Daan Frenkel

List of Publications by Citations

514 papers	36,985 citations	99 h-index	172 g-index
544 ext. papers	39,212 ext. citations	5.6 avg, IF	7.65 L-index

#	Paper	IF	Citations
514	Enhancement of protein crystal nucleation by critical density fluctuations. *Science*, **1997**, 277, 1975-8	33.3	1131
513	New Monte Carlo method to compute the free energy of arbitrary solids. Application to the fcc and hcp phases of hard spheres. *Journal of Chemical Physics*, **1984**, 81, 3188-3193	3.9	945
512	Configurational bias Monte Carlo: a new sampling scheme for flexible chains. *Molecular Physics*, **1992**, 75, 59-70	1.7	912
511	Prediction of absolute crystal-nucleation rate in hard-sphere colloids. *Nature*, **2001**, 409, 1020-3	50.4	768
510	Tracing the phase boundaries of hard spherocylinders. *Journal of Chemical Physics*, **1997**, 106, 666-687	3.9	624
509	Understanding Molecular Simulation. *Computers in Physics*, **1997**, 11, 351		621
508	Numerical calculation of the rate of crystal nucleation in a Lennard-Jones system at moderate undercooling. *Journal of Chemical Physics*, **1996**, 104, 9932-9947	3.9	604
507	Monte Carlo study of the isotropic and nematic phases of infinitely thin hard platelets. *Molecular Physics*, **1984**, 52, 1303-1334	1.7	576
506	The hard ellipsoid-of-revolution fluid. *Molecular Physics*, **1985**, 55, 1171-1192	1.7	425
505	Numerical evidence for bcc ordering at the surface of a critical fcc nucleus. *Physical Review Letters*, **1995**, 75, 2714-2717	7.4	420
504	Fluid–fluid coexistence in colloidal systems with short-ranged strongly directional attraction. *Journal of Chemical Physics*, **2003**, 118, 9882-9889	3.9	401
503	Molecular Dynamics Simulations **2002**, 63-107		391
502	Computer simulation study of gas–liquid nucleation in a Lennard-Jones system. *Journal of Chemical Physics*, **1998**, 109, 9901-9918	3.9	389
501	Receptor-mediated endocytosis of nanoparticles of various shapes. *Nano Letters*, **2011**, 11, 5391-5	11.5	384
500	Determination of phase diagrams for the hard-core attractive Yukawa system. *Journal of Chemical Physics*, **1994**, 101, 4093-4097	3.9	383
499	Novel scheme to study structural and thermal properties of continuously deformable molecules. *Journal of Physics Condensed Matter*, **1992**, 4, 3053-3076	1.8	356
498	Extended corresponding-states behavior for particles with variable range attractions. *Journal of Chemical Physics*, **2000**, 113, 2941-2944	3.9	353

497	Phase behavior of disklike hard-core mesogens. *Physical Review A*, **1992**, 45, 5632-5648	2.6	344
496	Computer simulation study of free energy barriers in crystal nucleation. *Journal of Chemical Physics*, **1992**, 96, 4655-4668	3.9	342
495	Thermodynamic stability of a smectic phase in a system of hard rods. *Nature*, **1988**, 332, 822-823	50.4	332
494	Entropy difference between crystal phases. *Nature*, **1997**, 388, 235-236	50.4	325
493	Monte Carlo Simulations **2002**, 23-61		324
492	Suppression of crystal nucleation in polydisperse colloids due to increase of the surface free energy. *Nature*, **2001**, 413, 711-3	50.4	322
491	Accelerating Monte Carlo Sampling **2002**, 389-408		316
490	Onset of heterogeneous crystal nucleation in colloidal suspensions. *Nature*, **2004**, 428, 404-6	50.4	314
489	Entropy-driven formation of a superlattice in a hard-sphere binary mixture. *Nature*, **1993**, 365, 35-37	50.4	288
488	Computer simulations in the Gibbs ensemble. *Molecular Physics*, **1989**, 68, 931-950	1.7	286
487	Simulating rare events in equilibrium or nonequilibrium stochastic systems. *Journal of Chemical Physics*, **2006**, 124, 024102	3.9	280
486	Numerical prediction of absolute crystallization rates in hard-sphere colloids. *Journal of Chemical Physics*, **2004**, 120, 3015-29	3.9	266
485	The steady state of heterogeneous catalysis, studied by first-principles statistical mechanics. *Physical Review Letters*, **2004**, 93, 116105	7.4	265
484	Colloids dispersed in polymer solutions. A computer simulation study. *Journal of Chemical Physics*, **1994**, 100, 6873-6887	3.9	263
483	Phase Diagram of a System of Hard Ellipsoids. *Physical Review Letters*, **1984**, 52, 287-290	7.4	262
482	Does C60 have a liquid phase?. *Nature*, **1993**, 365, 425-426	50.4	251
481	Dissipative particle dynamics for interacting systems. *Journal of Chemical Physics*, **2001**, 115, 5015-5026	3.9	247
480	Evidence for one-, two-, and three-dimensional order in a system of hard parallel spherocylinders. *Physical Review A*, **1987**, 36, 2929-2945	2.6	229

