Gren N Patey

List of Publications by Citations

191 papers	8,626 citations	54 h-index	81 g-index
194 ext. papers	8,980 ext. citations	3.6 avg, IF	6.2 L-index

#	Paper	IF	Citations
191	The solution of the hypernetted-chain approximation for fluids of nonspherical particles. A general method with application to dipolar hard spheres. *Journal of Chemical Physics*, **1985**, 82, 429-440	3.9	315
190	Orientational order in simple dipolar liquids: Computer simulation of a ferroelectric nematic phase. *Physical Review Letters*, **1992**, 68, 2043-2045	7.4	249
189	Dielectric Constants of Fluid Models: Statistical Mechanical Theory and its Quantitative Implementation. *Advances in Chemical Physics*, **2007**, 183-328		238
188	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	3.9	213
187	Fluids of polarizable hard spheres with dipoles and tetrahedral quadrupoles Integral equation results with application to liquid water. *Molecular Physics*, **1982**, 47, 1129-1151	1.7	173
186	Electrical double layers. II. Monte Carlo and HNC studies of image effects. *Journal of Chemical Physics*, **1982**, 76, 4615-4622	3.9	158
185	Ferroelectric liquid-crystal and solid phases formed by strongly interacting dipolar soft spheres. *Physical Review A*, **1992**, 46, 7783-7792	2.6	153
184	The interaction of two spherical colloidal particles in electrolyte solution. An application of the hypernetted-chain approximation. *Journal of Chemical Physics*, **1980**, 72, 5763-5771	3.9	148
183	Isotropic fluid phases of dipolar hard spheres. *Physical Review Letters*, **2000**, 84, 115-8	7.4	140
182	Charged hard spheres in dipolar hard sphere solvents. A model for electrolyte solutions. *Journal of Chemical Physics*, **1980**, 72, 1887-1899	3.9	138
181	An integral equation theory for the dense dipolar hard-sphere fluid. *Molecular Physics*, **1977**, 34, 427-440	1.7	137
180	Cavitation of a Lennard-Jones fluid between hard walls, and the possible relevance to the attraction measured between hydrophobic surfaces. *Journal of Chemical Physics*, **1993**, 98, 7236-7244	3.9	136
179	Structure and interaction in aqueous urea-trimethylamine-N-oxide solutions. *Journal of the American Chemical Society*, **2007**, 129, 4476-82	16.4	129
178	Hypernetted-chain closure with bridge diagrams. Asymmetric hard sphere mixtures. *Journal of Chemical Physics*, **1990**, 92, 4970-4982	3.9	122
177	The solution of the reference hypernetted-chain approximation for water-like models. *Molecular Physics*, **1988**, 65, 1105-1119	1.7	118
176	Structure and scattering in colloidal ferrofluids. *Physical Review E*, **2000**, 62, 5403-8	2.4	116
175	A Monte Carlo study of dipolar hard spheres The pair distribution function and the dielectric constant. *Molecular Physics*, **1977**, 34, 1077-1091	1.7	114

174	The free energy of spheres with dipoles: Monte Carlo with multistage sampling. *Chemical Physics Letters*, **1973**, 21, 297-300	2.5	107
173	The thermodynamic properties of electrolyte solutions: Some formal results. *Journal of Chemical Physics*, **1987**, 86, 5110-5116	3.9	105
172	The solution of the hypernetted chain and Percus□evick approximations for fluids of hard nonspherical particles. Results for hard ellipsoids of revolution. *Journal of Chemical Physics*, **1987**, 87, 1295-1306	3.9	99
171	On the theory and computer simulation of dipolar fluids. *Molecular Physics*, **1982**, 45, 733-746	1.7	92
170	Molecular solvent model for an electrical double layer: Reference hypernetted-chain (RHNC) results for solvent structure at a charged surface. *Journal of Chemical Physics*, **1988**, 88, 7826-7840	3.9	91
169	Theoretical results for aqueous electrolytes. Ion□on potentials of mean force and the solute-dependent dielectric constant. *Journal of Chemical Physics*, **1983**, 78, 5183-5190	3.9	88
168	Integral equation approximations for dipolar fluids. *Molecular Physics*, **1979**, 38, 219-239	1.7	88
167	Molecular solutes in nematic liquid crystals: Orientational order and electric field gradients. *Chemical Physics Letters*, **1983**, 99, 271-274	2.5	80
166	A Molecular Mechanism of Ice Nucleation on Model AgI Surfaces. *Journal of Physical Chemistry B*, **2015**, 119, 9049-55	3.4	77
165	An investigation of the influence of solute size and insertion conditions on solvation thermodynamics. *Journal of Chemical Physics*, **1997**, 106, 8165-8195	3.9	76
164	Ion solvation dynamics in water□ethanol and water□dimethylsulfoxide mixtures. *Journal of Chemical Physics*, **1999**, 110, 10937-10944	3.9	75
163	Density functional theory applied to the isotropic□ematic transition in model liquid crystals. *Journal of Chemical Physics*, **1988**, 89, 6941-6946	3.9	75
162	Orientational order in simple dipolar fluids: Density-functional theory and absolute-stability conditions. *Physical Review E*, **1993**, 47, 506-512	2.4	71
161	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	3.9	71
160	Heterogeneous Ice Nucleation Induced by Electric Fields. *Journal of Physical Chemistry Letters*, **2011** , 2, 2555-2559	6.4	69
159	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	3.9	69
158	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	2.6	68
157	The solution of the hypernetted-chain and Percus□evick approximations for fluids of hard spherocylinders. *Journal of Chemical Physics*, **1988**, 89, 5861-5868	3.9	67

