

Jens Glaser

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

109
papers

8,335
citations

37
h-index

91
g-index

116
ext. papers

9,466
ext. citations

8.1
avg, IF

6.58
L-index

#	Paper	IF	Citations
109	The emergence of valency in colloidal crystals through electron equivalents.. <i>Nature Materials</i> , 2022	27	10
108	Scaling SQL to the Supercomputer for Interactive Analysis of Simulation Data. <i>Communications in Computer and Information Science</i> , 2022 , 327-339	0.3	
107	Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor.. <i>ACS Pharmacology and Translational Science</i> , 2022 , 5, 255-265	5.9	1
106	Tuning Stoichiometry to Promote Formation of Binary Colloidal Superlattices.. <i>Physical Review Letters</i> , 2022 , 128, 188001	7.4	0
105	Inverse design of isotropic pair potentials using digital alchemy with a generalized Fourier potential. <i>European Physical Journal B</i> , 2021 , 94, 1	1.2	0
104	Effect of Particles of Irregular Size on the Microstructure and Structural Color of Self-Assembled Colloidal Crystals. <i>Langmuir</i> , 2021 , 37, 13300-13308	4	2
103	Formation of a single quasicrystal upon collision of multiple grains. <i>Nature Communications</i> , 2021 , 12, 5790	17.4	0
102	High-throughput virtual laboratory for drug discovery using massive datasets. <i>International Journal of High Performance Computing Applications</i> , 2021 , 35, 452-468	1.8	2
101	Moving beyond the constraints of chemistry via crystal structure discovery with isotropic multiwell pair potentials. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021 , 118,	11.5	4
100	Accelerated annealing of colloidal crystal monolayers by means of cyclically applied electric fields. <i>Scientific Reports</i> , 2021 , 11, 11042	4.9	1
99	Unexpected Dependence of Photonic Band Gap Size on Randomness in Self-Assembled Colloidal Crystals. <i>Physical Review Letters</i> , 2021 , 126, 208002	7.4	1
98	Anisotropic nanocrystal shape and ligand design for co-assembly. <i>Science Advances</i> , 2021 , 7,	14.3	5
97	Supercomputing Pipelines Search for Therapeutics Against COVID-19. <i>Computing in Science and Engineering</i> , 2021 , 23, 7-16	1.5	6
96	Particle shape tunes fragility in hard polyhedron glass-formers. <i>Soft Matter</i> , 2021 , 17, 600-610	3.6	1
95	Sculpting crystals one Burgers vector at a time: Toward colloidal lattice robot swarms. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021 , 118,	11.5	2
94	Synthesizable nanoparticle eigenshapes for colloidal crystals. <i>Nanoscale</i> , 2021 , 13, 13301-13309	7.7	
93	The role of complementary shape in protein dimerization. <i>Soft Matter</i> , 2021 , 17, 7376-7383	3.6	0

