Alan K Soper

List of Publications by Year
in descending order

93 papers	10,407 citations	41323 49 h-index	42364 92 g-index
93 all docs	93 docs citations	93 times ranked	7297 citing authors

#	Article	IF	Citations
1	Molecular segregation observed in a concentrated alcoholâ€“water solution. Nature, 2002, 416, 829-832.	13.7	862
2	Structures of High-Density and Low-Density Water. Physical Review Letters, 2000, 84, 2881-2884.	2.9	594
3	Siteâ€“site pair correlation functions of water from 25 to 400â€‰Â°C: Revised analysis of new and old diffraction data. Journal of Chemical Physics, 1997, 106, 247-254.	1.2	556
4	Effect of high salt concentrations on water structure. Nature, 1995, 378, 364-366.	13.7	417
5	Quantum Differences between Heavy and Light Water. Physical Review Letters, 2008, 101, 065502.	2.9	357
6	Partial structure factors from disordered materials diffraction data: An approach using empirical potential structure refinement. Physical Review B, 2005, 72, .	1.1	343
7	Structures of High and Low Density Amorphous Ice by Neutron Diffraction. Physical Review Letters, 2002, 88, 225503.	2.9	311
8	Perturbation of water structure due to monovalent ions in solution. Physical Chemistry Chemical Physics, 2007, 9, 2959.	1.3	303
9	Electron distribution in water. Journal of Chemical Physics, 2000, 112, 9206-9208.	1.2	290
10	Methanol-water solutions: A bi-percolating liquid mixture. Journal of Chemical Physics, 2004, 121, 6456-6462.	1.2	279
11	Hydration of methanol in aqueous solution. Physical Review Letters, 1993, 71, 4346-4349.	2.9	267
12	Tests of the empirical potential structure refinement method and a new method of application to neutron diffraction data on water. Molecular Physics, 2001, 99, 1503-1516.	0.8	261
13	A neutron diffraction study of dimethyl sulphoxideâ€“water mixtures. Journal of Chemical Physics, 1992, 97, 1320-1331.	1.2	241
14	A neutron diffraction study of hydration effects in aqueous solutions. Journal of Physics C: Solid State Physics, 1977, 10, 1793-1801.	1.5	210
15	The Radial Distribution Functions of Water as Derived from Radiation Total Scattering Experiments: Is There Anything We Can Say for Sure?. , 2013, 2013, 1-67.		208
16	Structural Investigation of Soluteâˆ’Solute Interactions in Aqueous Solutions of Tertiary Butanol. Journal of Physical Chemistry B, 1998, 102, 3551-3563.	1.2	202
17	Structure of a New Dense Amorphous Ice. Physical Review Letters, 2002, 89, 205503.	2.9	200
18	Impact of urea on water structure: a clue to its properties as a denaturant?. Biophysical Chemistry, 2003, 105, 649-666.	1.5	197

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19	Small-angle scattering and the structure of ambient liquid water. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 14003-14007.	3.3	178
20	Extracting the pair distribution function from white-beam X-ray total scattering data. Journal of Applied Crystallography, 2011, 44, 714-726.	1.9	175
21	Liquid Alumina: Detailed Atomic Coordination Determined from Neutron Diffraction Data Using Empirical Potential Structure Refinement. Physical Review Letters, 2001, 86, 4839-4842.	2.9	166
22	Joint structure refinement of x-ray and neutron diffraction data on disordered materials: application to liquid water. Journal of Physics Condensed Matter, 2007, 19, 335206.	0.7	158
23	The effect of apolar solutes on water structure: Alcohols and tetraalkylammonium ions. Journal of Chemical Physics, 1994, 101, 6116-6125.	1.2	153
24	Water ordering around methane during hydrate formation. Journal of Chemical Physics, 2000, 113, 6390-6397.	1.2	145
25	The structure of liquid methanol revisited: a neutron diffraction experiment at â˜'80 Â°C and +25 Â°C. Molecular Physics, 1999, 96, 1159-1168.	0.8	142
26	Chloride ions in aqueous solutions. Nature, 1980, 287, 714-716.	13.7	137
27	Search for memory effects in methane hydrate: Structure of water before hydrate formation and after hydrate decomposition. Journal of Chemical Physics, 2005, 123, 164507.	1.2	128
28	Pressure-dependent structures of amorphous red phosphorus and the origin of the first sharp diffraction peaks. Nature Materials, 2008, 7, 890-899.	13.3	124
29	NIMROD: The Near and InterMediate Range Order Diffractometer of the ISIS second target station. Review of Scientific Instruments, 2010, 81, 033905.	0.6	119
30	The local and intermediate range structures of the five amorphous ices at 80K and ambient pressure: A Faber-Ziman and Bhatia-Thornton analysis. Journal of Chemical Physics, 2006, 125, 194502.	1.2	117
31	Combined neutron diffraction and computer simulation study of liquid dimethyl sulphoxide. Journal of Chemical Physics, 1993, 99, 6836-6847.	1.2	116
32	Ions in water: The microscopic structure of concentrated hydroxide solutions. Journal of Chemical Physics, 2005, 122, 194509.	1.2	114
33	Hydrogen-Hydrogen Pair Correlation Function in Liquid Water. Physical Review Letters, 1982, 49, 471-474.	2.9	101
34	Excess Entropy in Alcoholâ˜'Water Solutions:Â A Simple Clustering Explanationâ€. Journal of Physical Chemistry B, 2006, 110, 3472-3476.	1.2	101
35	Inelasticity corrections for time-of-flight and fixed wavelength neutron diffraction experiments. Molecular Physics, 2009, 107, 1667-1684.	0.8	95
36	Structure of High-Density Amorphous Ice under Pressure. Physical Review Letters, 2002, 89, 285502.	2.9	93

