Gren N Patey

List of Publications by Year in descending order

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28190 54797 9,447 192 55 84 citations h-index g-index papers 194 194 194 3935 docs citations times ranked citing authors all docs

#	Article	IF	Citations
1	The solution of the hypernettedâ€chain approximation for fluids of nonspherical particles. A general method with application to dipolar hard spheres. Journal of Chemical Physics, 1985, 82, 429-440.	1.2	334
2	Orientational order in simple dipolar liquids: Computer simulation of a ferroelectric nematic phase. Physical Review Letters, 1992, 68, 2043-2045.	2.9	260
3	Dielectric Constants of Fluid Models: Statistical Mechanical Theory and its Quantitative Implementation. Advances in Chemical Physics, 2007, , 183-328.	0.3	260
4	On the molecular theory of aqueous electrolyte solutions. I. The solution of the RHNC approximation for models at finite concentration. Journal of Chemical Physics, 1988, 88, 7715-7738.	1.2	227
5	Fluids of polarizable hard spheres with dipoles and tetrahedral quadrupoles Integral equation results with application to liquid water. Molecular Physics, 1982, 47, 1129-1151.	0.8	179
6	Electrical double layers. II. Monte Carlo and HNC studies of image effects. Journal of Chemical Physics, 1982, 76, 4615-4622.	1.2	167
7	Ferroelectric liquid-crystal and solid phases formed by strongly interacting dipolar soft spheres. Physical Review A, 1992, 46, 7783-7792.	1.0	157
8	The interaction of two spherical colloidal particles in electrolyte solution. An application of the hypernetted $\hat{\epsilon}$ hain approximation. Journal of Chemical Physics, 1980, 72, 5763-5771.	1.2	155
9	An integral equation theory for the dense dipolar hard-sphere fluid. Molecular Physics, 1977, 34, 427-440.	0.8	147
10	Isotropic Fluid Phases of Dipolar Hard Spheres. Physical Review Letters, 2000, 84, 115-118.	2.9	147
11	Structure and Interaction in Aqueous Ureaâ^'Trimethylamine-N-oxide Solutions. Journal of the American Chemical Society, 2007, 129, 4476-4482.	6.6	146
12	Charged hard spheres in dipolar hard sphere solvents. A model for electrolyte solutions. Journal of Chemical Physics, 1980, 72, 1887-1899.	1.2	143
13	Cavitation of a Lennardâ€Jones fluid between hard walls, and the possible relevance to the attraction measured between hydrophobic surfaces. Journal of Chemical Physics, 1993, 98, 7236-7244.	1.2	143
14	Hypernettedâ€chain closure with bridge diagrams. Asymmetric hard sphere mixtures. Journal of Chemical Physics, 1990, 92, 4970-4982.	1.2	129
15	The free energy of spheres with dipoles: Monte Carlo with multistage sampling. Chemical Physics Letters, 1973, 21, 297-300.	1.2	127
16	Structure and scattering in colloidal ferrofluids. Physical Review E, 2000, 62, 5403-5408.	0.8	125
17	The solution of the reference hypernetted-chain approximation for water-like models. Molecular Physics, 1988, 65, 1105-1119.	0.8	122
18	The thermodynamic properties of electrolyte solutions: Some formal results. Journal of Chemical Physics, 1987, 86, 5110-5116.	1.2	118

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19	A Monte Carlo study of dipolar hard spheres The pair distribution function and the dielectric constant. Molecular Physics, 1977, 34, 1077-1091.	0.8	117
20	The solution of the hypernetted chain and Percus–Yevick approximations for fluids of hard nonspherical particles. Results for hard ellipsoids of revolution. Journal of Chemical Physics, 1987, 87, 1295-1306.	1.2	106
21	On the theory and computer simulation of dipolar fluids. Molecular Physics, 1982, 45, 733-746.	0.8	96