156	Why tert-butyl alcohol associates in aqueous solution but trimethylamine-N-oxide does not. *Journal of Physical Chemistry B*, **2006**, 110, 10514-8	3.4	66
155	Fluids of dipolar hard ellipsoids: Structural properties and isotropic□ematic phase transitions. *Journal of Chemical Physics*, **1989**, 91, 3045-3055	3.9	65
154	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, 10708-12	2.8	64
153	How Crystals Nucleate and Grow in Aqueous NaCl Solution. *Journal of Physical Chemistry Letters*, **2013**, 4, 573-8	6.4	63
152	Solvation energy of ions in dipolar solvents. *Journal of Chemical Physics*, **1983**, 79, 6294-6300	3.9	63
151	Structure of two-component clusters. *Journal of Chemical Physics*, **1994**, 101, 2432-2445	3.9	62
150	Simulation of water adsorption on kaolinite under atmospheric conditions. *Journal of Physical Chemistry A*, **2009**, 113, 7826-33	2.8	61
149	Integral equation approximations for fluids of hard spheres with linear quadrupoles. *Molecular Physics*, **1978**, 35, 1413-1428	1.7	61
148	NMR of deuterium in liquid crystal mixtures. *Chemical Physics Letters*, **1984**, 107, 426-430	2.5	60
147	Structural and dynamical properties of ionic liquids: the influence of ion size disparity. *Journal of Chemical Physics*, **2008**, 129, 064517	3.9	59
146	Theory of the electrical double layer: Ion size effects in a molecular solvent. *Journal of Chemical Physics*, **1989**, 91, 6367-6375	3.9	59
145	Aggregation in dilute aqueous tert-butyl alcohol solutions: insights from large-scale simulations. *Journal of Chemical Physics*, **2012**, 137, 034509	3.9	58
144	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	3.9	58
143	The influence of urea and trimethylamine-N-oxide on hydrophobic interactions. *Journal of Physical Chemistry B*, **2007**, 111, 7932-3	3.4	57
142	Monte Carlo calculation of y(r) for the hard-sphere fluid. *Molecular Physics*, **1977**, 34, 1623-1628	1.7	56
141	Rotational motion in molecular liquids. *Journal of Chemical Physics*, **1989**, 91, 7113-7129	3.9	55
140	Static dielectric properties of polarizable Stockmayer fluids. *Physica A: Statistical Mechanics and Its Applications*, **1981**, 108, 14-26	3.3	55
139	Simulations of Ice Nucleation by Kaolinite (001) with Rigid and Flexible Surfaces. *Journal of Physical Chemistry B*, **2016**, 120, 1726-34	3.4	54

