Ice Ih vs. ice III along the homogeneous nucleation line. Physical Chemistry Chemical Physics, 2019, 21, 5655-5660.  | 2.8                            | 10        |
| 14 | Seeding approach to bubble nucleation in superheated Lennard-Jones fluids. Physical Review E, 2019, 100, 052609.   | 2.1                            | 9         |
| 15 | Heterogeneous <i>versus</i> homogeneous crystal nucleation of hard spheres. Soft Matter, 2019, 15, 9625-9631.  | 2.7                            | 27        |
| 16 | A simulation study of homogeneous ice nucleation in supercooled salty water. Journal of Chemical<br>Physics, 2018, 148, 222811.  | 3.0                            | 33        |
| 17 | Phase boundaries, nucleation rates and speed of crystal growth of the water-to-ice transition under an electric field: a simulation study. Journal of Physics Condensed Matter, 2018, 30, 174002.  | 1.8                            | 12        |
| 18 | Calculation of the water-octanol partition coefficient of cholesterol for SPC, TIP3P, and TIP4P water.<br>Journal of Chemical Physics, 2018, 149, 224501.  | 3.0                            | 12        |

| #  | Article   | IF   | CITATIONS |
|----|---|------|-----------|
| 19 | Homogeneous Ice Nucleation Rate in Water Droplets. Journal of Physical Chemistry C, 2018, 122, 22892-22896.   | 3.1  | 25        |
| 20 | Viscosity and self-diffusion of supercooled and stretched water from molecular dynamics simulations. Journal of Chemical Physics, 2018, 149, 094503.  | 3.0  | 62        |
| 21 | NaCl nucleation from brine in seeded simulations: Sources of uncertainty in rate estimates. Journal of Chemical Physics, 2018, 148, 222838.   | 3.0  | 62        |
| 22 | Mechanosensitive Gold Colloidal Membranes Mediated by Supramolecular Interfacial Self-Assembly.<br>Journal of the American Chemical Society, 2017, 139, 1120-1128.                                | 13.7 | 24        |
| 23 | Brownian versus Newtonian devitrification of hard-sphere glasses. Physical Review E, 2017, 96, 020602.  | 2.1  | 4         |
| 24 | Role of Salt, Pressure, and Water Activity on Homogeneous Ice Nucleation. Journal of Physical Chemistry Letters, 2017, 8, 4486-4491.  | 4.6  | 33        |
| 25 | Avalanche mediated devitrification in a glass of pseudo hard-spheres. Journal of Statistical<br>Mechanics: Theory and Experiment, 2016, 2016, 094005.   | 2.3  | 12        |
| 26 | On the calculation of solubilities via direct coexistence simulations: Investigation of NaCl aqueous solutions and Lennard-Jones binary mixtures. Journal of Chemical Physics, 2016, 145, 154111. | 3.0  | 80        |
| 27 | New methods: general discussion. Faraday Discussions, 2016, 195, 521-556.   | 3.2  | 2         |
| 28 | Application to large systems: general discussion. Faraday Discussions, 2016, 195, 671-698.  | 3.2  | 4         |
| 29 | On the time required to freeze water. Journal of Chemical Physics, 2016, 145, 211922.   | 3.0  | 64        |
| 30 | Seeding approach to crystal nucleation. Journal of Chemical Physics, 2016, 144, 034501.   | 3.0  | 155       |
| 31 | Ice–Water Interfacial Free Energy for the TIP4P, TIP4P/2005, TIP4P/Ice, and mW Models As Obtained from the Mold Integration Technique. Journal of Physical Chemistry C, 2016, 120, 8068-8075.     | 3.1  | 79        |
| 32 | Interfacial Free Energy as the Key to the Pressure-Induced Deceleration of Ice Nucleation. Physical Review Letters, 2016, 117, 135702.  | 7.8  | 65        |
| 33 | Premelting-Induced Smoothening of the Ice-Vapor Interface. Physical Review Letters, 2016, 117, 096101.  | 7.8  | 39        |