22	Theoretical results for aqueous electrolytes. Ion–ion potentials of mean force and the soluteâ€dependent dielectric constant. Journal of Chemical Physics, 1983, 78, 5183-5190.	1.2	95
23	A Molecular Mechanism of Ice Nucleation on Model AgI Surfaces. Journal of Physical Chemistry B, 2015, 119, 9049-9055.	1.2	95
24	Integral equation approximations for dipolar fluids. Molecular Physics, 1979, 38, 219-239.	0.8	94
25	Molecular solvent model for an electrical double layer: Reference hypernettedâ€chain (RHNC) results for solvent structure at a charged surface. Journal of Chemical Physics, 1988, 88, 7826-7840.	1.2	94
26	How Crystals Nucleate and Grow in Aqueous NaCl Solution. Journal of Physical Chemistry Letters, 2013, 4, 573-578.	2.1	85
27	Molecular solutes in nematic liquid crystals: Orientational order and electric field gradients. Chemical Physics Letters, 1983, 99, 271-274.	1.2	83
28	Heterogeneous Ice Nucleation Induced by Electric Fields. Journal of Physical Chemistry Letters, 2011, 2, 2555-2559.	2.1	82
29	An investigation of the influence of solute size and insertion conditions on solvation thermodynamics. Journal of Chemical Physics, 1997, 106, 8165-8195.	1.2	80
30	Density functional theory applied to the isotropic–nematic transition in model liquid crystals. Journal of Chemical Physics, 1988, 89, 6941-6946.	1.2	78
31	lon solvation dynamics in water–methanol and water– dimethylsulfoxide mixtures. Journal of Chemical Physics, 1999, 110, 10937-10944.	1.2	77
32	On the molecular theory of aqueous electrolyte solutions. II. Structural and thermodynamic properties of different models at infinite dilution. Journal of Chemical Physics, 1988, 89, 5843-5851.	1.2	75
33	Whytert-Butyl Alcohol Associates in Aqueous Solution but Trimethylamine-N-oxide Does Not. Journal of Physical Chemistry B, 2006, 110, 10514-10518.	1.2	75
34	Interaction free energy between planar walls in dense fluids: An Ornstein-Zernike approach with results for hard-sphere, Lennard-Jones, and dipolar systems. Physical Review A, 1991, 44, 8224-8234.	1.0	74
35	Simulation of Water Adsorption on Kaolinite under Atmospheric Conditions. Journal of Physical Chemistry A, 2009, 113, 7826-7833.	1.1	73
36	Simulations of Ice Nucleation by Kaolinite (001) with Rigid and Flexible Surfaces. Journal of Physical Chemistry B, 2016, 120, 1726-1734.	1.2	73

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37	Adsorption and Structure of Water on Kaolinite Surfaces: Possible Insight into Ice Nucleation from Grand Canonical Monte Carlo Calculations. Journal of Physical Chemistry A, 2008, 112, 10708-10712.	1.1	72
38	Dynamics of molecular liquids: A comparison of different theories with application to wave vector dependent dielectric relaxation and ion solvation. Journal of Chemical Physics, 1990, 93, 1399-1411.	1.2	71
39	Orientational order in simple dipolar fluids: Density-functional theory and absolute-stability conditions. Physical Review E, 1993, 47, 506-512.	0.8	71
40	Solvation energy of ions in dipolar solvents. Journal of Chemical Physics, 1983, 79, 6294-6300.	1.2	70
41	The solution of the hypernettedâ€chain and Percus–Yevick approximations for fluids of hard spherocylinders. Journal of Chemical Physics, 1988, 89, 5861-5868.	1.2	70
42	Aggregation in dilute aqueous <i>tert</i> -butyl alcohol solutions: Insights from large-scale simulations. Journal of Chemical Physics, 2012, 137, 034509.	1.2	69
43	Fluids of dipolar hard ellipsoids: Structural properties and isotropic–nematic phase transitions. Journal of Chemical Physics, 1989, 91, 3045-3055.	1.2	68