138	Molecular dynamics simulations of ice nucleation by electric fields. *Journal of Physical Chemistry A*, **2012**, 116, 7057-64	2.8	54
137	Ion association and condensation in primitive models of electrolyte solutions. *Journal of Chemical Physics*, **1999**, 111, 9000-9008	3.9	51
136	Modeling and structure of mercury-water interfaces. *Journal of Chemical Physics*, **1997**, 107, 2122-2141	3.9	49
135	A comparison of liquid–vapor coexistence in charged hard sphere and charged hard dumbbell fluids. *Journal of Chemical Physics*, **1995**, 103, 8299-8301	3.9	49
134	A configuration bias Monte Carlo method for water. *Journal of Chemical Physics*, **1995**, 102, 7656-7663	3.9	49
133	Integral equation approximations for fluids of hard spheres with dipoles and quadrupoles. *Molecular Physics*, **1979**, 38, 1635-1654	1.7	49
132	An analysis of fluctuations in supercooled TIP4P/2005 water. *Journal of Chemical Physics*, **2013**, 138, 184502	3.9	48
131	Understanding the structure factor and isothermal compressibility of ambient water in terms of local structural environments. *Journal of Physical Chemistry B*, **2012**, 116, 12014-20	3.4	48
130	The influence of water on the structural and transport properties of model ionic liquids. *Journal of Chemical Physics*, **2010**, 132, 234510	3.9	48
129	Theory of ion solvation dynamics in mixed dipolar solvents. *Journal of Chemical Physics*, **1998**, 109, 3222-3231	3.9	47
128	Dielectric relaxation of electrolyte solutions: Is there really a kinetic dielectric decrement?. *Journal of Chemical Physics*, **1993**, 98, 4959-4966	3.9	47
127	The frequency dependent conductivity of electrolyte solutions. *Journal of Chemical Physics*, **1993**, 99, 2083-2094	3.9	47
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124	Monte Carlo simulations of the adsorption of CO2 on the MgO(100) surface. *Journal of Chemical Physics*, **2006**, 124, 114706	3.9	45
123	Coexistence and criticality of fluids with long-range potentials. *Journal of Chemical Physics*, **2001**, 114, 399	3.9	45
122	Molecular dynamics simulation of the plastic phase of solid methane. *Journal of Chemical Physics*, **1980**, 72, 5348-5356	3.9	45
121	Ion solvation dynamics in binary mixtures. *Journal of Chemical Physics*, **1997**, 106, 2782-2791	3.9	44

120	Liquid-vapor coexistence in fluids of dipolar hard dumbbells and spherocylinders. *Physical Review E*, **1999**, 59, 3065-3070	2.4	44
119	Orientational ordering in spatially disordered dipolar systems. *Physical Review Letters*, **1995**, 75, 2360-2363	7.4	44
118	Evidence that crystal nucleation in aqueous NaCl solution Occurs by the two-step mechanism. *Chemical Physics Letters*, **2013**, 587, 25-29	2.5	43
117	Structural and dynamical properties of ionic liquids: The influence of charge location. *Journal of Chemical Physics*, **2009**, 130, 104506	3.9	42
116	Hydrophobic interactions in urea-trimethylamine-N-oxide solutions. *Journal of Physical Chemistry B*, **2008**, 112, 11106-11	3.4	42
115	Molecular solvent model for an electrical double layer: Reference hypernetted chain results for potassium chloride solutions. *Journal of Chemical Physics*, **1989**, 90, 4513-4527	3.9	42
114	Critical comments on the nonlocal dielectric function employed in recent theories of the hydration force. *Chemical Physics Letters*, **1990**, 172, 69-72	2.5	42
113	Structure and properties of the metal liquid interface. *Journal of Chemical Physics*, **1994**, 101, 6271-6280	3.9	40
112	Simulations of water transport through carbon nanotubes: how different water models influence the conduction rate. *Journal of Chemical Physics*, **2014**, 141, 18C518	3.9	39
111	Structural and dynamical properties of ionic liquids: Competing influences of molecular properties. *Journal of Chemical Physics*, **2010**, 132, 154504	3.9	39
110	Structure of the metal-aqueous electrolyte solution interface. *Journal of Chemical Physics*, **1997**, 107, 4719-4728	3.9	39
109	Tracer diffusion in hard sphere fluids from molecular to hydrodynamic regimes. *Journal of Chemical Physics*, **2006**, 125, 204502	3.9	38
108	An investigation of dynamical density functional theory for solvation in simple mixtures. *Journal of Chemical Physics*, **1998**, 108, 6378-6386	3.9	38
107	Molecular solvent models of electrical double layers. *Electrochimica Acta*, **1991**, 36, 1677-1684	6.7	37
106	Fluids of Lennard-Jones spheres with dipoles and tetrahedral quadrupoles. *Molecular Physics*, **1984**, 51, 333-348	1.7	37
105	The solution of the reference hypernetted-chain approximation for Stockmayer fluids. *Molecular Physics*, **1985**, 55, 751-762	1.7	37
104	Molecular dynamics simulation of NaCl dissolution. *Journal of Physical Chemistry B*, **2015**, 119, 4275-83	3.4	36
103	Ferroelectric order in model discotic nematic liquid crystals. *Physical Review Letters*, **1996**, 76, 239-242	7.4	36