92	Open-source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. <i>AICHE Journal</i> , 2021 , 67, e17206	3.6	6
91	Thermodynamic Equilibrium of Binary Nanocrystal Superlattices. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 18936-18945	3.8	1
90	Shape-driven entropic self-assembly of an open, reconfigurable, binary host-guest colloidal crystal. <i>Soft Matter</i> , 2021 , 17, 2840-2848	3.6	3
89	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 5832-5852	6.1	71
88	Assembly of nanocrystal clusters by solvent evaporation: icosahedral order and the breakdown of the Maxwell regime. <i>Soft Matter</i> , 2020 , 16, 7350-7358	3.6	3
87	freud: A software suite for high throughput analysis of particle simulation data. <i>Computer Physics Communications</i> , 2020 , 254, 107275	4.2	42
86	Phase separation and state oscillation of active inertial particles. <i>Soft Matter</i> , 2020 , 16, 2847-2853	3.6	8
85	Efficient Phase Diagram Sampling by Active Learning. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 1275-1284	3.4	22
84	Effect of Defective Microstructure and Film Thickness on the Reflective Structural Color of Self-Assembled Colloidal Crystals. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 9842-9850	9.5	9
83	Scale-free, programmable design of morphable chain loops of kilobots and colloidal motors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 8700-8710	11.5	1
82	The alchemical energy landscape for a pentameric cluster. <i>Journal of Chemical Physics</i> , 2020 , 152, 014106	6.9	2
81	On the Thermodynamic Stability of Binary Superlattices of Polystyrene-Functionalized Nanocrystals. <i>Macromolecules</i> , 2020 , 53, 9929-9942	5.5	2
80	Pressure in rigid body molecular dynamics. <i>Computational Materials Science</i> , 2020 , 173, 109430	3.2	9
79	HOOMD-blue: A Python package for high-performance molecular dynamics and hard particle Monte Carlo simulations. <i>Computational Materials Science</i> , 2020 , 173, 109363	3.2	115
78	Unified memory in HOOMD-blue improves node-level strong scaling. <i>Computational Materials Science</i> , 2020 , 173, 109359	3.2	4
77	A mean-field approach to simulating anisotropic particles. <i>Journal of Chemical Physics</i> , 2020 , 153, 084106	6.9	2
76	Pinning dislocations in colloidal crystals with active particles that seek stacking faults. <i>Soft Matter</i> , 2020 , 16, 4182-4191	3.6	1
75	FCC \leftrightarrow BCC Phase Transitions in Convex and Concave Hard Particle Systems. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 9038-9043	3.4	6

74	Colloidal fibers and rings by cooperative assembly. <i>Nature Communications</i> , 2019 , 10, 3936	17.4	31
73	Identity crisis in alchemical space drives the entropic colloidal glass transition. <i>Nature Communications</i> , 2019 , 10, 64	17.4	12
72	Phase behavior and design rules for plastic colloidal crystals of hard polyhedra via consideration of directional entropic forces. <i>Soft Matter</i> , 2019 , 15, 5380-5389	3.6	6
71	Hierarchical self-assembly of hard cube derivatives. <i>Soft Matter</i> , 2019 , 15, 3733-3739	3.6	3
70	Supraparticle Nanoassemblies with Enzymes. <i>Chemistry of Materials</i> , 2019 , 31, 7493-7500	9.6	13
69	The entropic bond in colloidal crystals. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 16703-16710	11.5	21
68	Designing active particles for colloidal microstructure manipulation via strain field alchemy. <i>Soft Matter</i> , 2019 , 15, 6086-6096	3.6	4
67	Entropic colloidal crystallization pathways via fluid-fluid transitions and multidimensional prenucleation motifs. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 14843-14851	11.5	38
66	Principle of corresponding states for hard polyhedron fluids. <i>Molecular Physics</i> , 2019 , 117, 3518-3526	1.7	2
65	Influence of Softness on the Stability of Binary Colloidal Crystals. <i>ACS Nano</i> , 2019 , 13, 13829-13842	16.7	23
64	Alchemical molecular dynamics for inverse design. <i>Molecular Physics</i> , 2019 , 117, 3968-3980	1.7	7
63	Topological order in densely packed anisotropic colloids. <i>Physical Review E</i> , 2019 , 100, 032608	2.4	2
62	Dendrimer Ligand Directed Nanoplate Assembly. <i>ACS Nano</i> , 2019 , 13, 14241-14251	16.7	10
61	Supercharging enables organized assembly of synthetic biomolecules. <i>Nature Chemistry</i> , 2019 , 11, 204-212	7.6	48
60	How to Professionally Develop Reusable Scientific Software And When Not To. <i>Computing in Science and Engineering</i> , 2019 , 21, 66-79	1.5	6
59	Shapes within shapes: how particles arrange inside a cavity. <i>Soft Matter</i> , 2018 , 14, 3012-3017	3.6	6
58	Implementation of metal-friendly EAM/FS-type semi-empirical potentials in HOOMD-blue: A GPU-accelerated molecular dynamics software. <i>Journal of Computational Physics</i> , 2018 , 359, 352-360	4.1	6
57	Simple data and workflow management with the signac framework. <i>Computational Materials Science</i> , 2018 , 146, 220-229	3.2	62