44	Integral equation approximations for fluids of hard spheres with linear quadrupoles. Molecular Physics, 1978, 35, 1413-1428.	0.8	64
45	Molecular Dynamics Simulations of Ice Nucleation by Electric Fields. Journal of Physical Chemistry A, 2012, 116, 7057-7064.	1.1	64
46	Structure of twoâ€component clusters. Journal of Chemical Physics, 1994, 101, 2432-2445.	1.2	63
47	Structural and dynamical properties of ionic liquids: The influence of ion size disparity. Journal of Chemical Physics, 2008, 129, 064517.	1.2	63
48	NMR of deuterium in liquid crystal mixtures. Chemical Physics Letters, 1984, 107, 426-430.	1.2	62
49	The Influence of Urea and Trimethylamine-N-oxide on Hydrophobic Interactions. Journal of Physical Chemistry B, 2007, 111, 7932-7933.	1.2	62
50	Theory of the electrical double layer: Ion size effects in a molecular solvent. Journal of Chemical Physics, 1989, 91, 6367-6375.	1.2	61
51	Theoretical results for dielectric and structural properties of aqueous electrolytes. The influence of ion size and charge. Journal of Chemical Physics, 1983, 79, 4468-4474.	1.2	60
52	Rotational motion in molecular liquids. Journal of Chemical Physics, 1989, 91, 7113-7129.	1.2	60
53	The frequency dependent conductivity of electrolyte solutions. Journal of Chemical Physics, 1993, 99, 2083-2094.	1.2	59
54	Monte Carlo calculation ofy(r) for the hard-sphere fluid. Molecular Physics, 1977, 34, 1623-1628.	0.8	58

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55	Static dielectric properties of polarizable Stockmayer fluids. Physica A: Statistical Mechanics and Its Applications, 1981, 108, 14-26.	1.2	57
56	A configuration bias Monte Carlo method for water. Journal of Chemical Physics, 1995, 102, 7656-7663.	1.2	56
57	Understanding the Structure Factor and Isothermal Compressibility of Ambient Water in Terms of Local Structural Environments. Journal of Physical Chemistry B, 2012, 116, 12014-12020.	1.2	56
58	Integral equation approximations for fluids of hard spheres with dipoles and quadrupoles. Molecular Physics, 1979, 38, 1635-1654.	0.8	55
59	Modeling and structure of mercury-water interfaces. Journal of Chemical Physics, 1997, 107, 2122-2141.	1.2	54
60	Molecular dynamics simulation of the plastic phase of solid methane. Journal of Chemical Physics, 1980, 72, 5348-5356.	1.2	53
61	Evidence that crystal nucleation in aqueous NaCl solution Occurs by the two-step mechanism. Chemical Physics Letters, 2013, 587, 25-29.	1.2	53
62	lon association and condensation in primitive models of electrolyte solutions. Journal of Chemical Physics, 1999, 111, 9000-9008.	1.2	52
63	Monte Carlo simulations of the adsorption of CO2 on the MgO(100) surface. Journal of Chemical Physics, 2006, 124, 114706.	1.2	52
64	Simulations of water transport through carbon nanotubes: How different water models influence the conduction rate. Journal of Chemical Physics, 2014, 141, 18C518.	1.2	52
65	A comparison of liquid–vapor coexistence in charged hard sphere and charged hard dumbbell fluids. Journal of Chemical Physics, 1995, 103, 8299-8301.	1.2	51
66	Orientational Ordering in Spatially Disordered Dipolar Systems. Physical Review Letters, 1995, 75, 2360-2363.	2.9	51
67	An analysis of fluctuations in supercooled TIP4P/2005 water. Journal of Chemical Physics, 2013, 138, 184502.	1.2	51
68	Computer simulation and theoretical results for a polar-polarizable fluid. Molecular Physics, 1985, 55, 65-76.	0.8	50
69	Dielectric relaxation of electrolyte solutions: Is there really a kinetic dielectric decrement?. Journal of Chemical Physics, 1993, 98, 4959-4966.	1.2	50