479	Molecular dynamics studies of orientational and collision-induced light scattering in molecular fluids. *Journal of Chemical Physics*, **1980**, 72, 2801-2818	3.9	220
478	Ab initio molecular dynamics with excited electrons. *Physical Review Letters*, **1994**, 73, 2599-2602	7.4	213
477	Designing super selectivity in multivalent nano-particle binding. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 10963-8	11.5	212
476	Melting line of Yukawa system by computer simulation. *Journal of Chemical Physics*, **1991**, 94, 2269-2271	3.9	209
475	Evidence for algebraic orientational order in a two-dimensional hard-core nematic. *Physical Review A*, **1985**, 31, 1776-1787	2.6	205
474	Phase diagram of a system of hard spherocylinders by computer simulation. *Physical Review A*, **1990**, 41, 3237-3244	2.6	201
473	Phase behavior of two-dimensional hard rod fluids. *Journal of Chemical Physics*, **2000**, 112, 10034-10041	3.9	192
472	Ab initio Molecular Dynamics Simulation of Laser Melting of Silicon. *Physical Review Letters*, **1996**, 77, 3149-3152	7.4	186
471	Finite-size corrections to the free energies of crystalline solids. *Journal of Chemical Physics*, **2000**, 112, 5339-5342	3.9	183
470	Structure of hard-core models for liquid crystals. *The Journal of Physical Chemistry*, **1988**, 92, 3280-3284		182
469	Depletion effects in binary hard-sphere fluids. *Journal of Physics Condensed Matter*, **1996**, 8, 10799-10821	1.8	181
468	Hard Convex Body Fluids. *Advances in Chemical Physics*, **2007**, 1-166		179
467	Prediction of an expanded-to-condensed transition in colloidal crystals. *Physical Review Letters*, **1994**, 72, 2211-2214	7.4	175
466	Homogeneous nucleation and the Ostwald step rule. *Physical Chemistry Chemical Physics*, **1999**, 1, 2191-2196	3.6	170
465	Forward flux sampling-type schemes for simulating rare events: efficiency analysis. *Journal of Chemical Physics*, **2006**, 124, 194111	3.9	169
464	Direct simulation of phase equilibria of chain molecules. *Journal of Physics Condensed Matter*, **1992**, 4, L255-L259	1.8	165
463	Surface-induced melting and freezing II. A semi-empirical Landau-type model. *Surface Science*, **1990**, 239, 282-300	1.8	162
462	Entropy-driven phase transitions. *Physica A: Statistical Mechanics and Its Applications*, **1999**, 263, 26-38	3.3	161

461	Calculation of the chemical potential in the Gibbs ensemble. *Molecular Physics*, **1989**, 68, 951-958	1.7	161
460	Self-consistent dissipative particle dynamics algorithm. *Europhysics Letters*, **1998**, 42, 377-382	1.6	152
459	Numerical study of the phase behavior of rodlike colloids with attractive interactions. *Journal of Chemical Physics*, **1997**, 107, 1551-1564	3.9	150
458	Order through entropy. *Nature Materials*, **2015**, 14, 9-12	27	149
457	Computer simulation of hard-core models for liquid crystals. *Molecular Physics*, **1987**, 60, 1-20	1.7	149
456	Evidence for smectic order in a fluid of hard parallel spherocylinders. *Physical Review Letters*, **1986**, 57, 1452-1455	7.4	148
455	Isostructural solid-solid transition in crystalline systems with short-ranged interaction. *Physical Review E*, **1994**, 50, 4880-4890	2.4	147
454	Phase separation in binary hard-core mixtures. *Journal of Chemical Physics*, **1994**, 101, 3179-3189	3.9	137
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452	Polymer Crystallization Driven by Anisotropic Interactions1-35		135
451	Rate of homogeneous crystal nucleation in molten NaCl. *Journal of Chemical Physics*, **2005**, 122, 194501	3.9	135
450	Nematic□sotropic transition in polydisperse systems of infinitely thin hard platelets. *Journal of Chemical Physics*, **1999**, 110, 6553-6559	3.9	135
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448	Computer simulation of solid-liquid coexistence in binary hard sphere mixtures. *Molecular Physics*, **1991**, 72, 679-697	1.7	134
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446	Evidence for an Orientationally Ordered Two-Dimensional Fluid Phase from Molecular-Dynamics Calculations. *Physical Review Letters*, **1979**, 42, 1632-1635	7.4	132
445	Quantitative prediction of crystal-nucleation rates for spherical colloids: a computational approach. *Annual Review of Physical Chemistry*, **2004**, 55, 333-61	15.7	131
444	Simulation of the adhesive-hard-sphere model. *Molecular Physics*, **1988**, 64, 403-424	1.7	131

443	Vapor–liquid equilibria of the two-dimensional Lennard-Jones fluid(s). *Journal of Chemical Physics*, **1991**, 94, 5663-5668	3.9	130
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438	Computer simulation of polymer-induced clustering of colloids. *Physical Review Letters*, **1991**, 67, 1110-1113	7.4	126
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433	Influence of polydispersity on the phase behavior of colloidal liquid crystals: A Monte Carlo simulation study. *Journal of Chemical Physics*, **1998**, 109, 6193-6199	3.9	118
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431	Crucial role of nonspecific interactions in amyloid nucleation. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 17869-74	11.5	116
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429	Calculation of the melting point of NaCl by molecular simulation. *Journal of Chemical Physics*, **2003**, 118, 728-735	3.9	108
428	The hard ellipsoid-of-revolution fluid. *Molecular Physics*, **1985**, 55, 1193-1215	1.7	108
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425	Living clusters and crystals from low-density suspensions of active colloids. *Physical Review Letters*, **2013**, 111, 245702	7.4	106
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406	Crystal nucleation of colloidal suspensions under shear. *Physical Review Letters*, **2004**, 93, 068303	7.4	91
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403	Effect of Nutrient Diffusion and Flow on Coral Morphology. *Physical Review Letters*, **1996**, 77, 2328-2331	7.4	90
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