Daan Frenkel

List of Publications by Year
in descending order

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530 papers	42,673 citations	1792 103 h-index	3563 181 g-index
544 all docs	544 docs citations	544 times ranked	20306 citing authors

#	Article	IF	Citations
1	Enhancement of Protein Crystal Nucleation by Critical Density Fluctuations. Science, 1997, 277, 1975-1978.	6.0	1,262
2	Understanding Molecular Simulation. Computers in Physics, 1997, 11, 351-354.	0.6	1,063
3	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.	1.2	1,060
4	Configurational bias Monte Carlo: a new sampling scheme for flexible chains. Molecular Physics, 1992, 75, 59-70.	0.8	1,016
5	Prediction of absolute crystal-nucleation rate in hard-sphere colloids. Nature, 2001, 409, 1020-1023.	13.7	865
6	Tracing the phase boundaries of hard spherocylinders. Journal of Chemical Physics, 1997, 106, 666-687.	1.2	708
7	Numerical calculation of the rate of crystal nucleation in a Lennardâ€Jones system at moderate undercooling. Journal of Chemical Physics, 1996, 104, 9932-9947.	1.2	679
8	Monte Carlo study of the isotropic and nematic phases of infinitely thin hard platelets. Molecular Physics, 1984, 52, 1303-1334.	0.8	618
9	Numerical Evidence for bcc Ordering at the Surface of a Critical fcc Nucleus. Physical Review Letters, 1995, 75, 2714-2717.	2.9	463
10	The hard ellipsoid-of-revolution fluid. Molecular Physics, 1985, 55, 1171-1192.	0.8	457
11	Fluidâ€“fluid coexistence in colloidal systems with short-ranged strongly directional attraction. Journal of Chemical Physics, 2003, 118, 9882-9889.	1.2	452
12	Molecular Dynamics Simulations. , 2002, , 63-107.		441
13	Receptor-Mediated Endocytosis of Nanoparticles of Various Shapes. Nano Letters, 2011, 11, 5391-5395.	4.5	441
14	Computer simulation study of gasâ€“liquid nucleation in a Lennard-Jones system. Journal of Chemical Physics, 1998, 109, 9901-9918.	1.2	426
15	Monte Carlo Simulations. , 2002, , 23-61.		414
16	Determination of phase diagrams for the hardâ€core attractive Yukawa system. Journal of Chemical Physics, 1994, 101, 4093-4097.	1.2	410
17	Extended corresponding-states behavior for particles with variable range attractions. Journal of Chemical Physics, 2000, 113, 2941-2944.	1.2	404
18	Entropy difference between crystal phases. Nature, 1997, 388, 235-236.	13.7	396

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19	Novel scheme to study structural and thermal properties of continuously deformable molecules. Journal of Physics Condensed Matter, 1992, 4, 3053-3076.	0.7	384
20	Suppression of crystal nucleation in polydisperse colloids due to increase of the surface free energy. Nature, 2001, 413, 711-713.	13.7	370
21	Phase behavior of disklike hard-core mesogens. Physical Review A, 1992, 45, 5632-5648.	1.0	368
22	Computer simulation study of free energy barriers in crystal nucleation. Journal of Chemical Physics, 1992, 96, 4655-4668.	1.2	367
23	Onset of heterogeneous crystal nucleation in colloidal suspensions. Nature, 2004, 428, 404-406.	13.7	355
24	Thermodynamic stability of a smectic phase in a system of hard rods. Nature, 1988, 332, 822-823.	13.7	354
25	Entropy-driven formation of a superlattice in a hard-sphere binary mixture. Nature, 1993, 365, 35-37.	13.7	321
26	Accelerating Monte Carlo Sampling. , 2002, , 389-408.		316
27	Simulating rare events in equilibrium or nonequilibrium stochastic systems. Journal of Chemical Physics, 2006, 124, 024102.	1.2	314
28	Computer simulations in the Gibbs ensemble. Molecular Physics, 1989, 68, 931-950.	0.8	311
29	Numerical prediction of absolute crystallization rates in hard-sphere colloids. Journal of Chemical Physics, 2004, 120, 3015-3029.	1.2	303
30	Dissipative particle dynamics for interacting systems. Journal of Chemical Physics, 2001, 115, 5015-5026.	1.2	296
31	Phase Diagram of a System of Hard Ellipsoids. Physical Review Letters, 1984, 52, 287-290.	2.9	294
32	The Steady State of Heterogeneous Catalysis, Studied by First-Principles Statistical Mechanics. Physical Review Letters, 2004, 93, 116105.	2.9	289
33	Colloids dispersed in polymer solutions. A computer simulation study. Journal of Chemical Physics, 1994, 100, 6873-6887.	1.2	274
34	Does C60 have a liquid phase?. Nature, 1993, 365, 425-426.	13.7	273
35	Designing super selectivity in multivalent nano-particle binding. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 10963-10968.	3.3	273
36	Evidence for one-, two-, and three-dimensional order in a system of hard parallel spherocylinders. Physical Review A, 1987, 36, 2929-2945.	1.0	244