70	Theory of ion solvation dynamics in mixed dipolar solvents. Journal of Chemical Physics, 1998, 109, 3222-3231.	1.2	49
71	The influence of water on the structural and transport properties of model ionic liquids. Journal of Chemical Physics, 2010, 132, 234510.	1,2	49
72	Coexistence and criticality of fluids with long-range potentials. Journal of Chemical Physics, 2001, 114, 399.	1.2	48

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73	Simulated conduction rates of water through a (6,6) carbon nanotube strongly depend on bulk properties of the model employed. Journal of Chemical Physics, 2016, 144, 184502.	1.2	47
74	Vapour–liquid phase transition of dipolar particles. Molecular Physics, 2009, 107, 403-413.	0.8	46
75	Structure and properties of the metal–liquid interface. Journal of Chemical Physics, 1994, 101, 6271-6280.	1.2	45
76	Ion solvation dynamics in binary mixtures. Journal of Chemical Physics, 1997, 106, 2782-2791.	1.2	45
77	Hydrophobic Interactions in Ureaâ^'Trimethylamine- <i>N</i> -oxide Solutions. Journal of Physical Chemistry B, 2008, 112, 11106-11111.	1.2	45
78	Structural and dynamical properties of ionic liquids: The influence of charge location. Journal of Chemical Physics, 2009, 130, 104506.	1.2	45
79	Liquid-vapor coexistence in fluids of dipolar hard dumbbells and spherocylinders. Physical Review E, 1999, 59, 3065-3070.	0.8	44
80	Structural and dynamical properties of ionic liquids: Competing influences of molecular properties. Journal of Chemical Physics, 2010, 132, 154504.	1.2	44
81	Molecular solvent model for an electrical double layer: Reference hypernetted chain results for potassium chloride solutions. Journal of Chemical Physics, 1989, 90, 4513-4527.	1.2	43
82	Critical comments on the nonlocal dielectric function employed in recent theories of the hydration force. Chemical Physics Letters, 1990, 172, 69-72.	1.2	43
83	Structure of the metal-aqueous electrolyte solution interface. Journal of Chemical Physics, 1997, 107, 4719-4728.	1.2	43
84	Molecular Dynamics Simulation of NaCl Dissolution. Journal of Physical Chemistry B, 2015, 119, 4275-4283.	1.2	43
85	The solution of the reference hypernetted-chain approximation for Stockmayer fluids. Molecular Physics, 1985, 55, 751-762.	0.8	42
86	Molecular solvent models of electrical double layers. Electrochimica Acta, 1991, 36, 1677-1684.	2.6	42
87	Tracer diffusion in hard sphere fluids from molecular to hydrodynamic regimes. Journal of Chemical Physics, 2006, 125, 204502.	1.2	42
88	Birth of NaCl Crystals: Insights from Molecular Simulations. Journal of Physical Chemistry B, 2016, 120, 9076-9087.	1.2	41
89	The application of integral equation theories to fluids of nonspherical particles near a uniform planar wall. Journal of Chemical Physics, 1991, 95, 5281-5288.	1.2	40
90	Microscopic theory of solvation dynamics in dipolar liquids. Journal of Chemical Physics, 1993, 99, 4926-4931.	1.2	39

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91	Ferroelectric and dipolar glass phases of noncrystalline systems. Physical Review E, 1997, 56, 562-570.	0.8	39
92	Fluids of Lennard-Jones spheres with dipoles and tetrahedral quadrupoles. Molecular Physics, 1984, 51, 333-348.	0.8	38
93	The relative motion of ions in solution. I. Microdynamical models and intermolecular dipolar spin relaxation. Journal of Chemical Physics, 1984, 80, 6253-6266.	1.2	38
94	Ferroelectric Order in Model Discotic Nematic Liquid Crystals. Physical Review Letters, 1996, 76, 239-242.	2.9	38
