

# Roland Roth

## List of Publications by Year in descending order

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106  
papers

4,824  
citations

94415

37  
h-index

98792

67  
g-index

108  
all docs

108  
docs citations

108  
times ranked

2536  
citing authors

#	ARTICLE	IF	CITATIONS
1	Intrusion and extrusion of liquids in highly confining media: bridging fundamental research to applications. <i>Advances in Physics: X</i> , 2022, 7, .	4.1	9
2	Dynamical Density Functional Theory for the Drying and Stratification of Binary Colloidal Dispersions. <i>Langmuir</i> , 2021, 37, 1399-1409.	3.5	16
3	Phase behaviour of a simple fluid confined in a periodic porous material. <i>Molecular Physics</i> , 2021, 119, .	1.7	2
4	Gas-liquid phase transition in a binary mixture with an interaction that creates constant density profiles. <i>Journal of Chemical Physics</i> , 2021, 154, 204905.	3.0	3
5	Liquid-liquid phase separation in an inhomogeneous ternary colloid-polymer mixture. <i>Journal of Chemical Physics</i> , 2021, 154, 224504.	3.0	3
6	Bubble formation in nanopores: a matter of hydrophobicity, geometry, and size. <i>Advances in Physics: X</i> , 2020, 5, 1817780.	4.1	15
7	Statics and dynamics of a finite two-dimensional colloidal system with competing attractive critical Casimir and repulsive magnetic dipole interactions. <i>Physical Review E</i> , 2020, 102, 042608.	2.1	7
8	Toward a density-functional theory for the Jagla fluid. <i>Physical Review E</i> , 2020, 102, 062112.	2.1	7
9	Remnants of the disappearing critical point in chain-forming patchy fluids. <i>Journal of Chemical Physics</i> , 2020, 152, 111101.	3.0	6
10	Morphological thermodynamics for hard bodies from a controlled expansion. <i>Philosophical Magazine</i> , 2020, 100, 2614-2635.	1.6	0
11	Enhanced protein adsorption upon bulk phase separation. <i>Scientific Reports</i> , 2020, 10, 10349.	3.3	11
12	On the decay of the pair correlation function and the line of vanishing excess isothermal compressibility in simple fluids. <i>Journal of Chemical Physics</i> , 2019, 151, 014501.	3.0	14
13	Microphase separation in a two-dimensional colloidal system with competing attractive critical Casimir and repulsive magnetic dipole interactions. <i>Physical Review E</i> , 2019, 100, 052602.	2.1	12
14	Morphometric Approach to Many-Body Correlations in Hard Spheres. <i>Physical Review Letters</i> , 2019, 122, 068004.	7.8	16
15	Many-body correlations from integral geometry. <i>Physical Review E</i> , 2019, 100, 062126.	2.1	1
16	Classical density functional theory meets Monte-Carlo simulations. <i>Molecular Physics</i> , 2018, 116, 3323-3330.	1.7	3
17	Solvent-Mediated Interactions Close to the Fisher-Widom Line. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3556-3561.	2.6	6
18	Bulk dynamics of Brownian hard disks: Dynamical density functional theory versus experiments on two-dimensional colloidal hard spheres. <i>Journal of Chemical Physics</i> , 2018, 148, 104501.	3.0	22