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37	Evidence for algebraic orientational order in a two-dimensional hard-core nematic. Physical Review A, 1985, 31, 1776-1787.	1.0	241
38	Molecular dynamics studies of orientational and collisionâ€induced light scattering in molecular fluids. Journal of Chemical Physics, 1980, 72, 2801-2818.	1.2	229
39	Ab InitioMolecular Dynamics with Excited Electrons. Physical Review Letters, 1994, 73, 2599-2602.	2.9	227
40	Phase diagram of a system of hard spherocylinders by computer simulation. Physical Review A, 1990, 41, 3237-3244.	1.0	221
41	Melting line of Yukawa system by computer simulation. Journal of Chemical Physics, 1991, 94, 2269-2271.	1.2	220
42	Ab initioMolecular Dynamics Simulation of Laser Melting of Silicon. Physical Review Letters, 1996, 77, 3149-3152.	2.9	216
43	Phase behavior of two-dimensional hard rod fluids. Journal of Chemical Physics, 2000, 112, 10034-10041.	1.2	215
44	Hard Convex Body Fluids. Advances in Chemical Physics, 2007, , 1-166.	0.3	205
45	Order through entropy. Nature Materials, 2015, 14, 9-12.	13.3	205
46	Depletion effects in binary hard-sphere fluids. Journal of Physics Condensed Matter, 1996, 8, 10799-10821.	0.7	199
47	Finite-size corrections to the free energies of crystalline solids. Journal of Chemical Physics, 2000, 112, 5339-5342.	1.2	199
48	Homogeneous nucleation and the Ostwald step rule. Physical Chemistry Chemical Physics, 1999, 1, 2191-2196.	1.3	196
49	Structure of hard-core models for liquid crystals. The Journal of Physical Chemistry, 1988, 92, 3280-3284.	2.9	193
50	Direct simulation of phase equilibria of chain molecules. Journal of Physics Condensed Matter, 1992, 4, L255-L259.	0.7	190
51	Prediction of an expanded-to-condensed transition in colloidal crystals. Physical Review Letters, 1994, 72, 2211-2214.	2.9	185
52	Forward flux sampling-type schemes for simulating rare events: Efficiency analysis. Journal of Chemical Physics, 2006, 124, 194111.	1.2	183
53	Entropy-driven phase transitions. Physica A: Statistical Mechanics and Its Applications, 1999, 263, 26-38.	1.2	182
54	Surface-induced melting and freezing II. A semi-empirical Landau-type model. Surface Science, 1990, 239, 282-300.	0.8	179