56	Ordered Networks of Gold Nanoparticles Crosslinked by Dithiol-Oligomers. <i>Particle and Particle Systems Characterization</i> , 2018 , 35, 1800097	3.1	5
55	Strain fields in repulsive colloidal crystals. <i>Physical Review Materials</i> , 2018 , 2,	3.2	8
54	rowan: A Python package for working with quaternions. <i>Journal of Open Source Software</i> , 2018 , 3, 787	5.2	4
53	Calculation of critical nucleation rates by the persistent embryo method: application to quasi hard sphere models. <i>Soft Matter</i> , 2018 , 14, 9185-9193	3.6	5
52	Inverse design of simple pair potentials for the self-assembly of complex structures. <i>Journal of Chemical Physics</i> , 2018 , 149, 204102	3.9	24
51	Why large icosahedral viruses need scaffolding proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 10971-10976	11.5	47
50	Universal folding pathways of polyhedron nets. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E6690-E6696	11.5	9
49	Shape-dependent ordering of gold nanocrystals into large-scale superlattices. <i>Nature Communications</i> , 2017 , 8, 14038	17.4	114
48	GPU accelerated Discrete Element Method (DEM) molecular dynamics for conservative, faceted particle simulations. <i>Journal of Computational Physics</i> , 2017 , 334, 460-467	4.1	26
47	Clathrate colloidal crystals. <i>Science</i> , 2017 , 355, 931-935	33.3	121
46	Non-close-packed three-dimensional quasicrystals. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 234005.8	5.8	18
45	Capping Ligand Vortices as "Atomic Orbitals" in Nanocrystal Self-Assembly. <i>ACS Nano</i> , 2017 , 11, 11273-11282	11.2	33
44	Tunable emergent structures and traveling waves in mixtures of passive and contact-triggered-active particles. <i>Soft Matter</i> , 2017 , 13, 6332-6339	3.6	7
43	Shape and Symmetry Determine Two-Dimensional Melting Transitions of Hard Regular Polygons. <i>Physical Review X</i> , 2017 , 7,	9.1	38
42	Quasicrystalline nanocrystal superlattice with partial matching rules. <i>Nature Materials</i> , 2017 , 16, 214-219	27	96
41	Using depletion to control colloidal crystal assemblies of hard cuboctahedra. <i>Soft Matter</i> , 2016 , 12, 5199-5204	3.204	23
40	Efficient neighbor list calculation for molecular simulation of colloidal systems using graphics processing units. <i>Computer Physics Communications</i> , 2016 , 203, 45-52	4.2	35
39	Scalable Metropolis Monte Carlo for simulation of hard shapes. <i>Computer Physics Communications</i> , 2016 , 204, 21-30	4.2	50

38	Universal Phenomenology of Symmetric Diblock Copolymers near the OrderDisorder Transition. <i>Macromolecules</i> , 2015 , 48, 819-839	5.5	69
37	Shape allophiles improve entropic assembly. <i>Soft Matter</i> , 2015 , 11, 7250-6	3.6	13
36	Strong scaling of general-purpose molecular dynamics simulations on GPUs. <i>Computer Physics Communications</i> , 2015 , 192, 97-107	4.2	441
35	Metastable orientational order of colloidal discoids. <i>Nature Communications</i> , 2015 , 6, 8507	17.4	28
34	Computational self-assembly of a one-component icosahedral quasicrystal. <i>Nature Materials</i> , 2015 , 14, 109-16	27	110
33	Rational design of nanomaterials from assembly and reconfigurability of polymer-tethered nanoparticles. <i>MRS Communications</i> , 2015 , 5, 397-406	2.7	30
32	A parallel algorithm for implicit depletant simulations. <i>Journal of Chemical Physics</i> , 2015 , 143, 184110	3.9	13
31	Simultaneous Nano- and Microscale Control of Nanofibrous Microspheres Self-Assembled from Star-Shaped Polymers. <i>Advanced Materials</i> , 2015 , 27, 3947-52	24	55
30	Binding kinetics of lock and key colloids. <i>Journal of Chemical Physics</i> , 2015 , 142, 174909	3.9	28
29	Terminal supraparticle assemblies from similarly charged protein molecules and nanoparticles. <i>Nature Communications</i> , 2014 , 5, 3593	17.4	81
28	Understanding shape entropy through local dense packing. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, E4812-21	11.5	159
27	Collective and Single-Chain Correlations in Disordered Melts of Symmetric Diblock Copolymers: Quantitative Comparison of Simulations and Theory. <i>Macromolecules</i> , 2014 , 47, 851-869	5.5	44
26	Entropically patchy particles: engineering valence through shape entropy. <i>ACS Nano</i> , 2014 , 8, 931-40	16.7	143
25	Universality of block copolymer melts. <i>Physical Review Letters</i> , 2014 , 113, 068302	7.4	84
24	Massively parallel Monte Carlo for many-particle simulations on GPUs. <i>Journal of Computational Physics</i> , 2013 , 254, 27-38	4.1	48
23	Shape alloys of nanorods and nanospheres from self-assembly. <i>Nano Letters</i> , 2013 , 13, 4980-8	11.5	87
22	Competition of shape and interaction patchiness for self-assembling nanoplates. <i>Nature Chemistry</i> , 2013 , 5, 466-73	17.6	253
21	A directional entropic force approach to assemble anisotropic nanoparticles into superlattices. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 13980-4	16.4	80

