List of Publications by Year in descending order

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IENIS CLASED

#	Article	IF	CITATIONS
1	Anisotropy of building blocks and their assembly into complex structures. Nature Materials, 2007, 6, 557-562.	13.3	2,440
2	Predictive Self-Assembly of Polyhedra into Complex Structures. Science, 2012, 337, 453-457.	6.0	882
3	Self-Assembly of CdTe Nanocrystals into Free-Floating Sheets. Science, 2006, 314, 274-278.	6.0	824
4	Self-Assembly of Patchy Particles. Nano Letters, 2004, 4, 1407-1413.	4.5	722
5	Strong scaling of general-purpose molecular dynamics simulations on GPUs. Computer Physics Communications, 2015, 192, 97-107.	3.0	546
6	HOOMD-blue: A Python package for high-performance molecular dynamics and hard particle Monte Carlo simulations. Computational Materials Science, 2020, 173, 109363.	1.4	326
7	Competition of shape and interaction patchiness for self-assembling nanoplates. Nature Chemistry, 2013, 5, 466-473.	6.6	278
8	Understanding shape entropy through local dense packing. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E4812-21.	3.3	199
9	Crystalline Assemblies and Densest Packings of a Family of Truncated Tetrahedra and the Role of Directional Entropic Forces. ACS Nano, 2012, 6, 609-614.	7.3	190
10	Entropically Patchy Particles: Engineering Valence through Shape Entropy. ACS Nano, 2014, 8, 931-940.	7.3	175
11	Rigid body constraints realized in massively-parallel molecular dynamics on graphics processing units. Computer Physics Communications, 2011, 182, 2307-2313.	3.0	164
12	Clathrate colloidal crystals. Science, 2017, 355, 931-935.	6.0	162
13	Pseudo-random number generation for Brownian Dynamics and Dissipative Particle Dynamics simulations on GPU devices. Journal of Computational Physics, 2011, 230, 7191-7201.	1.9	148
14	Shape-dependent ordering of gold nanocrystals into large-scale superlattices. Nature Communications, 2017, 8, 14038.	5.8	141
15	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. Journal of Chemical Information and Modeling, 2020, 60, 5832-5852.	2.5	134
16	freud: A software suite for high throughput analysis of particle simulation data. Computer Physics Communications, 2020, 254, 107275.	3.0	133
17	Role of isostaticity and load-bearing microstructure in the elasticity of yielded colloidal gels. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 16029-16034.	3.3	132
18	Computational self-assembly of a one-component icosahedral quasicrystal. Nature Materials, 2015, 14, 109-116.	13.3	129

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19	Glass transition and rheological redundancy in F-actin solutions. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 20199-20203.	3.3	120
20	Quasicrystalline nanocrystal superlattice with partial matching rules. Nature Materials, 2017, 16, 214-219.	13.3	114
21	Shape Alloys of Nanorods and Nanospheres from Self-Assembly. Nano Letters, 2013, 13, 4980-4988.	4.5	104
22	Universality of Block Copolymer Melts. Physical Review Letters, 2014, 113, 068302.	2.9	102
23	Terminal supraparticle assemblies from similarly charged protein molecules and nanoparticles. Nature Communications, 2014, 5, 3593.	5.8	97
24	Simple data and workflow management with the signac framework. Computational Materials Science, 2018, 146, 220-229.	1.4	91
25	A Directional Entropic Force Approach to Assemble Anisotropic Nanoparticles into Superlattices. Angewandte Chemie - International Edition, 2013, 52, 13980-13984.	7.2	90
26	Universal Phenomenology of Symmetric Diblock Copolymers near the Order–Disorder Transition. Macromolecules, 2015, 48, 819-839.	2.2	83
27	Phase diagram of hard tetrahedra. Journal of Chemical Physics, 2011, 135, 194101.	1.2	76
28	Why large icosahedral viruses need scaffolding proteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10971-10976.	3.3	72
29	The glassy wormlike chain. New Journal of Physics, 2007, 9, 416-416.	1.2	71
30	Supercharging enables organized assembly of synthetic biomolecules. Nature Chemistry, 2019, 11, 204-212.	6.6	70
31	Scalable Metropolis Monte Carlo for simulation of hard shapes. Computer Physics Communications, 2016, 204, 21-30.	3.0	69
32	Simultaneous Nano―and Microscale Control of Nanofibrous Microspheres Selfâ€Assembled from Starâ€Shaped Polymers. Advanced Materials, 2015, 27, 3947-3952.	11.1	63
33	Shape and Symmetry Determine Two-Dimensional Melting Transitions of Hard Regular Polygons. Physical Review X, 2017, 7, .	2.8	61
34	Colloidal fibers and rings by cooperative assembly. Nature Communications, 2019, 10, 3936.	5.8	61
35	Entropic colloidal crystallization pathways via fluid–fluid transitions and multidimensional prenucleation motifs. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 14843-14851.	3.3	60
36	Massively parallel Monte Carlo for many-particle simulations on GPUs. Journal of Computational Physics, 2013, 254, 27-38.	1.9	58