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55	Calculation of the chemical potential in the Gibbs ensemble. Molecular Physics, 1989, 68, 951-958.	0.8	178
56	Self-consistent dissipative particle dynamics algorithm. Europhysics Letters, 1998, 42, 377-382.	0.7	167
57	Liquid network connectivity regulates the stability and composition of biomolecular condensates with many components. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 13238-13247.	3.3	167
58	Numerical study of the phase behavior of rodlike colloids with attractive interactions. Journal of Chemical Physics, 1997, 107, 1551-1564.	1.2	164
59	Evidence for Smectic Order in a Fluid of Hard Parallel Spherocylinders. Physical Review Letters, 1986, 57, 1452-1455.	2.9	160
60	Computer simulation of hard-core models for liquid crystals. Molecular Physics, 1987, 60, 1-20.	0.8	158
61	Crucial role of nonspecific interactions in amyloid nucleation. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17869-17874.	3.3	157
62	Isostructural solid-solid transition in crystalline systems with short-ranged interaction. Physical Review E, 1994, 50, 4880-4890.	0.8	155
63	Vaporâ€“liquid equilibria of the twoâ€dimensional Lennardâ€Jones fluid(s). Journal of Chemical Physics, 1991, 94, 5663-5668.	1.2	154
64	Phase separation in binary hardâ€core mixtures. Journal of Chemical Physics, 1994, 101, 3179-3189.	1.2	153
65	Polymer Crystallization Driven by Anisotropic Interactions. , 0, , 1-35.		149
66	Simulation of homogeneous crystal nucleation close to coexistence. Faraday Discussions, 1996, 104, 93.	1.6	148
67	Simulation of the adhesive-hard-sphere model. Molecular Physics, 1988, 64, 403-424.	0.8	147
68	Can stacking faults in hard-sphere crystals anneal out spontaneously?. Journal of Chemical Physics, 1999, 110, 4589-4592.	1.2	147
69	Rate of homogeneous crystal nucleation in molten NaCl. Journal of Chemical Physics, 2005, 122, 194501.	1.2	145
70	Line Tension Controls Wall-Induced Crystal Nucleation in Hard-Sphere Colloids. Physical Review Letters, 2003, 91, 015703.	2.9	144
71	QUANTITATIVE PREDICTION OF CRYSTAL-NUCLEATION RATES FOR SPHERICAL COLLOIDS: A Computational Approach. Annual Review of Physical Chemistry, 2004, 55, 333-361.	4.8	144
72	Computer simulation of solid-liquid coexistence in binary hard sphere mixtures. Molecular Physics, 1991, 72, 679-697.	0.8	143

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73	Nematicâ€“isotropic transition in polydisperse systems of infinitely thin hard platelets. Journal of Chemical Physics, 1999, 110, 6553-6559.	1.2	143
74	Light-induced actuating nanotransducers. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 5503-5507.	3.3	143
75	Onsager's spherocylinders revisited. The Journal of Physical Chemistry, 1987, 91, 4912-4916.	2.9	142
76	Evidence for an Orientationally Ordered Two-Dimensional Fluid Phase from Molecular-Dynamics Calculations. Physical Review Letters, 1979, 42, 1632-1635.	2.9	139
77	Computer simulation of polymer-induced clustering of colloids. Physical Review Letters, 1991, 67, 1110-1113.	2.9	139
78	Monte Carlo Study of the Isotropic-Nematic Transition in a Fluid of Thin Hard Disks. Physical Review Letters, 1982, 49, 1089-1092.	2.9	138
79	Monte Carlo simulation of two-dimensional hard ellipses. Physical Review A, 1990, 42, 2126-2136.	1.0	137
80	Phase diagram of the adhesive hard sphere fluid. Journal of Chemical Physics, 2004, 121, 535.	1.2	137
81	Force Barriers for Membrane Tube Formation. Physical Review Letters, 2005, 94, 068101.	2.9	137
82	Chromatin Unfolding by Epigenetic Modifications Explained by Dramatic Impairment of Internucleosome Interactions: A Multiscale Computational Study. Journal of the American Chemical Society, 2015, 137, 10205-10215.	6.6	135
83	The Lennard-Jones potential: when (not) to use it. Physical Chemistry Chemical Physics, 2020, 22, 10624-10633.	1.3	133
84	Harvesting graphics power for MD simulations. Molecular Simulation, 2008, 34, 259-266.	0.9	131
85	Influence of polydispersity on the phase behavior of colloidal liquid crystals: A Monte Carlo simulation study. Journal of Chemical Physics, 1998, 109, 6193-6199.	1.2	130
86	Simulation of Shish-Kebab Crystallite Induced by a Single Prealigned Macromolecule. Macromolecules, 2002, 35, 7172-7174.	2.2	130
87	Competition of Percolation and Phase Separation in a Fluid of Adhesive Hard Spheres. Physical Review Letters, 2003, 90, 135702.	2.9	130
88	Structure factors of polydisperse systems of hard spheres: A comparison of Monte Carlo simulations and Percusâ€“Yevick theory. Journal of Chemical Physics, 1986, 84, 4625-4630.	1.2	127
89	Field-Induced Self-Assembly of Suspended Colloidal Membranes. Physical Review Letters, 2009, 103, 228301.	2.9	127
90	Evidence for entropy-driven demixing in hard-core fluids. Physical Review Letters, 1994, 72, 298-300.	2.9	121