| 34 | Lattice mold technique for the calculation of crystal nucleation rates. Faraday Discussions, 2016, 195, 569-582.  | 3.2  | 4         |
| 35 | Competition between ices Ih and Ic in homogeneous water freezing. Journal of Chemical Physics, 2015, 143, 134504.   | 3.0  | 65        |
| 36 | Interfacial free energy of the NaCl crystal-melt interface from capillary wave fluctuations. Journal of Chemical Physics, 2015, 142, 134706.  | 3.0  | 11        |

| #  | Article   | IF   | CITATIONS |
|----|---|------|-----------|
| 37 | The crystal-fluid interfacial free energy and nucleation rate of NaCl from different simulation methods. Journal of Chemical Physics, 2015, 142, 194709.            | 3.0  | 59        |
| 38 | Mediated by a liquid. Nature Materials, 2015, 14, 15-16.  | 27.5 | 11        |
| 39 | Avalanches mediate crystallization in a hard-sphere glass. Proceedings of the National Academy of<br>Sciences of the United States of America, 2014, 111, 75-80.    | 7.1  | 52        |
| 40 | Field-induced sublimation in perfect two-dimensional colloidal crystals. Physical Review E, 2014, 89, 012306.   | 2.1  | 12        |
| 41 | Homogeneous ice nucleation evaluated for several water models. Journal of Chemical Physics, 2014, 141, 18C529.  | 3.0  | 128       |
| 42 | The mold integration method for the calculation of the crystal-fluid interfacial free energy from simulations. Journal of Chemical Physics, 2014, 141, 134709.      | 3.0  | 58        |
| 43 | Computer simulation study of surface wave dynamics at the crystal-melt interface. Journal of Chemical Physics, 2014, 141, 034701.                                   | 3.0  | 25        |
| 44 | Exposing a dynamical signature of the freezing transition through the sound propagation gap. Nature Communications, 2014, 5, 5503.                                  | 12.8 | 8         |
| 45 | Nucleation free-energy barriers with Hybrid Monte-Carlo/Umbrella Sampling. Physical Chemistry Chemical Physics, 2014, 16, 24913-24919.                              | 2.8  | 13        |
| 46 | A study of the ice–water interface using the TIP4P/2005 water model. Physical Chemistry Chemical Physics, 2014, 16, 22159-22166.                                    | 2.8  | 41        |
| 47 | Disjoining Pressure, Healing Distance, and Film Height Dependent Surface Tension of Thin Wetting<br>Films. Journal of Physical Chemistry C, 2014, 118, 22079-22089. | 3.1  | 16        |
| 48 | On fluid-solid direct coexistence simulations: The pseudo-hard sphere model. Journal of Chemical Physics, 2013, 139, 144502.  | 3.0  | 92        |
| 49 | Homogeneous Ice Nucleation at Moderate Supercooling from Molecular Simulation. Journal of the American Chemical Society, 2013, 135, 15008-15017.                    | 13.7 | 256       |
| 50 | Calculation of the melting point of alkali halides by means of computer simulations. Journal of<br>Chemical Physics, 2012, 137, 104507.                             | 3.0  | 41        |
| 51 | Solubility of NaCl in water by molecular simulation revisited. Journal of Chemical Physics, 2012, 136, 244508.  | 3.0  | 133       |
| 52 | From compact to fractal crystalline clusters in concentrated systems of monodisperse hard spheres.<br>Soft Matter, 2012, 8, 4960.                                   | 2.7  | 27        |
| 53 | Phase diagram of trivalent and pentavalent patchy particles. Journal of Physics Condensed Matter, 2012, 24, 064113.   | 1.8  | 26        |
| 54 | Sheet-like assemblies of spherical particles with point-symmetrical patches. Journal of Chemical Physics, 2012, 136, 144706.  | 3.0  | 22        |

| #  | Article  | IF  | CITATIONS |