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37	Computer simulation as a tool for the interpretation of total scattering data from glasses and liquids. Molecular Simulation, 2012, 38, 1171-1185.	0.9	90
38	Water and Trehalose: How Much Do They Interact with Each Other?. Journal of Physical Chemistry B, 2010, 114, 4904-4908.	1.2	80
39	Neutron diffraction study of high density supercritical water. Journal of Chemical Physics, 1998, 109, 3180-3184.	1.2	78
40	Recent water myths. Pure and Applied Chemistry, 2010, 82, 1855-1867.	0.9	77
41	The structure of liquid hydrogen chloride. Molecular Physics, 1981, 42, 399-410.	0.8	76
42	Structure of 2 molar NaOH in aqueous solution from neutron diffraction and empirical potential structure refinement. Physical Review B, 2006, 74, .	1.1	75
43	Formation of Methane Hydrate in the Presence of Natural and Synthetic Nanoparticles. Journal of the American Chemical Society, 2018, 140, 3277-3284.	6.6	73
44	The Three-Dimensional Structure of Water Confined in Nanoporous Vycor Glass. Journal of Physical Chemistry B, 2007, 111, 5610-5620.	1.2	72
45	Structure and Hydration ofl-Proline in Aqueous Solutions. Journal of Physical Chemistry B, 2007, 111, 4568-4580.	1.2	70
46	Segregation in aqueous methanol enhanced by cooling and compression. Journal of Chemical Physics, 2005, 122, 174514.	1.2	69
47	Orientational correlations in liquid acetone and dimethyl sulfoxide: A comparative study. Journal of Chemical Physics, 2006, 124, 074502.	1.2	68
48	Multiscale Approach to the Structural Study of Water Confined in MCM41. Journal of Physical Chemistry B, 2009, 113, 16169-16177.	1.2	66
49	Molecular Insight Into the Hydrogen Bonding and Micro-Segregation of a Cryoprotectant Molecule. Journal of Physical Chemistry B, 2012, 116, 13898-13904.	1.2	60
50	Axial Structure of the Pd(II) Aqua Ion in Solution. Journal of the American Chemical Society, 2012, 134, 962-967.	6.6	50
51	Structural Studies on the Hydration ofl-Glutamic Acid in Solution. Journal of Physical Chemistry B, 2006, 110, 21251-21258.	1.2	49
52	Preference for Isolated Water Molecules in a Concentrated Glycerolâ€“Water Mixture. Journal of Physical Chemistry B, 2011, 115, 7799-7807.	1.2	49
53	The excluded volume effect in confined fluids and liquid mixtures. Journal of Physics Condensed Matter, 1997, 9, 2399-2410.	0.7	48
54	The Hydration of the Neurotransmitter Acetylcholine in Aqueous Solution. Biophysical Journal, 2006, 91, 2371-2380.	0.2	42