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91	Living Clusters and Crystals from Low-Density Suspensions of Active Colloids. Physical Review Letters, 2013, 111, 245702.	2.9	121
92	Phase Transitions in Biological Systems with Many Components. Biophysical Journal, 2017, 112, 683-691.	0.2	121
93	The hard ellipsoid-of-revolution fluid. Molecular Physics, 1985, 55, 1193-1215.	0.8	120
94	Calculation of the melting point of NaCl by molecular simulation. Journal of Chemical Physics, 2003, 118, 728-735.	1.2	119
95	Modeling the Phase Diagram of Carbon. Physical Review Letters, 2005, 94, 145701.	2.9	119
96	Phase diagram of Hertzian spheres. Journal of Chemical Physics, 2009, 131, 044514.	1.2	119
97	Numerical study of the phase diagram of a mixture of spherical and rodlike colloids. Journal of Chemical Physics, 1994, 101, 9869-9875.	1.2	118
98	Quasibinary amorphous phase in a three-dimensional system of particles with repulsive-shoulder interactions. Journal of Chemical Physics, 2008, 129, 064512.	1.2	116
99	Computer Simulations of Freezing and Supercooled Liquids. Annual Review of Physical Chemistry, 1980, 31, 491-521.	4.8	115
100	Role of long-range interactions in the melting of a metallic surface. Physical Review B, 1989, 40, 1353-1356.	1.1	115
101	Intramolecular Nucleation Model for Polymer Crystallization. Macromolecules, 2003, 36, 8178-8183.	2.2	113
102	Simulations: The dark side. European Physical Journal Plus, 2013, 128, 1.	1.2	113
103	Molecular dynamics simulation using hard particles. Computer Physics Reports, 1989, 9, 301-353.	2.3	112
104	Partial enthalpies and related quantities in mixtures from computer simulation. Chemical Physics Letters, 1987, 136, 35-41.	1.2	111
105	Molecular dynamics study of the dynamical properties of an assembly of infinitely thin hard rods. Molecular Physics, 1983, 49, 503-541.	0.8	110
106	The crucial effect of early-stage gelation on the mechanical properties of cement hydrates. Nature Communications, 2016, 7, 12106.	5.8	109
107	Phase separation in binary hard-core mixtures: An exact result. Physical Review Letters, 1992, 68, 3363-3365.	2.9	108
108	An enhanced version of the heat exchange algorithm with excellent energy conservation properties. Journal of Chemical Physics, 2015, 143, 124104.	1.2	108

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109	Effect of Nutrient Diffusion and Flow on Coral Morphology. Physical Review Letters, 1996, 77, 2328-2331.	2.9	107
110	Enhanced stability of layered phases in parallel hard spherocylinders due to addition of hard spheres. Physical Review E, 2000, 62, 3925-3933.	0.8	107
111	Spatiotemporal control and superselectivity in supramolecular polymers using multivalency. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 12203-12208.	3.3	106
112	Re-entrant melting as a design principle for DNA-coated colloids. Nature Materials, 2012, 11, 518-522.	13.3	104
113	Designing multivalent probes for tunable superselective targeting. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 5579-5584.	3.3	104
114	Computing stationary distributions in equilibrium and nonequilibrium systems with forward flux sampling. Journal of Chemical Physics, 2007, 127, 114109.	1.2	102
115	The stability of the AB 13 crystal in a binary hard sphere system. Molecular Physics, 1993, 79, 105-120.	0.8	101
116	Invited Lecture. Columnar ordering as an excluded-volume effect. Liquid Crystals, 1989, 5, 929-940.	0.9	100
117	Crystal Nucleation of Colloidal Suspensions under Shear. Physical Review Letters, 2004, 93, 068303.	2.9	99
118	Waterlike thermodynamic anomalies in a repulsive-shoulder potential system. Physical Review E, 2009, 79, 051202.	0.8	99
119	On the anisotropy of diffusion in nematic liquid crystals: test of a modified affine transformation model via molecular dynamics. Molecular Physics, 1991, 74, 765-774.	0.8	98
120	Dislocation Unbinding in Dense Two-Dimensional Crystals. Physical Review Letters, 1995, 74, 2519-2522.	2.9	98
121	Evidence for Out-of-Equilibrium Crystal Nucleation in Suspensions of Oppositely Charged Colloids. Physical Review Letters, 2007, 99, 055501.	2.9	97
122	Rational design of self-assembly pathways for complex multicomponent structures. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 6313-6318.	3.3	97
123	COLLOIDAL SYSTEMS: Playing Tricks with Designer "Atoms". Science, 2002, 296, 65-66.	6.0	96
124	A general theory of DNA-mediated and other valence-limited colloidal interactions. Journal of Chemical Physics, 2012, 137, 094108.	1.2	96
125	Nonperiodic solid phase in a two-dimensional hard-dimer system. Physical Review Letters, 1991, 66, 3168-3171.	2.9	95
126	Simulation study of the isotropic-to-nematic transitions of semiflexible polymers. Physical Review E, 1995, 51, 5891-5898.	0.8	95