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37	Collective and Single-Chain Correlations in Disordered Melts of Symmetric Diblock Copolymers: Quantitative Comparison of Simulations and Theory. Macromolecules, 2014, 47, 851-869.	2.2	56
38	Efficient neighbor list calculation for molecular simulation of colloidal systems using graphics processing units. Computer Physics Communications, 2016, 203, 45-52.	3.0	53
39	Stability of the double gyroid phase to nanoparticle polydispersity in polymer-tethered nanosphere systems. Soft Matter, 2010, 6, 1693.	1.2	46
40	Capping Ligand Vortices as "Atomic Orbitals―in Nanocrystal Self-Assembly. ACS Nano, 2017, 11, 11273-11282.	7.3	43
41	The entropic bond in colloidal crystals. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 16703-16710.	3.3	42
42	Metastable orientational order of colloidal discoids. Nature Communications, 2015, 6, 8507.	5.8	40
43	GPU accelerated Discrete Element Method (DEM) molecular dynamics for conservative, faceted particle simulations. Journal of Computational Physics, 2017, 334, 460-467.	1.9	38
44	The emergence of valency in colloidal crystals through electron equivalents. Nature Materials, 2022, 21, 580-587.	13.3	37
45	Rational design of nanomaterials from assembly and reconfigurability of polymer-tethered nanoparticles. MRS Communications, 2015, 5, 397-406.	0.8	36
46	Test of a scaling hypothesis for the structure factor of disordered diblock copolymer melts. Soft Matter, 2012, 8, 11310.	1.2	34
47	Efficient Phase Diagram Sampling by Active Learning. Journal of Physical Chemistry B, 2020, 124, 1275-1284.	1.2	33
48	Tube Width Fluctuations in F-Actin Solutions. Physical Review Letters, 2010, 105, 037801.	2.9	30
49	Generalised Einstein relation for hot Brownian motion. Europhysics Letters, 2011, 96, 60009.	0.7	30
50	Inverse design of simple pair potentials for the self-assembly of complex structures. Journal of Chemical Physics, 2018, 149, 204102.	1.2	30
51	Thermal and athermal three-dimensional swarms of self-propelled particles. Physical Review E, 2012, 86, 011136.	0.8	29
52	Influence of Softness on the Stability of Binary Colloidal Crystals. ACS Nano, 2019, 13, 13829-13842.	7.3	29
53	Binding kinetics of lock and key colloids. Journal of Chemical Physics, 2015, 142, 174909.	1.2	28
54	Using depletion to control colloidal crystal assemblies of hard cuboctahedra. Soft Matter, 2016, 12, 5199-5204.	1.2	27