95	An investigation of dynamical density functional theory for solvation in simple mixtures. Journal of Chemical Physics, 1998, 108, 6378-6386.	1.2	38
96	Observations of High-Density Ferroelectric Ordered Water in Kaolinite Trenches using Monte Carlo Simulations. Journal of Physical Chemistry A, 2010, 114, 8396-8405.	1.1	38
97	Long-range attractions between solutes in near-critical fluids. Physical Review A, 1992, 45, 7621-7623.	1.0	37
98	An Accurate Equation of State for Fluids and Solids. Journal of Physical Chemistry B, 2009, 113, 11977-11987.	1.2	36
99	Ground state configurations of model molecular clusters. Journal of Chemical Physics, 1994, 100, 2213-2219.	1.2	35
100	Ice nucleation by electric surface fields of varying range and geometry. Journal of Chemical Physics, 2013, 139, 144501.	1.2	35
101	Fluctuations and local ice structure in model supercooled water. Journal of Chemical Physics, 2015, 143, 094504.	1.2	35
102	Water Adsorption on Kaolinite Surfaces Containing Trenches. Journal of Physical Chemistry A, 2010, 114, 2171-2178.	1.1	34
103	Association and Microheterogeneity in Aqueous 2-Butoxyethanol Solutions. Journal of Physical Chemistry B, 2011, 115, 15323-15331.	1.2	34
104	Simulations of Ice Nucleation by Model Agl Disks and Plates. Journal of Physical Chemistry B, 2016, 120, 2291-2299.	1.2	33
105	On the molecular theory of aqueous electrolyte solutions. III. A comparison between Born–Oppenheimer and McMillan–Mayer levels of description. Journal of Chemical Physics, 1988, 89, 7478-7484.	1.2	32
106	A theoretical study of the solid–electrolyte solution interface. I. Structure of a hard sphere ion–dipole mixture near an uncharged hard wall. Journal of Chemical Physics, 1988, 89, 4994-5009.	1.2	32
107	Solvation dynamics in electrolyte solutions. Journal of Chemical Physics, 1994, 100, 1552-1558.	1.2	32
108	Molecular solvent model for an electrical double layer: Reference hypernettedâ€chain results for ion behavior at infinite dilution. Journal of Chemical Physics, 1988, 89, 3285-3294.	1.2	31

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109	Dielectric relaxation of electrolyte solutions: Molecular dynamics and theoretical results for ions in simple dipolar solvents. Journal of Chemical Physics, 1994, 100, 8385-8391.	1.2	30
110	Integral equation theory for dipolar hard sphere fluids with fluctuating orientational order. Journal of Chemical Physics, 2000, 112, 3832-3844.	1.2	30
111	A molecular dynamics investigation of the influence of water structure on ion conduction through a carbon nanotube. Journal of Chemical Physics, 2017, 146, 074502.	1.2	30
112	Dielectric relaxation of electrolyte solutions. Journal of Chemical Physics, 1991, 94, 6795-6806.	1.2	28
113	A generalized Gaussian overlap model for fluids of anisotropic particles. Journal of Chemical Physics, 1995, 102, 9040-9047.	1.2	28
114	Ion Solvation in a Waterâ^'Urea Mixture. Journal of Physical Chemistry B, 2010, 114, 613-619.	1.2	28
115	The solution of the Percus–Yevick approximation for fluids with angleâ€dependent pair interactions. A general method with results for dipolar hard spheres. Journal of Chemical Physics, 1986, 85, 7307-7311.	1.2	27
116	Gas-liquid coexistence and demixing in systems with highly directional pair potentials. Physical Review E, 1998, 57, 5682-5686.	0.8	27
117	Ion association in model ionic fluids. Physical Review E, 1999, 60, 1063-1066.	0.8	27
118	Understanding electrofreezing in water simulations. Journal of Chemical Physics, 2014, 141, 074501.	1.2	27
119	Structure of the metalâ€electrolyte solution interface: Theoretical results for simple models. Journal of Chemical Physics, 1995, 102, 1024-1033.	1.2	26