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127	Intrinsic disorder modulates protein self-assembly and aggregation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 6951-6956.	3.3	95
128	Calculation of liquid-crystal Frank constants by computer simulation. Physical Review A, 1988, 37, 1813-1816.	1.0	92
129	Speed-up of Monte Carlo simulations by sampling of rejected states. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 17571-17575.	3.3	92
130	Superselective Targeting Using Multivalent Polymers. Journal of the American Chemical Society, 2014, 136, 1722-1725.	6.6	92
131	Relative stability of columnar and crystalline phases in a system of parallel hard spherocylinders. Physical Review A, 1991, 43, 4334-4343.	1.0	91
132	Numerical calculation of the rate of homogeneous gasâ€“liquid nucleation in a Lennard-Jones system. Journal of Chemical Physics, 1999, 110, 1591-1599.	1.2	91
133	Discrete solution of the electrokinetic equations. Journal of Chemical Physics, 2004, 121, 973-986.	1.2	91
134	Structural, dynamical, electronic, and bonding properties of laser-heated silicon: Anab initiomolecular-dynamics study. Physical Review B, 1997, 56, 3806-3812.	1.1	90
135	Physical determinants of the self-replication of protein fibrils. Nature Physics, 2016, 12, 874-880.	6.5	90
136	Crystallization of weakly charged colloidal spheres: a numerical study. Journal of Physics Condensed Matter, 2002, 14, 7667-7680.	0.7	89
137	Numerical Simulation of Crystal Nucleation in Colloids. Advances in Polymer Science, 0, , 149-208.	0.4	87
138	Homogeneous Bubble Nucleation Driven by Local Hot Spots: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2009, 113, 3776-3784.	1.2	86
139	A parameter-free, solid-angle based, nearest-neighbor algorithm. Journal of Chemical Physics, 2012, 136, 234107.	1.2	86
140	Soft condensed matter. Physica A: Statistical Mechanics and Its Applications, 2002, 313, 1-31.	1.2	84
141	Gibbs, Boltzmann, and negative temperatures. American Journal of Physics, 2015, 83, 163-170.	0.3	83
142	Simulation of diffusion in a two-dimensional lattice-gas cellular automaton: A test of mode-coupling theory. Physical Review Letters, 1989, 63, 2165-2168.	2.9	82
143	Unexpected length dependence of the solubility of chain molecules. Molecular Physics, 1992, 75, 983-988.	0.8	82
144	Two-step vapor-crystal nucleation close below triple point. Journal of Chemical Physics, 2008, 129, 204505.	1.2	82