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101	The application of integral equation theories to fluids of nonspherical particles near a uniform planar wall. *Journal of Chemical Physics*, **1991**, 95, 5281-5288	3.9	36
100	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	3.9	36
99	An accurate equation of state for fluids and solids. *Journal of Physical Chemistry B*, **2009**, 113, 11977-87	3.4	35
98	Long-range attractions between solutes in near-critical fluids. *Physical Review A*, **1992**, 45, 7621-7623	2.6	35
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95	Observations of high-density ferroelectric ordered water in kaolinite trenches using Monte Carlo simulations. *Journal of Physical Chemistry A*, **2010**, 114, 8396-405	2.8	33
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93	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	3.9	32
92	Fluctuations and local ice structure in model supercooled water. *Journal of Chemical Physics*, **2015**, 143, 094504	3.9	31
91	Solvation dynamics in electrolyte solutions. *Journal of Chemical Physics*, **1994**, 100, 1552-1558	3.9	31
90	Integral equation theory for dipolar hard sphere fluids with fluctuating orientational order. *Journal of Chemical Physics*, **2000**, 112, 3832-3844	3.9	30
89	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	3.9	30
88	Association and microheterogeneity in aqueous 2-butoxyethanol solutions. *Journal of Physical Chemistry B*, **2011**, 115, 15323-31	3.4	29
87	Molecular solvent model for an electrical double layer: Reference hypernetted-chain results for ion behavior at infinite dilution. *Journal of Chemical Physics*, **1988**, 89, 3285-3294	3.9	29
86	Simulations of Ice Nucleation by Model AgI Disks and Plates. *Journal of Physical Chemistry B*, **2016**, 120, 2291-9	3.4	28
85	Ice nucleation by electric surface fields of varying range and geometry. *Journal of Chemical Physics*, **2013**, 139, 144501	3.9	28

84	Water adsorption on kaolinite surfaces containing trenches. *Journal of Physical Chemistry A*, **2010**, 114, 2171-8	2.8	28
83	Birth of NaCl Crystals: Insights from Molecular Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 9076-87	3.4	27
82	Ion solvation in a water-urea mixture. *Journal of Physical Chemistry B*, **2010**, 114, 613-9	3.4	26
81	Liquid crystal phases of dipolar discotic particles. *Physical Review E*, **1997**, 55, 447-454	2.4	26
80	Gas-liquid coexistence and demixing in systems with highly directional pair potentials. *Physical Review E*, **1998**, 57, 5682-5686	2.4	26
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78	Dielectric relaxation of electrolyte solutions: Molecular dynamics and theoretical results for ions in simple dipolar solvents. *Journal of Chemical Physics*, **1994**, 100, 8385-8391	3.9	26
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75	Understanding electrofreezing in water simulations. *Journal of Chemical Physics*, **2014**, 141, 074501	3.9	24
74	A generalized Gaussian overlap model for fluids of anisotropic particles. *Journal of Chemical Physics* , **1995**, 102, 9040-9047	3.9	24
73	Dielectric relaxation of electrolyte solutions. *Journal of Chemical Physics*, **1991**, 94, 6795-6806	3.9	24
72	Structure of the metal-electrolyte solution interface: Theoretical results for simple models. *Journal of Chemical Physics*, **1995**, 102, 1024-1033	3.9	23
71	On the existence of exact conditions in the theory of electrical double layers. *Journal of Chemical Physics*, **1992**, 96, 3767-3771	3.9	23
70	The interaction between macroparticles in molecular fluids. *Journal of Chemical Physics*, **1990**, 93, 7360-7368	3.9	23
69	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	2.6	23
68	A molecular dynamics investigation of the influence of water structure on ion conduction through a carbon nanotube. *Journal of Chemical Physics*, **2017**, 146, 074502	3.9	22
67	Demixing and the force between parallel plates immersed in binary liquid mixtures. *Journal of Chemical Physics*, **2001**, 114, 7182-7188	3.9	22