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19	Reentrant Phase Behavior in Protein Solutions Induced by Multivalent Salts: Strong Effect of Anions $Cl^{sup>1</sup>}$ Versus $NO_3^{sup>3</sup>}$ . Journal of Physical Chemistry B, 2018, 122, 11978-11985.	2.6	33
20	Bulk structural information from density functionals for patchy particles. Journal of Chemical Physics, 2018, 149, 224503.	3.0	8
21	Nonequilibrium phase transitions of sheared colloidal microphases: Results from dynamical density functional theory. Physical Review E, 2018, 97, 062602.	2.1	16
22	Mean-field density functional theory of a nanoconfined classical, three-dimensional Heisenberg fluid. II. The interplay between molecular packing and orientational order. Journal of Chemical Physics, 2018, 149, 054704.	3.0	6
23	Thermodynamics of the hard-disk fluid at a planar hard wall: Generalized scaled-particle theory and Monte Carlo simulation. Journal of Chemical Physics, 2018, 149, 084701.	3.0	9
24	Microscopic density functional theory for monolayers of diblock copolymers. Journal of Chemical Physics, 2018, 149, 064902.	3.0	1
25	Structure factors in a two-dimensional binary colloidal hard sphere system. Molecular Physics, 2018, 116, 3245-3257.	1.7	22
26	Strong Isotope Effects on Effective Interactions and Phase Behavior in Protein Solutions in the Presence of Multivalent Ions. Journal of Physical Chemistry B, 2017, 121, 1731-1739.	2.6	38
27	Massively parallel GPU-accelerated minimization of classical density functional theory. Journal of Chemical Physics, 2017, 147, 064508.	3.0	24
28	Multivalent-Ion-Activated Protein Adsorption Reflecting Bulk Reentrant Behavior. Physical Review Letters, 2017, 119, 228001.	7.8	33
29	Phase behavior and bulk structural properties of a microphase former with anisotropic competing interactions: A density functional theory study. Physical Review E, 2017, 96, 042607.	2.1	6
30	Bubble gating in biological ion channels: A density functional theory study. Physical Review E, 2017, 95, 062407.	2.1	11
31	A numerical efficient way to minimize classical density functional theory. Journal of Chemical Physics, 2016, 144, 074105.	3.0	20
32	New developments in classical density functional theory. Journal of Physics Condensed Matter, 2016, 28, 240401.	1.8	71
33	Shells of charge: a density functional theory for charged hard spheres. Journal of Physics Condensed Matter, 2016, 28, 244006.	1.8	40
34	Structural relaxation and diffusion in a model colloid-polymer mixture: dynamical density functional theory and simulation. Journal of Physics Condensed Matter, 2016, 28, 455101.	1.8	11
35	Gyroid phase of fluids with spherically symmetric competing interactions. Physical Review E, 2016, 93, 062146.	2.1	33
36	Cation-Induced Hydration Effects Cause Lower Critical Solution Temperature Behavior in Protein Solutions. Journal of Physical Chemistry B, 2016, 120, 7731-7736.	2.6	49

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37	Density functional theory for polymeric systems in 2D. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 244010.	1.8	4
38	Modeling diffusion in colloidal suspensions by dynamical density functional theory using fundamental measure theory of hard spheres. <i>Physical Review E</i> , 2015, 92, 022151.	2.1	26
39	Communication: Dynamical density functional theory for dense suspensions of colloidal hard spheres. <i>Journal of Chemical Physics</i> , 2015, 143, 181105.	3.0	25
40	Parameterising the surface free energy and excess adsorption of a hard-sphere fluid at a planar hard wall. <i>Molecular Physics</i> , 2015, 113, 1091-1096.	1.7	5
41	Solid-liquid interfaces of ionic liquid solutions—Interfacial layering and bulk correlations. <i>Journal of Chemical Physics</i> , 2015, 142, 164707.	3.0	56
42	Fundamental measure theory for the inhomogeneous hard-sphere system based on Santos' consistent free energy. <i>Physical Review E</i> , 2015, 91, 052121.	2.1	12
43	Solvation of a sponge-like geometry. <i>Pure and Applied Chemistry</i> , 2014, 86, 173-179.	1.9	1
44	Shaping the Skin: The Interplay of Mesoscale Geometry and Corneocyte Swelling. <i>Physical Review Letters</i> , 2014, 112, 038102.	7.8	16
45	Protein cluster formation in aqueous solution in the presence of multivalent metal ions — a light scattering study. <i>Soft Matter</i> , 2014, 10, 894-902.	2.7	55
46	Domain and Interdomain Energetics Underlying Gating in Shaker -Type K V Channels. <i>Biophysical Journal</i> , 2014, 107, 1841-1852.	0.5	9
47	Effective interactions in protein—salt solutions approaching liquid—liquid phase separation. <i>Journal of Molecular Liquids</i> , 2014, 200, 20-27.	4.9	50
48	Communication: Radial distribution functions in a two-dimensional binary colloidal hard sphere system. <i>Journal of Chemical Physics</i> , 2014, 140, 161106.	3.0	59
49	Ion-activated attractive patches as a mechanism for controlled protein interactions. <i>Scientific Reports</i> , 2014, 4, 7016.	3.3	94
50	A morphometric approach for the accurate solvation thermodynamics of proteins and ligands. <i>Journal of Computational Chemistry</i> , 2013, 34, 1969-1974.	3.3	9
51	Light-induced phase transitions of colloidal monolayers with crystalline order. <i>Soft Matter</i> , 2013, 9, 9230.	2.7	24
52	Geometrical Aspects of Drying in a Capped Capillary: a DFT Study. <i>Journal of the Physical Society of Japan</i> , 2012, 81, SA009.	1.6	5
53	Evaluation of protein—ligand binding free energy focused on its entropic components. <i>Journal of Computational Chemistry</i> , 2012, 33, 550-560.	3.3	26
54	Polyhedral colloidal —rocks—™: low-dimensional networks. <i>Soft Matter</i> , 2012, 8, 1163-1167.	2.7	18

