Mark A Miller

List of Publications by Year
in descending order

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Version: 2024-02-01

55 papers	3,498 citations	159358 30 h-index	168136 53 g-index
56 all docs	56 docs citations	56 times ranked	2602 citing authors

#	Article	IF	Citations
1	Archetypal energy landscapes. Nature, 1998, 394, 758-760.	13.7	528
2	The double-funnel energy landscape of the 38-atom Lennard-Jones cluster. Journal of Chemical Physics, 1999, 110, 6896-6906.	1.2	279
3	Evolution of the potential energy surface with size for Lennard-Jones clusters. Journal of Chemical Physics, 1999, 111, 8417-8428.	1.2	222
4	Thermodynamics and the global optimization of Lennard-Jones clusters. Journal of Chemical Physics, 1998, 109, 8143-8153.	1.2	178
5	Reversible self-assembly of patchy particles into monodisperse icosahedral clusters. Journal of Chemical Physics, 2007, 127, 085106.	1.2	176
6	Energy Landscapes: From Clusters to Biomolecules. Advances in Chemical Physics, 2007, , 1-111.	0.3	153
7	Phase diagram of the adhesive hard sphere fluid. Journal of Chemical Physics, 2004, 121, 535.	1.2	137
8	The formation of cyclic water complexes by sequential ring insertion: Experiment and theory. Journal of Chemical Physics, 2002, 117, 1109-1122.	1.2	134
9	Competition of Percolation and Phase Separation in a Fluid of Adhesive Hard Spheres. Physical Review Letters, 2003, 90, 135702.	2.9	130
10	Energy landscape of a model protein. Journal of Chemical Physics, 1999, 111, 6610-6616.	1.2	115
11	Structural relaxation in Morse clusters: Energy landscapes. Journal of Chemical Physics, 1999, 110, 328-334.	1.2	114
12	Depletion-Induced Percolation in Networks of Nanorods. Physical Review Letters, 2007, 98, 108303.	2.9	104
13	Structural relaxation in atomic clusters: Master equation dynamics. Physical Review E, 1999, 60, 3701-3718.	0.8	86
14	Role of Configurational Gating in Intracomplex Electron Transfer from Cytochrome c to the Radical Cation in Cytochrome c Peroxidase. Biochemistry, 1999, 38, 6846-6854.	1.2	70
15	Knot theory in modern chemistry. Chemical Society Reviews, 2016, 45, 6432-6448.	18.7	70
16	The vanishing limit of the square-well fluid: The adhesive hard-sphere model as a reference system. Journal of Chemical Physics, 2008, 128, 134513.	1.2	67
17	Design of a Rutheniumâ"CytochromecDerivative To Measure Electron Transfer to the Radical Cation and Oxyferryl Heme in CytochromecPeroxidaseâ€. Biochemistry, 1996, 35, 15107-15119.	1.2	64
18	Percolation in suspensions of hard nanoparticles: From spheres to needles. Europhysics Letters, 2015, 111, 56004.	0.7	61