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55	Temperature-Dependent Segregation in Alcoholâ€“Water Binary Mixtures Is Driven by Water Clustering. Journal of Physical Chemistry B, 2018, 122, 7884-7894.	1.2	41
56	Radical re-appraisal of water structure in hydrophilic confinement. Chemical Physics Letters, 2013, 590, 1-15.	1.2	40
57	Highly compressed water structure observed in a perchlorate aqueous solution. Nature Communications, 2017, 8, 919.	5.8	39
58	Is water one liquid or two?. Journal of Chemical Physics, 2019, 150, 234503.	1.2	38
59	Pronounced Microheterogeneity in a Sorbitolâ€“Water Mixture Observed through Variable Temperature Neutron Scattering. Journal of Physical Chemistry B, 2012, 116, 4439-4447.	1.2	36
60	Local and long-range structure of water in a perfluorinated ionomer membrane. Macromolecules, 1992, 25, 3106-3109.	2.2	34
61	The structure of aqueous solutions of tertiary butanol. Journal of Physics Condensed Matter, 2000, 12, A123-A128.	0.7	33
62	Water: Two Liquids Divided by a Common Hydrogen Bond. Journal of Physical Chemistry B, 2011, 115, 14014-14022.	1.2	32
63	Comment on â€œMaxima in the thermodynamic response and correlation functions of deeply supercooled waterâ€. Science, 2018, 360, .	6.0	32
64	Density profile of water confined in cylindrical pores in MCM-41 silica. Journal of Physics Condensed Matter, 2012, 24, 064107.	0.7	27
65	Low-Density Water Structure Observed in a Nanosegregated Cryoprotectant Solution at Low Temperatures from 285 to 238 K. Journal of Physical Chemistry B, 2016, 120, 4439-4448.	1.2	26
66	Trehalose in Water Revisited. Journal of Physical Chemistry B, 2018, 122, 7365-7374.	1.2	26
67	Water/Cosolvent Attraction Induced Phase Separation: A Molecular Picture of Cononsolvency. Macromolecules, 2019, 52, 457-464.	2.2	25
68	On the uniqueness of structure extracted from diffraction experiments on liquids and glasses. Journal of Physics Condensed Matter, 2007, 19, 415108.	0.7	24
69	High-pressure neutron diffraction on fluid carbon tetrafluoride and interpretation by reverse Monte Carlo simulations. Journal of Chemical Physics, 1997, 107, 10667-10674.	1.2	21
70	Investigation on the structure of liquid N-methylformamideâ€“dimethylsulfoxide mixtures. Chemical Physics, 2011, 381, 21-28.	0.9	20
71	Density minimum in supercooled confined water. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, E1192; author reply E1193-4.	3.3	20
72	Structural evidence for solvent-stabilisation by aspartic acid as a mechanism for halophilic protein stability in high salt concentrations. Physical Chemistry Chemical Physics, 2016, 18, 18054-18062.	1.3	18

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73	Freezing of Aqueous Solutions and Chemical Stability of Amorphous Pharmaceuticals: Water Clusters Hypothesis. Journal of Pharmaceutical Sciences, 2019, 108, 36-49.	1.6	18
74	Network structure and concentration fluctuations in a series of elemental, binary, and tertiary liquids and glasses. Journal of Physics Condensed Matter, 2010, 22, 404210.	0.7	17
75	Water in a Soft Confinement: Structure of Water in Amorphous Sorbitol. Journal of Physical Chemistry B, 2016, 120, 7289-7296.	1.2	17
76	Density profile of nitrogen in cylindrical pores of MCM-41. Chemical Physics Letters, 2017, 683, 529-535.	1.2	17
77	Boroxol rings from diffraction data on vitreous boron trioxide. Journal of Physics Condensed Matter, 2011, 23, 365402.	0.7	16
78	Ice crystallization observed in highly supercooled confined water. Physical Chemistry Chemical Physics, 2019, 21, 4931-4938.	1.3	13
79	Disordered Atom Molecular Potential for Water Parameterized against Neutron Diffraction Data. Application to the Structure of Ice Ih. Journal of Physical Chemistry B, 2015, 119, 9244-9253.	1.2	12
80	Segregated water observed in a putative fish embryo cryopreservative. Royal Society Open Science, 2016, 3, 150655.	1.1	12
81	Hydrophilic Association in a Dilute Glutamine Solution Persists Independent of Increasing Temperature. Journal of Physical Chemistry B, 2015, 119, 15644-15651.	1.2	11
82	Coarse-grained empirical potential structure refinement: Application to a reverse aqueous micelle. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 1652-1660.	1.1	11
83	Experimental and modeling evidence for structural crossover in supercritical CO2. Physical Review E, 2020, 101, 052109.	0.8	11
84	TrimethylamineN-oxide (TMAO) resists the compression of water structure by magnesium perchlorate: terrestrial kosmotropevs.Martian chaotrope. Physical Chemistry Chemical Physics, 2020, 22, 4924-4937.	1.3	10
85	Empirical potential structure refinement of semi-crystalline polymer systems: polytetrafluoroethylene and polychlorotrifluoroethylene. Journal of Physics Condensed Matter, 2013, 25, 454219.	0.7	9
86	Solute Specific Perturbations to Water Structure and Dynamics in Tertiary Aqueous Solution. Journal of Physical Chemistry B, 2020, 124, 10983-10993.	1.2	9
87	The Structure of Water and Aqueous Systems. Experimental Methods in the Physical Sciences, 2017, 49, 135-211.	0.1	8
88	Bridging Structure, Dynamics, and Thermodynamics: An Example Study on Aqueous Potassium Halides. Journal of Physical Chemistry B, 2021, 125, 12774-12786.	1.2	8
89	Neutron diffraction study of aqueous Laponite suspensions at the NIMROD diffractometer. Physical Review E, 2014, 90, 032301.	0.8	7
90	Biomolecular self-assembly under extreme Martian mimetic conditions. Molecular Physics, 2019, 117, 3398-3407.	0.8	7

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91	Adsorption of simple gases into the porous glass MCM-41. Journal of Chemical Physics, 2021, 154, 184503.	1.2	6
92	Comment on â€œOxygen as a Site Specific Probe of the Structure of Water and Oxide Materialsâ€• Physical Review Letters, 2012, 108, 259603; discussion 259604.	2.9	3
93	Through the looking glass and into the liquid. Molecular Physics, 2019, 117, 3197-3206.	0.8	1