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55	The role of cluster formation and metastable liquid-liquid phase separation in protein crystallization. <i>Faraday Discussions</i> , 2012, 159, 313.	3.2	70
56	Charge-controlled metastable liquid-liquid phase separation in protein solutions as a universal pathway towards crystallization. <i>Soft Matter</i> , 2012, 8, 1313-1316.	2.7	83
57	Communication: Fundamental measure theory for hard disks: Fluid and solid. <i>Journal of Chemical Physics</i> , 2012, 136, 081101.	3.0	46
58	Fluid of discs with competing interactions. <i>Molecular Physics</i> , 2011, 109, 2897-2905.	1.7	14
59	Depletion potentials in highly size-asymmetric binary hard-sphere mixtures: Comparison of simulation results with theory. <i>Physical Review E</i> , 2011, 84, 061136.	2.1	44
60	Drying in a capped capillary. <i>Molecular Physics</i> , 2011, 109, 1159-1167.	1.7	31
61	Morphometric approach to thermodynamic quantities of solvation of complex molecules: Extension to multicomponent solvent. <i>Journal of Chemical Physics</i> , 2011, 135, 045103.	3.0	17
62	Free-energy function for discriminating the native fold of a protein from misfolded decoys. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 2161-2171.	2.6	28
63	Fundamental measure theory for hard-sphere mixtures: a review. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 063102.	1.8	446
64	Free-energy function based on an all-atom model for proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 77, 950-961.	2.6	32
65	Depletion interaction of two spheres - Full density functional theory vs. morphometric results. <i>Europhysics Letters</i> , 2009, 85, 36003.	2.0	27
66	Selectivity in binary fluid mixtures: Static and dynamical properties. <i>Physical Review E</i> , 2009, 80, 021409.	2.1	26
67	Solvation Free Energy of and Solvent Mediated Force on Proteins. <i>Biophysical Journal</i> , 2009, 96, 387a-388a.	0.5	0
68	Bubbles, Gating, and Anesthetics in Ion Channels. <i>Biophysical Journal</i> , 2008, 94, 4282-4298.	0.5	82
69	Water and ice in contact with octadecyl-trichlorosilane functionalized surfaces: A high resolution x-ray reflectivity study. <i>Journal of Chemical Physics</i> , 2008, 128, 244705.	3.0	75
70	Solvation of Proteins: Linking Thermodynamics to Geometry. <i>Physical Review Letters</i> , 2007, 99, 128101.	7.8	65
71	Experimental Observation of Structural Crossover in Binary Mixtures of Colloidal Hard Spheres. <i>Physical Review Letters</i> , 2007, 98, 198303.	7.8	42
72	Physical basis for characterizing native structures of proteins. <i>Chemical Physics Letters</i> , 2007, 437, 112-116.	2.6	37