|----|--|-----|-----------|
| 55 | Crystallization and aging in hard-sphere glasses. Journal of Physics Condensed Matter, 2011, 23, 194117.   | 1.8 | 18        |
| 56 | Crystallization and aging in hard-sphere glasses. Journal of Physics Condensed Matter, 2011, 23, 319501.   | 1.8 | 2         |
| 57 | Crystallization Mechanism of Hard Sphere Classes. Physical Review Letters, 2011, 106, 215701.  | 7.8 | 65        |
| 58 | Crystallization of tetrahedral patchy particles <i>in silico</i> . Journal of Chemical Physics, 2011, 134, 174502.   | 3.0 | 116       |
| 59 | Monte Carlo and event-driven dynamics of Brownian particles with orientational degrees of freedom.<br>Journal of Chemical Physics, 2011, 135, 124106.                              | 3.0 | 32        |
| 60 | Dynamic Monte Carlo versus Brownian dynamics: A comparison for self-diffusion and crystallization in colloidal fluids. Journal of Chemical Physics, 2010, 132, 194102.             | 3.0 | 109       |
| 61 | Phase diagram of a tetrahedral patchy particle model for different interaction ranges. Journal of<br>Chemical Physics, 2010, 132, .  | 3.0 | 116       |
| 62 | Stabilization of Nanoparticle Shells by Competing Interactions. Journal of Physical Chemistry C, 2010, 114, 7780-7786.   | 3.1 | 20        |
| 63 | Can the isotropic-smectic transition of colloidal hard rods occur via nucleation and growth?.<br>Faraday Discussions, 2010, 144, 253-269.  | 3.2 | 17        |
| 64 | Colloidal Gels Assembled via a Temporary Interfacial Scaffold. Physical Review Letters, 2009, 103, 255502.   | 7.8 | 60        |
| 65 | Role of the Range in the Fluidâ^'Crystal Coexistence for a Patchy Particle Model. Journal of Physical<br>Chemistry B, 2009, 113, 15133-15136.                                      | 2.6 | 47        |
| 66 | Hard spheres: crystallization and glass formation. Philosophical Transactions Series A, Mathematical,<br>Physical, and Engineering Sciences, 2009, 367, 4993-5011.                 | 3.4 | 191       |
| 67 | Triple points and coexistence properties of the dense phases of water calculated using computer simulation. Physical Chemistry Chemical Physics, 2009, 11, 556-562.                | 2.8 | 26        |
| 68 | Crystallization of Hard-Sphere Glasses. Physical Review Letters, 2009, 103, 135704.  | 7.8 | 174       |
| 69 | Determination of phase diagrams via computer simulation: methodology and applications to water, electrolytes and proteins. Journal of Physics Condensed Matter, 2008, 20, 153101.  | 1.8 | 209       |
| 70 | Gel Formation in Suspensions of Oppositely Charged Colloids: Mechanism and Relation to the<br>Equilibrium Phase Diagram. Journal of Physical Chemistry B, 2008, 112, 10861-10872.  | 2.6 | 51        |
| 71 | Irreducible Finite-Size Effects in the Surface Free Energy of NaCl Crystals from Crystal-Nucleation<br>Data. Physical Review Letters, 2008, 100, 036103.                           | 7.8 | 32        |
| 72 | Out-of-equilibrium processes in suspensions of oppositely charged colloids: liquid-to-crystal nucleation and gel formation. Journal of Physics Condensed Matter, 2008, 20, 494247. | 1.8 | 26        |

| #  | Article  | IF  | CITATIONS |
|----|--|-----|-----------|
| 73 | Crystallization and gelation in colloidal systems with short-ranged attractive interactions. Physical Review E, 2008, 78, 041402.  | 2.1 | 62        |
| 74 | Solubility of KF and NaCl in water by molecular simulation. Journal of Chemical Physics, 2007, 126, 014507.  | 3.0 | 107       |
| 75 | Evidence for Out-of-Equilibrium Crystal Nucleation in Suspensions of Oppositely Charged Colloids.<br>Physical Review Letters, 2007, 99, 055501.  | 7.8 | 97        |