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55	Supraparticle Nanoassemblies with Enzymes. Chemistry of Materials, 2019, 31, 7493-7500.	3.2	24
56	High-throughput virtual laboratory for drug discovery using massive datasets. International Journal of High Performance Computing Applications, 2021, 35, 452-468.	2.4	24
57	Non-close-packed three-dimensional quasicrystals. Journal of Physics Condensed Matter, 2017, 29, 234005.	0.7	22
58	Dendrimer Ligand Directed Nanoplate Assembly. ACS Nano, 2019, 13, 14241-14251.	7.3	22
59	Effect of Defective Microstructure and Film Thickness on the Reflective Structural Color of Self-Assembled Colloidal Crystals. ACS Applied Materials & Interfaces, 2020, 12, 9842-9850.	4.0	22
60	A theory of entropic bonding. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	22
61	Phase separation and state oscillation of active inertial particles. Soft Matter, 2020, 16, 2847-2853.	1.2	21
62	Pressure in rigid body molecular dynamics. Computational Materials Science, 2020, 173, 109430.	1.4	19
63	Supercomputing Pipelines Search for Therapeutics Against COVID-19. Computing in Science and Engineering, 2021, 23, 7-16.	1.2	19
64	Anisotropic nanocrystal shape and ligand design for co-assembly. Science Advances, 2021, 7, .	4.7	19
65	A parallel algorithm for implicit depletant simulations. Journal of Chemical Physics, 2015, 143, 184110.	1.2	18
66	Shape allophiles improve entropic assembly. Soft Matter, 2015, 11, 7250-7256.	1.2	18
67	Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor. ACS Pharmacology and Translational Science, 2022, 5, 255-265.	2.5	17
68	Universal folding pathways of polyhedron nets. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E6690-E6696.	3.3	16
69	Identity crisis in alchemical space drives the entropic colloidal glass transition. Nature Communications, 2019, 10, 64.	5.8	16
70	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	1.8	16
71	A mean-field approach to simulating anisotropic particles. Journal of Chemical Physics, 2020, 153, 084106.	1.2	13
72	Tube-width fluctuations of entangled stiff polymers. Physical Review E, 2011, 84, 051801.	0.8	12

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73	Tunable emergent structures and traveling waves in mixtures of passive and contact-triggered-active particles. Soft Matter, 2017, 13, 6332-6339.	1.2	11
74	Phase behavior and design rules for plastic colloidal crystals of hard polyhedra via consideration of directional entropic forces. Soft Matter, 2019, 15, 5380-5389.	1.2	11
75	Strain fields in repulsive colloidal crystals. Physical Review Materials, 2018, 2, .	0.9	11
76	Dynamic structure factor of a stiff polymer in a glassy solution. European Physical Journal E, 2008, 26, 123-36.	0.7	10
77	Shapes within shapes: how particles arrange inside a cavity. Soft Matter, 2018, 14, 3012-3017.	1.2	10
78	FCC ↔ BCC Phase Transitions in Convex and Concave Hard Particle Systems. Journal of Physical Chemistry B, 2019, 123, 9038-9043.	1.2	10
79	Moving beyond the constraints of chemistry via crystal structure discovery with isotropic multiwell pair potentials. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	10
80	Unexpected Dependence of Photonic Band Gap Size on Randomness in Self-Assembled Colloidal Crystals. Physical Review Letters, 2021, 126, 208002.	2.9	10
81	How to Professionally Develop Reusable Scientific Software—And When Not To. Computing in Science and Engineering, 2019, 21, 66-79.	1.2	9
82	Shape-driven entropic self-assembly of an open, reconfigurable, binary host–guest colloidal crystal. Soft Matter, 2021, 17, 2840-2848.	1.2	9
83	Folding and stability of helical bundle proteins from coarseâ€grained models. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1200-1211.	1.5	8
84	Alchemical molecular dynamics for inverse design. Molecular Physics, 2019, 117, 3968-3980.	0.8	8
85	Implementation of metal-friendly EAM/FS-type semi-empirical potentials in HOOMD-blue: A GPU-accelerated molecular dynamics software. Journal of Computational Physics, 2018, 359, 352-360.	1.9	7
86	Ordered Networks of Gold Nanoparticles Crosslinked by Dithiolâ€Oligomers. Particle and Particle Systems Characterization, 2018, 35, 1800097.	1.2	7
87	Thermodynamic Equilibrium of Binary Nanocrystal Superlattices. Journal of Physical Chemistry C, 2021, 125, 18936-18945.	1.5	7
88	Effect of Particles of Irregular Size on the Microstructure and Structural Color of Self-Assembled Colloidal Crystals. Langmuir, 2021, 37, 13300-13308.	1.6	7
89	Particle anisotropy tunes emergent behavior in active colloidal systems. Soft Matter, 2022, 18, 1044-1053.	1.2	7
90	Tuning Stoichiometry to Promote Formation of Binary Colloidal Superlattices. Physical Review Letters, 2022, 128, 188001.	2.9	7