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19	Why Is It So Difficult To Simulate Entropies, Free Energies, and Their Differences?. Accounts of Chemical Research, 2001, 34, 607-614.	7.6	53
20	Simulating colloids with BaxterÂs adhesive hard sphere model. Journal of Physics Condensed Matter, 2004, 16, S4901-S4912.	0.7	52
21	Reversible gelation and dynamical arrest of dipolar colloids. Europhysics Letters, 2007, 78, 26002.	0.7	52
22	Patchy sticky hard spheres: Analytical study and Monte Carlo simulations. Journal of Chemical Physics, 2007, 127, 234507.	1.2	46
23	Dynamical arrest in low density dipolar colloidal gels. Journal of Chemical Physics, 2009, 130, 114507.	1.2	46
24	Identifying the Physiological Electron Transfer Site of CytochromecPeroxidase by Structure-Based Engineeringâ€. Biochemistry, 1996, 35, 667-673.	1.2	44
25	Novel Structural Motifs in Clusters of Dipolar Spheres:â€‰ Knots, Links, and Coils. Journal of Physical Chemistry B, 2005, 109, 23109-23112.	1.2	43
26	Efficient free energy calculations by variationally optimized metric scaling: Concepts and applications to the volume dependence of cluster free energies and to solidâ€“solid phase transitions. Journal of Chemical Physics, 2000, 113, 7035-7046.	1.2	42
27	Isomerization dynamics and ergodicity in Ar7. Journal of Chemical Physics, 1997, 107, 8568-8574.	1.2	39
28	Importance of Metastable States in the Free Energy Landscapes of Polypeptide Chains. Physical Review Letters, 2007, 99, 178104.	2.9	39
29	Automated Coarse-Grained Mapping Algorithm for the Martini Force Field and Benchmarks for Membraneâ€“Water Partitioning. Journal of Chemical Theory and Computation, 2021, 17, 5777-5791.	2.3	35
30	Energy landscapes, structural topologies and rearrangement mechanisms in clusters of dipolar particles. Soft Matter, 2013, 9, 5407.	1.2	32
31	Should one adjust the maximum step size in a Metropolis Monte Carlo simulation?. Chemical Physics Letters, 2000, 331, 278-284.	1.2	31
32	Crystallization of Deformable Spherical Colloids. Physical Review Letters, 2010, 105, 088305.	2.9	30
33	On structural correlations in the percolation of hard-core particles. Journal of Chemical Physics, 2009, 131, 066101.	1.2	22
34	Quantification of Stereochemical Communication in Metalâ€“Organic Assemblies. Angewandte Chemie - International Edition, 2016, 55, 10616-10620.	7.2	21
35	Design strategies for self-assembly of discrete targets. Journal of Chemical Physics, 2015, 143, 044905.	1.2	19
36	Tunneling conductivity in composites of attractive colloids. Journal of Chemical Physics, 2012, 136, 164903.	1.2	16

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37	Continuum percolation of polydisperse rods in quadrupole fields: Theory and simulations. Journal of Chemical Physics, 2018, 148, 034903.	1.2	16
38	Controlling the Folding and Substrate-Binding of Proteins Using Polymer Brushes. Physical Review Letters, 2012, 108, 208104.	2.9	14
39	Depletion-interaction effects on the tunneling conductivity of nanorod suspensions. Physical Review E, 2013, 88, 042140.	0.8	14
40	Optimising minimal building blocks for addressable self-assembly. Soft Matter, 2017, 13, 7780-7792.	1.2	13
41	Structure, rearrangements and evaporation of rotating atomic clusters. Molecular Physics, 1996, 89, 533-554.	0.8	11
42	Control of Superselectivity by Crowding in Three-Dimensional Hosts. Physical Review Letters, 2021, 126, 028002.	2.9	9
43	Structural trends in clusters of quadrupolar spheres. Molecular Physics, 2008, 106, 1655-1664.	0.8	8
44	Density Functional Theory for Baxterâ€™s Sticky Hard Spheres in Confinement. Physical Review Letters, 2012, 108, 047801.	2.9	8
45	Structure and stability of charged clusters. Journal of Physics Condensed Matter, 2012, 24, 284130.	0.7	8
46	Dynamics and thermodynamics of decay in charged clusters. Molecular Physics, 2015, 113, 2428-2434.	0.8	8
47	Quantification of Stereochemical Communication in Metalâ€“Organic Assemblies. Angewandte Chemie, 2016, 128, 10774-10778.	1.6	8
48	Phase transitions on non-uniformly curved surfaces: coupling between phase and location. Soft Matter, 2020, 16, 8069-8077.	1.2	7
49	Nucleation on a sphere: the roles of curvature, confinement and ensemble. Molecular Physics, 2018, 116, 3008-3019.	0.8	6
50	Controlling Fragment Competition on Pathways to Addressable Self-Assembly. Journal of Physical Chemistry B, 2018, 122, 9815-9825.	1.2	5
51	Nearest-neighbor connectedness theory: A general approach to continuum percolation. Physical Review E, 2021, 103, 042115.	0.8	5
52	Topological characteristics of model gels. Journal of Physics Condensed Matter, 2010, 22, 104109.	0.7	4
53	Knots in soft condensed matter. Journal of Physics Condensed Matter, 2015, 27, 350301.	0.7	2
54	Controlling polymorphism: general discussion. Faraday Discussions, 0, 235, 508-535.	1.6	2

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55	Colloidal clusters on curved surfaces. Frontiers of Nanoscience, 2022, , 129-150.	0.3	0