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73	A new generalization of the Carnahan-Starling equation of state to additive mixtures of hard spheres. <i>Journal of Chemical Physics</i> , 2006, 124, 154506.	3.0	60
74	Density functional theory for hard-sphere mixtures: the White Bear version mark II. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 8413-8425.	1.8	165
75	Capillary evaporation in pores. <i>Journal of Physics Condensed Matter</i> , 2006, 18, 6517-6530.	1.8	26
76	On the energetics of protein folding in aqueous solution. <i>Chemical Physics Letters</i> , 2006, 432, 275-280.	2.6	32
77	Depletion potential between large spheres immersed in a multicomponent mixture of small spheres. <i>Journal of Chemical Physics</i> , 2006, 125, 084910.	3.0	37
78	From pair correlations to pair interactions: An exact relation in one-dimensional systems. <i>Europhysics Letters</i> , 2006, 74, 8-14.	2.0	9
79	Morphometric Approach to the Solvation Free Energy of Complex Molecules. <i>Physical Review Letters</i> , 2006, 97, 078101.	7.8	143
80	Effect of many-body interactions on the bulk and interfacial phase behavior of a model colloid-polymer mixture. <i>Physical Review E</i> , 2006, 73, 041404.	2.1	82
81	Curvature expansion of density profiles. <i>Europhysics Letters</i> , 2005, 69, 832-838.	2.0	26
82	Fluid mixtures at curved walls. <i>Journal of Physics Condensed Matter</i> , 2005, 17, S3463-S3468.	1.8	9
83	Physics of Size Selectivity. <i>Physical Review Letters</i> , 2005, 95, 247801.	7.8	56
84	Bulk and inhomogeneous mixtures of hard rods and excluded-volume polymer: A density functional approach. <i>Physical Review E</i> , 2005, 71, 011510.	2.1	9
85	Homogeneous and inhomogeneous hard-sphere mixtures: manifestations of structural crossover. <i>Molecular Physics</i> , 2005, 103, 3009-3023.	1.7	52
86	General methods for free-volume theory. <i>Journal of Chemical Physics</i> , 2005, 122, 214502.	3.0	79
87	Decay of correlation functions in hard-sphere mixtures: Structural crossover. <i>Journal of Chemical Physics</i> , 2004, 121, 7869.	3.0	41
88	Nonanalytic curvature contributions to solvation free energies: Influence of drying. <i>Journal of Chemical Physics</i> , 2004, 121, 12074-12084.	3.0	49
89	Morphological Thermodynamics of Fluids: Shape Dependence of Free Energies. <i>Physical Review Letters</i> , 2004, 93, 160601.	7.8	175
90	Wetting at curved substrates: Non-analytic behavior of interfacial properties. <i>Europhysics Letters</i> , 2003, 62, 815-821.	2.0	36

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91	The Asakura-Oosawa model in the protein limit: the role of many-body interactions. Journal of Physics Condensed Matter, 2003, 15, S3429-S3442.	1.8	38
92	Depletion potentials near geometrically structured substrates. Europhysics Letters, 2003, 63, 233-239.	2.0	39
93	Entropic wetting of a colloidal rod-sphere mixture. Europhysics Letters, 2003, 63, 549-555.	2.0	25
94	Microscopic theory of solvent-mediated long-range forces: Influence of wetting. Europhysics Letters, 2002, 59, 526-532.	2.0	21
95	Fundamental measure theory for hard-sphere mixtures revisited: the White Bear version. Journal of Physics Condensed Matter, 2002, 14, 12063-12078.	1.8	509
96	The depletion potential in non-additive hard-sphere mixtures. Europhysics Letters, 2001, 53, 271-277.	2.0	45
97	Generalized depletion potentials. Journal of Physics Condensed Matter, 2001, 13, L777-L784.	1.8	32
98	Depletion potential in hard-sphere mixtures: Theory and applications. Physical Review E, 2000, 62, 5360-5377.	2.1	283
99	Binary hard-sphere fluids near a hard wall. Physical Review E, 2000, 62, 6926-6936.	2.1	83
100	Depletion potential in hard-sphere fluids. Europhysics Letters, 1999, 47, 398-404.	2.0	88
101	Understanding Depletion Forces beyond Entropy. Physical Review Letters, 1999, 83, 3960-3963.	7.8	113
102	Depletion Forces near Curved Surfaces. Physical Review Letters, 1999, 83, 448-451.	7.8	75
103	Frustrated antiferromagnetic quantum spin chains for spin length $S > 1$ . Physical Review B, 1998, 58, 9264-9268.	3.2	25
104	Variational and density-matrix renormalization-group studies of the frustrated antiferromagnetic Heisenberg $S=1$ quantum spin chain. Physical Review B, 1997, 55, 8928-8939.	3.2	42
105	First Order Transition in the Frustrated Antiferromagnetic Heisenberg $S=1$ Quantum Spin Chain. Physical Review Letters, 1996, 77, 5142-5145.	7.8	75
106	Inside and out: surface thermodynamics from positive to negative curvature. Journal of Chemical Physics, 0, , .	3.0	1