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145	Simulation of nucleation in almost hard-sphere colloids: The discrepancy between experiment and simulation persists. Journal of Chemical Physics, 2011, 134, 134901.	1.2	82
146	Numerical Evidence for Nucleated Self-Assembly of DNA Brick Structures. Physical Review Letters, 2014, 112, 238103.	2.9	82
147	The effect of chain stiffness on the phase behaviour of isolated homopolymers. Journal of Chemical Physics, 1998, 108, 2134-2142.	1.2	81
148	Algebraic Decay of Velocity Fluctuations in a Confined Fluid. Physical Review Letters, 1997, 78, 3785-3788.	2.9	80
149	The role of long-range forces in the phase behavior of colloids and proteins. Europhysics Letters, 1999, 48, 332-338.	0.7	80
150	Monte Carlo study of hard pentagons. Physical Review E, 2005, 71, 036138.	0.8	80
151	Free energy changes on freezing and melting ductile metals. Molecular Physics, 1993, 80, 801-814.	0.8	79
152	Transverse interlayer order in lyotropic smectic liquid crystals. Physical Review E, 1995, 52, R1277-R1280.	0.8	79
153	Location of melting point at 300 K of nitrogen by Monte Carlo simulation. Journal of Chemical Physics, 1990, 92, 7570-7575.	1.2	75
154	Recent advances in the modelling and simulation of electrokinetic effects: bridging the gap between atomistic and macroscopic descriptions. Physical Chemistry Chemical Physics, 2010, 12, 9566.	1.3	75
155	Numerical study of DNA-functionalized microparticles and nanoparticles: Explicit pair potentials and their implications for phase behavior. Journal of Chemical Physics, 2011, 134, 084702.	1.2	75
156	Mobile Linkers on DNA-Coated Colloids: Valency without Patches. Physical Review Letters, 2014, 113, 128303.	2.9	75
157	Liquid-crystalline ordering of antimicrobial peptideâ€“DNA complexes controls TLR9 activation. Nature Materials, 2015, 14, 696-700.	13.3	75
158	Protein Shape and Crowding Drive Domain Formation and Curvature in Biological Membranes. Biophysical Journal, 2008, 94, 640-647.	0.2	74
159	Design Rule for Colloidal Crystals of DNA-Functionalized Particles. Physical Review Letters, 2011, 107, 045902.	2.9	74
160	Kinetics of spontaneous filament nucleation via oligomers: Insights from theory and simulation. Journal of Chemical Physics, 2016, 145, 211926.	1.2	73
161	Self-Assembly of Structures with Addressable Complexity. Journal of the American Chemical Society, 2016, 138, 2457-2467.	6.6	73
162	Computational methodology for solubility prediction: Application to the sparingly soluble solutes. Journal of Chemical Physics, 2017, 146, 214110.	1.2	71

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163	Optimal multivalent targeting of membranes with many distinct receptors. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7210-7215.	3.3	71
164	Elastic constants of hard-sphere crystals. Physical Review Letters, 1987, 59, 1169-1169.	2.9	70
165	Pore nucleation in mechanically stretched bilayer membranes. Journal of Chemical Physics, 2005, 123, 154701.	1.2	68
166	Molecular simulations of droplet coalescence in oil/water/surfactant systems. Journal of Chemical Physics, 2007, 127, 134701.	1.2	68
167	Numerical Calculation of Granular Entropy. Physical Review Letters, 2014, 112, 098002.	2.9	68
168	Modeling flexible amphiphilic bilayers: A solvent-free off-lattice Monte Carlo study. Journal of Chemical Physics, 2005, 122, 234711.	1.2	67
169	Observation of dynamical precursors of the isotropic-nematic transition by computer simulation. Physical Review Letters, 1987, 58, 1748-1750.	2.9	66
170	A Simple Lattice Model That Captures Protein Folding, Aggregation and Amyloid Formation. PLoS ONE, 2014, 9, e85185.	1.1	66
171	Calculation of partial enthalpies of an argon-krypton mixture by NPT molecular dynamics. Chemical Physics, 1989, 129, 213-224.	0.9	65
172	Demixing in hard ellipsoid rod-plate mixtures. Journal of Chemical Physics, 1997, 106, 9270-9275.	1.2	65
173	Kinetic Monte Carlo simulations of the growth of polymer crystals. Journal of Chemical Physics, 1999, 110, 2692-2702.	1.2	65
174	Phase Behavior and Selectivity of DNA-Linked Nanoparticle Assemblies. Physical Review Letters, 2004, 92, 068302.	2.9	65
175	Efficient schemes to compute diffusive barrier crossing rates. Molecular Physics, 1997, 90, 925-942.	0.8	64
176	Phase Coexistence of Cluster Crystals: Beyond the Gibbs Phase Rule. Physical Review Letters, 2007, 99, 235702.	2.9	63
177	Connecting Macroscopic Observables and Microscopic Assembly Events in Amyloid Formation Using Coarse Grained Simulations. PLoS Computational Biology, 2012, 8, e1002692.	1.5	63
178	Longâ€time tails in angular momentum correlations. Journal of Chemical Physics, 1995, 103, 1582-1587.	1.2	62
179	Do Hydrodynamic Dispersion Coefficients Exist?. Physical Review Letters, 1996, 77, 4552-4555.	2.9	62
180	Relation between Molecular Shape and the Morphology of Self-Assembling Aggregates: A Simulation Study. Biophysical Journal, 2011, 101, 1432-1439.	0.2	62