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65	Stability of binary mixtures: Supersaturation limits of aqueous alkali halide solutions. *Journal of Chemical Physics*, **1994**, 100, 3827-3842	3.9	22
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61	Structure formation in dipolar fluids driven by rotating fields. *Journal of Chemical Physics*, **2000**, 112, 9828-9833	3.9	20
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59	Charge ordering induces a smectic phase in oblate ionic liquid crystals. *Physical Review Letters*, **2010**, 105, 137801	7.4	19
58	A mean field theory for fluids of multipolar particles in contact with a polarizable wall. *Journal of Chemical Physics*, **1992**, 97, 4372-4379	3.9	19
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56	Remarks on the forces between macroscopic particles in solution. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1996**, 100, 885-888		18
55	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	3.9	17
54	Water adsorption in ion-bearing nanopores. *Journal of Chemical Physics*, **2007**, 126, 024703	3.9	17
53	Liquid–vapor criticality in a fluid of charged hard dumbbells. *Journal of Chemical Physics*, **2003**, 119, 7952-7956	3.9	17
52	Dielectric relaxation of chained ferrofluids. *Journal of Chemical Physics*, **2002**, 116, 6731-6737	3.9	17
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50	Dielectric relaxation of liquid mixtures. *Journal of Chemical Physics*, **1991**, 94, 6785-6794	3.9	16
49	Dynamical properties of a ferroelectric nematic liquid crystal. *Physical Review E*, **1993**, 47, 2954-2957	2.4	15

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46	Crystallization of dipolar spheres: A discussion of second-order density functional theory. *Journal of Chemical Physics*, **2000**, 112, 10949-10956	3.9	14
45	Continuum electrostatic interactions between planar lattices of dipoles and the possible relevance to the hydration force. *Physical Review A*, **1991**, 43, 2953-2962	2.6	14
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43	A configuration bias Monte Carlo method for ionic solutions. *Journal of Chemical Physics*, **1994**, 100, 8265-8270	3.9	13
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41	The composition of liquid methane–nitrogen aerosols in Titan's lower atmosphere from Monte Carlo simulations. *Icarus*, **2011**, 212, 779-789	3.8	12
40	Orientational order in model dipolar fluids. *Physical Review E*, **1999**, 60, 4280-4	2.4	12
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38	Comparison of simulation and experimental results for a model aqueous tert-butanol solution. *Journal of Chemical Physics*, **2017**, 147, 024503	3.9	11
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36	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	3.9	11
35	Simulations of water structure and the possibility of ice nucleation on selected crystal planes of K-feldspar. *Journal of Chemical Physics*, **2019**, 150, 214501	3.9	10
34	Mechanism of Urea Crystal Dissolution in Water from Molecular Dynamics Simulation. *Journal of Physical Chemistry B*, **2018**, 122, 1213-1222	3.4	10
33	A Monte Carlo study of model electrorheological fluids. *Journal of Chemical Physics*, **1999**, 111, 3278-3287	3.9	10
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29	How distributed charge reduces the melting points of model ionic salts. *Journal of Chemical Physics*, **2014**, 140, 104504	3.9	7
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27	Surfactant-stabilized structures in confined liquids. *Journal of Chemical Physics*, **2003**, 119, 8676-8685	3.9	7
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25	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	3.9	6
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19	Bridging the gap between phenomenology and microscopic theory: asymptotes in nematic colloids. *Physical Review E*, **2008**, 77, 041701	2.4	5
18	Colloidal interactions in nematic fluids. *Physical Review E*, **2006**, 73, 020701	2.4	5
17	Unified Description of Diffusion Coefficients from Small to Large Molecules in Organic-Water Mixtures. *Journal of Physical Chemistry A*, **2020**, 124, 2301-2308	2.8	4
16	Structure and adsorption of water in nonuniform cylindrical nanopores. *Journal of Chemical Physics*, **2010**, 133, 224703	3.9	4
15	Constant-volume heat capacity in a near-critical fluid from Monte Carlo simulations. *Journal of Chemical Physics*, **2004**, 121, 8956-9	3.9	4
14	Colloid-induced structure in liquid crystal media. *Journal of Chemical Physics*, **2005**, 122, 124907	3.9	4
13	The crystallization of alkali halides from aqueous solution: An application of density-functional theory. *Journal of Chemical Physics*, **1991**, 95, 485-493	3.9	4

12	The influence of ion hydration on nucleation and growth of LiF crystals in aqueous solution. *Journal of Chemical Physics*, **2018**, 148, 024507	3.9	3
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8	Molecular Simulations of Feldspar Surfaces Interacting with Aqueous Inorganic Solutions: Interfacial Water/Ion Structure and Implications for Ice Nucleation. *ACS Earth and Space Chemistry*, **2021**, 5, 2169-2183	3.2	3
7	Nematic-fluid structure in wall-field geometry. II. The direct correlation function. *Journal of Chemical Physics*, **2006**, 125, 34903	3.9	2
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