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91	Hierarchical self-assembly of hard cube derivatives. Soft Matter, 2019, 15, 3733-3739.	1.2	6
92	Unified memory in HOOMD-blue improves node-level strong scaling. Computational Materials Science, 2020, 173, 109359.	1.4	6
93	Assembly of nanocrystal clusters by solvent evaporation: icosahedral order and the breakdown of the Maxwell regime. Soft Matter, 2020, 16, 7350-7358.	1.2	6
94	Scale-free, programmable design of morphable chain loops of kilobots and colloidal motors. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 8700-8710.	3.3	6
95	On the Thermodynamic Stability of Binary Superlattices of Polystyrene-Functionalized Nanocrystals. Macromolecules, 2020, 53, 9929-9942.	2.2	6
96	Calculation of critical nucleation rates by the persistent embryo method: application to quasi hard sphere models. Soft Matter, 2018, 14, 9185-9193.	1.2	5
97	Designing active particles for colloidal microstructure manipulation <i>via</i> strain field alchemy. Soft Matter, 2019, 15, 6086-6096.	1.2	5
98	Sculpting crystals one Burgers vector at a time: Toward colloidal lattice robot swarms. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	5
99	Accelerated annealing of colloidal crystal monolayers by means of cyclically applied electric fields. Scientific Reports, 2021, 11, 11042.	1.6	5
100	rowan: A Python package for working with quaternions. Journal of Open Source Software, 2018, 3, 787.	2.0	5
101	Topological order in densely packed anisotropic colloids. Physical Review E, 2019, 100, 032608.	0.8	3
102	Pinning dislocations in colloidal crystals with active particles that seek stacking faults. Soft Matter, 2020, 16, 4182-4191.	1.2	3
103	The role of complementary shape in protein dimerization. Soft Matter, 2021, 17, 7376-7383.	1.2	3
104	A route to hierarchical assembly of colloidal diamond. Soft Matter, 2022, 18, 304-311.	1.2	3
105	Structural Color Spectral Response of Dense Structures of Discoidal Particles Generated by Evaporative Assembly. Journal of Physical Chemistry B, 2022, 126, 1315-1324.	1.2	3
106	Fluctuations of Stiff Polymers and Cell Mechanics. , 0, , .		2
107	Principle of corresponding states for hard polyhedron fluids. Molecular Physics, 2019, 117, 3518-3526.	0.8	2
108	Particle shape tunes fragility in hard polyhedron glass-formers. Soft Matter, 2021, 17, 600-610.	1.2	2

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109	Formation of a single quasicrystal upon collision of multiple grains. Nature Communications, 2021, 12, 5790.	5.8	2
110	The alchemical energy landscape for a pentameric cluster. Journal of Chemical Physics, 2020, 152, 014106.	1.2	2
111	Inverse design of isotropic pair potentials using digital alchemy with a generalized Fourier potential. European Physical Journal B, 2021, 94, 1.	0.6	2
112	Nanocomposite tectons as unifying systems for nanoparticle assembly. Soft Matter, 2022, 18, 2176-2192.	1.2	2
113	DYNAMICS OF STICKY POLYMER SOLUTIONS. , 2008, , .		1
114	Synthesizable nanoparticle eigenshapes for colloidal crystals. Nanoscale, 2021, 13, 13301-13309.	2.8	0