120	Liquid crystal phases of dipolar discotic particles. Physical Review E, 1997, 55, 447-454.	0.8	26
121	Phase behavior of ionic solutions: Comparison of the primitive and explicit solvent models. Journal of Chemical Physics, 1999, 110, 1633-1637.	1.2	26
122	The interaction between macroparticles in molecular fluids. Journal of Chemical Physics, 1990, 93, 7360-7368.	1.2	25
123	On the existence of exact conditions in the theory of electrical double layers. Journal of Chemical Physics, 1992, 96, 3767-3771.	1.2	25
124	Molecular solvent model for an electrical double layer: Effects of ionic polarizability. Journal of Chemical Physics, 1993, 99, 3990-3997.	1.2	24
125	Demixing and the force between parallel plates immersed in binary liquid mixtures. Journal of Chemical Physics, 2001, 114, 7182-7188.	1.2	24
126	Molecular theory of orientationally ordered liquids: Exact formal expressions and the application of integral-equation methods with results for ferrofluids. Physical Review A, 1988, 38, 4772-4788.	1.0	23

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127	On the molecular theory of aqueous electrolyte solutions. IV. Effects of solvent polarizability. Journal of Chemical Physics, 1990, 92, 1345-1358.	1.2	23
128	Stability of binary mixtures: Supersaturation limits of aqueous alkali halide solutions. Journal of Chemical Physics, 1994, 100, 3827-3842.	1.2	23
129	Simulations of water structure and the possibility of ice nucleation on selected crystal planes of K-feldspar. Journal of Chemical Physics, 2019, 150, 214501.	1.2	23
130	Ferroelectric order in positionally frozen dipolar systems. Journal of Chemical Physics, 2001, 115, 4718-4731.	1.2	22
131	Charge Ordering Induces a Smectic Phase in Oblate Ionic Liquid Crystals. Physical Review Letters, 2010, 105, 137801.	2.9	22
132	Dielectric relaxation of dipolar liquids. Journal of Chemical Physics, 1993, 99, 2068-2073.	1.2	21
133	A configuration bias Monte Carlo method for ionic solutions. Journal of Chemical Physics, 1994, 100, 8265-8270.	1.2	21
134	Structure formation in dipolar fluids driven by rotating fields. Journal of Chemical Physics, 2000, 112, 9828-9833.	1.2	21
135	A mean field theory for fluids of multipolar particles in contact with a polarizable wall. Journal of Chemical Physics, 1992, 97, 4372-4379.	1.2	20
136	Forces between like-charged walls in electrolyte solution: Molecular solvent effects at the McMillan–Mayer level. Journal of Chemical Physics, 2000, 112, 8939-8949.	1.2	20
137	Nonequilibrium molecular dynamics simulations of a simple dipolar fluid under shear flow. Journal of Chemical Physics, 2002, 117, 2747-2761.	1.2	20
138	Melting point trends and solid phase behaviors of model salts with ion size asymmetry and distributed cation charge. Journal of Chemical Physics, 2015, 143, 024508.	1.2	20
139	Structures and rearrangements of LiCl clusters. Journal of Chemical Physics, 2006, 124, 244506.	1.2	19
140	Structural behavior of aqueous <i>t</i> -butanol solutions from large-scale molecular dynamics simulations. Journal of Chemical Physics, 2019, 150, 184504.	1.2	19
141	Unified Description of Diffusion Coefficients from Small to Large Molecules in Organic–Water Mixtures. Journal of Physical Chemistry A, 2020, 124, 2301-2308.	1.1	19
142	The relative motion of ions in solution. II. An NMR relaxation study of attractive ions in water at low ionic strength. Journal of Chemical Physics, 1984, 80, 6267-6273.	1.2	18
143	Dielectric relaxation of liquid mixtures. Journal of Chemical Physics, 1991, 94, 6785-6794.	1.2	18