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181	Long-time tails of the velocity autocorrelation function in two- and three-dimensional lattice-gas cellular automata: A test of mode-coupling theory. Physical Review A, 1990, 41, 4277-4284.	1.0	61
182	A computer simulation investigation into the stability of theAB2superlattice in a binary hard sphere system. Molecular Physics, 1993, 80, 987-995.	0.8	61
183	Infinitely thin disks exhibit a first order nematic-columnar phase transition. Physical Review E, 1998, 57, 4824-4826.	0.8	61
184	Multiple occupancy crystals formed by purely repulsive soft particles. Journal of Physics Condensed Matter, 2008, 20, 494245.	0.7	61
185	Application of lattice-gas cellular automata to the Brownian motion of solids in suspension. Physical Review Letters, 1988, 60, 975-978.	2.9	60
186	Coil-Globule Transition in Gas-Liquid Nucleation of Polar Fluids. Physical Review Letters, 1998, 81, 3695-3698.	2.9	60
187	Do cylinders exhibit a cubatic phase?. Journal of Chemical Physics, 1999, 110, 11652-11659.	1.2	59
188	Stretching the Frontiers: Exploring the Relationships Between Entrepreneurship and Ethics. Journal of Business Ethics, 2005, 60, 207-209.	3.7	59
189	Homogeneous nucleation under shear in a two-dimensional Ising model: Cluster growth, coalescence, and breakup. Journal of Chemical Physics, 2008, 129, 134704.	1.2	59
190	State-of-the-art models for the phase diagram of carbon and diamond nucleation. Molecular Physics, 2008, 106, 2011-2038.	0.8	58
191	Large Difference in the Elastic Properties of fcc and hcp Hard-Sphere Crystals. Physical Review Letters, 2003, 90, 255501.	2.9	57
192	Confinement free energy of semiflexible polymers. Physica A: Statistical Mechanics and Its Applications, 1993, 193, 374-393.	1.2	56
193	First-order nematic-smectic phase transition for hard spherocylinders in the limit of infinite aspect ratio. Physical Review E, 1997, 56, R6260-R6263.	0.8	56
194	Thermodynamics and kinetics of phase separation of protein-RNA mixtures by a minimal model. Biophysical Journal, 2021, 120, 1219-1230.	0.2	56
195	Isostructural solid - solid transitions in systems with a repulsive `shoulder' potential. Journal of Physics Condensed Matter, 1997, 9, 381-387.	0.7	55
196	Intracellular Release of Endocytosed Nanoparticles Upon a Change of Ligandâ€“Receptor Interaction. ACS Nano, 2012, 6, 10598-10605.	7.3	55
197	Theory and simulation of DNA-coated colloids: a guide for rational design. Physical Chemistry Chemical Physics, 2016, 18, 6373-6393.	1.3	55
198	Virtual-Move Parallel Tempering. ChemPhysChem, 2005, 6, 1779-1783.	1.0	54

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199	Disordered Flanks Prevent Peptide Aggregation. PLoS Computational Biology, 2008, 4, e1000241.	1.5	54
200	Discotic liquid crystals Physical parameters of some 2,3,7,8,12,13-hexa(alkanoyloxy)truxenes. Observation of a re-entrant isotropic phase in a pure disc-like mesogen. Liquid Crystals, 1988, 3, 1087-1104.	0.9	53
201	Evidence for faster-than-tâ^'1decay of the velocity autocorrelation function in a 2D fluid. Physical Review Letters, 1991, 66, 1591-1594.	2.9	53
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