20	Folding and stability of helical bundle proteins from coarse-grained models. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013 , 81, 1200-11	4.2	8
19	Thermal and athermal three-dimensional swarms of self-propelled particles. <i>Physical Review E</i> , 2012 , 86, 011136	2.4	17
18	Test of a scaling hypothesis for the structure factor of disordered diblock copolymer melts. <i>Soft Matter</i> , 2012 , 8, 11310	3.6	30
17	Crystalline assemblies and densest packings of a family of truncated tetrahedra and the role of directional entropic forces. <i>ACS Nano</i> , 2012 , 6, 609-14	16.7	155
16	Predictive self-assembly of polyhedra into complex structures. <i>Science</i> , 2012 , 337, 453-7	33.3	746
15	Role of isostaticity and load-bearing microstructure in the elasticity of yielded colloidal gels. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 16029-34	11.5	111
14	Pseudo-random number generation for Brownian Dynamics and Dissipative Particle Dynamics simulations on GPU devices. <i>Journal of Computational Physics</i> , 2011 , 230, 7191-7201	4.1	115
13	Rigid body constraints realized in massively-parallel molecular dynamics on graphics processing units. <i>Computer Physics Communications</i> , 2011 , 182, 2307-2313	4.2	125
12	Generalised Einstein relation for hot Brownian motion. <i>Europhysics Letters</i> , 2011 , 96, 60009	1.6	26
11	Tube-width fluctuations of entangled stiff polymers. <i>Physical Review E</i> , 2011 , 84, 051801	2.4	11
10	Phase diagram of hard tetrahedra. <i>Journal of Chemical Physics</i> , 2011 , 135, 194101	3.9	67
9	Fluctuations of Stiff Polymers and Cell Mechanics 2010 ,		1
8	Tube width fluctuations in F-actin solutions. <i>Physical Review Letters</i> , 2010 , 105, 037801	7.4	27
7	Stability of the double gyroid phase to nanoparticle polydispersity in polymer-tethered nanosphere systems. <i>Soft Matter</i> , 2010 , 6, 1693	3.6	40
6	Dynamic structure factor of a stiff polymer in a glassy solution. <i>European Physical Journal E</i> , 2008 , 26, 123-36	1.5	9
5	Anisotropy of building blocks and their assembly into complex structures. <i>Nature Materials</i> , 2007 , 6, 557-562	22.0	2201
4	The glassy wormlike chain. <i>New Journal of Physics</i> , 2007 , 9, 416-416	2.9	60
3	Glass transition and rheological redundancy in F-actin solutions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 20199-203	11.5	107

- 2 Self-assembly of CdTe nanocrystals into free-floating sheets. *Science*, **2006**, 314, 274-8 33.3 772
- 1 Self-Assembly of Patchy Particles. *Nano Letters*, **2004**, 4, 1407-1413 11.5 631