144	Remarks on the forces between macroscopic particles in solution. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1996, 100, 885-888.	0.9	18

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145	Dielectric relaxation of chained ferrofluids. Journal of Chemical Physics, 2002, 116, 6731-6737.	1.2	18
146	Effects of Inorganic Ions on Ice Nucleation by the Al Surface of Kaolinite Immersed in Water. Journal of Physical Chemistry B, 2020, 124, 4605-4618.	1.2	18
147	Continuum electrostatic interactions between planar lattices of dipoles and the possible relevance to the hydration force. Physical Review A, 1991, 43, 2953-2962.	1.0	17
148	Liquid–vapor criticality in a fluid of charged hard dumbbells. Journal of Chemical Physics, 2003, 119, 7952-7956.	1.2	17
149	Water adsorption in ion-bearing nanopores. Journal of Chemical Physics, 2007, 126, 024703.	1.2	17
150	Dynamical properties of a ferroelectric nematic liquid crystal. Physical Review E, 1993, 47, 2954-2957.	0.8	15
151	First passage times of driven DNA hairpin unzipping. Physical Biology, 2005, 2, 166-174.	0.8	15
152	Comparison of simulation and experimental results for a model aqueous tert-butanol solution. Journal of Chemical Physics, 2017, 147, 024503.	1.2	15
153	Molecular Simulations of Feldspar Surfaces Interacting with Aqueous Inorganic Solutions: Interfacial Water/lon Structure and Implications for Ice Nucleation. ACS Earth and Space Chemistry, 2021, 5, 2169-2183.	1.2	15
154	Crystallization of dipolar spheres: A discussion of second-order density functional theory. Journal of Chemical Physics, 2000, 112, 10949-10956.	1.2	14
155	Structure and aggregation in model tetramethylurea solutions. Journal of Chemical Physics, 2014, 141, 064502.	1.2	14
156	Orientational order in model dipolar fluids. Physical Review E, 1999, 60, 4280-4284.	0.8	13
157	Forces between chemically patterned plates immersed in binary liquid mixtures. Journal of Chemical Physics, 2002, 117, 3391-3397.	1.2	12
158	The composition of liquid methane–nitrogen aerosols in Titan's lower atmosphere from Monte Carlo simulations. Icarus, 2011, 212, 779-789.	1.1	12
159	Mechanism of Urea Crystal Dissolution in Water from Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2018, 122, 1213-1222.	1.2	12
160	How Microscopic Features of Mineral Surfaces Critically Influence Heterogeneous Ice Nucleation. Journal of Physical Chemistry C, 2021, 125, 10723-10737.	1.5	12
161	The relative motion of ions in solution. III. An NMR relaxation study of repulsive ions in water at low ionic strength. Journal of Chemical Physics, 1985, 83, 307-311.	1.2	11
162	A Monte Carlo study of model electrorheological fluids. Journal of Chemical Physics, 1999, 111, 3278-3287.	1.2	11

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163	Forces between like-charged walls in an electrolyte solution: A comparison of McMillan–Mayer results for several models. Journal of Chemical Physics, 2000, 113, 2851-2855.	1.2	10
164	Activity coefficients of model aqueous electrolyte solutions: Sensitivity to the short range part of the interionic potential. Journal of Chemical Physics, 1991, 94, 6782-6784.	1.2	9
165	Nanoscopic Liquid Bridges between Chemically Patterned Atomistic Wallsâ€. Journal of Physical Chemistry B, 2006, 110, 3764-3772.	1.2	9
166	Crystal structures of model lithium halides in bulk phase and in clusters. Journal of Chemical Physics, 2017, 146, 154501.	1.2	9
167	How distributed charge reduces the melting points of model ionic salts. Journal of Chemical Physics, 2014, 140, 104504.	1.2	8