| 76 | Investigation of the Salting Out of Methane from Aqueous Electrolyte Solutions Using Computer Simulations. Journal of Physical Chemistry B, 2007, 111, 8993-9000.  | 2.6 | 36        |
| 77 | lce: A fruitful source of information about liquid water. Journal of Molecular Liquids, 2007, 136, 214-220.  | 4.9 | 15        |
| 78 | A potential model for methane in water describing correctly the solubility of the gas and the properties of the methane hydrate. Journal of Chemical Physics, 2006, 125, 074510.                                       | 3.0 | 139       |
| 79 | Non-Markovian melting: a novel procedure to generate initial liquid like phases for small molecules for use in computer simulation studies. Computer Physics Communications, 2005, 170, 137-143.                       | 7.5 | 1         |
| 80 | Radial distribution functions and densities for the SPC/E, TIP4P and TIP5P models for liquid water and ices Ih, Ic, II, III, IV, V, VI, VII, VIII, IX, XI and XII. Physical Chemistry Chemical Physics, 2005, 7, 1450. | 2.8 | 111       |
| 81 | Rate of homogeneous crystal nucleation in molten NaCl. Journal of Chemical Physics, 2005, 122, 194501.   | 3.0 | 145       |
| 82 | Can simple models describe the phase diagram of water?. Journal of Physics Condensed Matter, 2005,<br>17, S3283-S3288.   | 1.8 | 72        |
| 83 | The range of meta stability of ice-water melting for two simple models of water. Molecular Physics, 2005, 103, 1-5.  | 1.7 | 54        |
| 84 | A potential model for the study of ices and amorphous water: TIP4P/Ice. Journal of Chemical Physics, 2005, 122, 234511.  | 3.0 | 1,041     |
| 85 | The melting temperature of the most common models of water. Journal of Chemical Physics, 2005, 122, 114507.  | 3.0 | 338       |
| 86 | Tracing the phase diagram of the four-site water potential (TIP4P). Journal of Chemical Physics, 2004, 121, 1165-1166.   | 3.0 | 73        |
| 87 | Combinatorial entropy and phase diagram of partially ordered ice phases. Journal of Chemical Physics, 2004, 121, 10145-10158.  | 3.0 | 54        |
| 88 | Formation of high density amorphous ice by decompression of ice VII and ice VIII at 135 K. Journal of Chemical Physics, 2004, 121, 11907-11911.  | 3.0 | 24        |
| 89 | Molecular modeling of flexible molecules. Vapor–liquid and fluid–solid equilibria. Journal of<br>Molecular Liquids, 2004, 113, 37-51.  | 4.9 | 12        |
| 90 | Computer simulation study of the global phase behavior of linear rigid Lennard-Jones chain molecules: Comparison with flexible models. Journal of Chemical Physics, 2004, 120, 3957-3968.                              | 3.0 | 27        |

| #  | Article  | IF  | CITATIONS |
|----|--|-----|-----------|
| 91 | Phase Diagram of Water from Computer Simulation. Physical Review Letters, 2004, 92, 255701.  | 7.8 | 264       |
| 92 | The properties of fully flexible Lennard-Jones chains in the solid phase: Wertheim theory and simulation. Molecular Physics, 2003, 101, 2241-2255.                           | 1.7 | 17        |
| 93 | Fluid–solid equilibria of flexible and linear rigid tangent chains from Wertheim's thermodynamic perturbation theory. Journal of Chemical Physics, 2003, 119, 10958-10971.   | 3.0 | 17        |
| 94 | Equation of state of model branched alkanes: Theoretical predictions and configurational bias Monte<br>Carlo simulations. Journal of Chemical Physics, 2001, 115, 6220-6235. | 3.0 | 15        |
| 95 | The virial coefficients of the pearl-necklace model. Journal of Chemical Physics, 2000, 113, 10398-10409.  | 3.0 | 24        |