168	Why α-Alumina Is an Effective Ice Nucleus. Journal of Physical Chemistry C, 2019, 123, 26424-26431.	1.5	8
169	Surfactant-stabilized structures in confined liquids. Journal of Chemical Physics, 2003, 119, 8676-8685.	1.2	7
170	Surface-Induced Ordering of Nematics in an External Field: The Strong Influence of Tilted Walls. Physical Review Letters, 2004, 92, 185508.	2.9	7
171	The interaction of patterned solutes in binary solvent mixtures. Journal of Chemical Physics, 2006, 124, 094901.	1.2	7
172	Influence of Urea on <i>tert</i> -Butyl Alcohol Aggregation in Aqueous Solutions. Journal of Physical Chemistry B, 2012, 116, 4991-5001.	1.2	7
173	Unraveling the Mechanism of Ice Nucleation by Mica (001) Surfaces. Journal of Physical Chemistry C, 2021, 125, 26927-26941.	1.5	7
174	Orientational ordering and disordering of a simple dipolar fluid under shear flow. Journal of Chemical Physics, 2002, 117, 9016-9027.	1.2	6
175	Molecular dynamics simulations of a ferroelectric nematic liquid under shear flow. Journal of Chemical Physics, 2002, 117, 8551-8564.	1.2	6
176	The constant-volume heat capacity of near-critical fluids with long-range interactions: A discussion of different Monte Carlo estimates. Journal of Chemical Physics, 2003, 118, 4164-4168.	1.2	6
177	Shearing of nanoscopic bridges in two-component thin liquid layers between chemically patterned walls. Journal of Chemical Physics, 2004, 121, 6508-6517.	1.2	6
178	Nematic fluid structure in wall-field geometry. Journal of Chemical Physics, 2005, 122, 034703.	1.2	6
179	The crystallization of alkali halides from aqueous solution: An application of densityâ€functional theory. Journal of Chemical Physics, 1991, 95, 485-493.	1.2	5
180	Colloidal interactions in nematic fluids. Physical Review E, 2006, 73, 020701.	0.8	5

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181	Bridging the gap between phenomenology and microscopic theory: Asymptotes in nematic colloids. Physical Review E, 2008, 77, 041701.	0.8	5
182	Constant-volume heat capacity in a near-critical fluid from Monte Carlo simulations. Journal of Chemical Physics, 2004, 121, 8956-8959.	1.2	4
183	Colloid-induced structure in liquid crystal media. Journal of Chemical Physics, 2005, 122, 124907.	1.2	4
184	Structure and adsorption of water in nonuniform cylindrical nanopores. Journal of Chemical Physics, 2010, 133, 224703.	1.2	4
185	Solvent phase behavior and the interaction of uniform and patterned solutes. Journal of Chemical Physics, 2005, 123, 194505.	1.2	3
186	The influence of ion hydration on nucleation and growth of LiF crystals in aqueous solution. Journal of Chemical Physics, 2018, 148, 024507.	1.2	3
187	Ice Nucleation by the Primary Prism Face of Silver Iodide. Journal of Physical Chemistry C, 2022, 126, 6716-6723.	1.5	3
188	Nematic-fluid structure in wall-field geometry. II. The direct correlation function. Journal of Chemical Physics, 2006, 125, 034903.	1.2	2
189	Analysis of the relative stability of lithium halide crystal structures: Density functional theory and classical models. Journal of Chemical Physics, 2021, 154, 184507.	1.2	2
190	A simple model of spin transitions in polymeric materials. Journal of Physics Condensed Matter, 1998, 10, 10909-10917.	0.7	1
191	Wall–colloid interaction in nematic solvents: external field effects. Journal of Physics Condensed Matter, 2009, 21, 245105.	0.7	1
192	The composition of ternary N2/CH4/C2H6 cloud droplets under Titan conditions: Monte Carlo simulations and experiment. Molecular Physics, 2013, 111, 2233-2242.	0.8	1