Jose L F Abascal

List of Publications by Year
in descending order

93	10,342	81743	40881
papers	citations	39 h-index	93 g-index

94	94	94	6090
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Madrid-2019 force field for electrolytes in water using TIP4P/2005 and scaled charges: Extension to the ions Fâ^', Brâ^', Iâ^', Rb+, and Cs+. Journal of Chemical Physics, 2022, 156, 044505.	1.2	36
2	â€œIn Silicoâ€•Seawater. Journal of Chemical Theory and Computation, 2021, 17, 1715-1725.	2.3	20
3	Effect of dissolved salt on the anomalies of water at negative pressure. Journal of Chemical Physics, 2020, 152, 194501.	1.2	4
4	Scaled charges at work: Salting out and interfacial tension of methane with electrolyte solutions from computer simulations. Fluid Phase Equilibria, 2020, 513, 112548.	1.4	33
5	A force field of Li+, Na+, K+, Mg2+, Ca2+, Clâ^', and SO42â^' in aqueous solution based on the TIP4P/2005 water model and scaled charges for the ions. Journal of Chemical Physics, 2019, 151, 134504.	1.2	166
6	Estimating the solubility of 1:1 electrolyte aqueous solutions: the chemical potential difference rule. Molecular Physics, 2017, 115, 1301-1308.	0.8	21
7	Two-structure thermodynamics for the TIP4P/2005 model of water covering supercooled and deeply stretched regions. Journal of Chemical Physics, 2017, 146, 034502.	1.2	107
8	A potential model for sodium chloride solutions based on the TIP4P/2005 water model. Journal of Chemical Physics, 2017, 147, 104501.	1.2	82
9	A comprehensive scenario of the thermodynamic anomalies of water using the TIP4P/2005 model. Journal of Chemical Physics, 2016, 145, 054505.	1.2	48
10	Molecular mechanism for cavitation in water under tension. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 13582-13587.	3.3	110
11	Equation of state for water and its line of density maxima down to â^'120 MPa. Physical Chemistry Chemical Physics, 2016, 18, 5896-5900.	1.3	45
12	Bubble nucleation in simple and molecular liquids via the largest spherical cavity method. Journal of Chemical Physics, 2015, 142, 154903.	1.2	15
13	Detecting vapour bubbles in simulations of metastable water. Journal of Chemical Physics, 2014, 141, 18C511.	1.2	19
14	Anomalies in bulk supercooled water at negative pressure. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 7936-7941.	3.3	103
15	Nucleation free-energy barriers with Hybrid Monte-Carlo/Umbrella Sampling. Physical Chemistry Chemical Physics, 2014, 16, 24913-24919.	1.3	13
16	Homogeneous Ice Nucleation at Moderate Supercooling from Molecular Simulation. Journal of the American Chemical Society, 2013, 135, 15008-15017.	6.6	256
17	Homogeneous bubble nucleation in water at negative pressure: A Voronoi polyhedra analysis. Journal of Chemical Physics, 2013, 138, 084508.	1.2	35
18	Determining the phase diagram of water from direct coexistence simulations: The phase diagram of the TIP4P/2005 model revisited. Journal of Chemical Physics, 2013, 139, 154505.	1.2	61

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19	A flexible model for water based on TIP4P/2005. Journal of Chemical Physics, 2011, 135, 224516.	1.2	153
20	Note: Equation of state and compressibility of supercooled water: Simulations and experiment. Journal of Chemical Physics, 2011, 134, 186101.	1.2	52
21	Physics and chemistry of water and ice. Physical Chemistry Chemical Physics, 2011, 13, 19660.	1.3	12
22	Simulating water with rigid non-polarizable models: a general perspective. Physical Chemistry Chemical Physics, 2011, 13, 19663.	1.3	749
23	The shear viscosity of rigid water models. Journal of Chemical Physics, 2010, 132, 096101.	1.2	276
24	Widom line and the liquidâ€“liquid critical point for the TIP4P/2005 water model. Journal of Chemical Physics, 2010, 133, 234502.	1.2	267
25	Heat capacity of water: A signature of nuclear quantum effects. Journal of Chemical Physics, 2010, 132, 046101.	1.2	90
26	Anomalies in water as obtained from computer simulations of the TIP4P/2005 model: density maxima, and density, isothermal compressibility and heat capacity minima. Molecular Physics, 2009, 107, 365-374.	0.8	153
27	Triple points and coexistence properties of the dense phases of water calculated using computer simulation. Physical Chemistry Chemical Physics, 2009, 11, 556-562.	1.3	26
28	What ice can teach us about water interactions: a critical comparison of the performance of different water models. Faraday Discussions, 2009, 141, 251-276.	1.6	375
29	Determination of phase diagrams via computer simulation: methodology and applications to water, electrolytes and proteins. Journal of Physics Condensed Matter, 2008, 20, 153101.	0.7	209
30	Dipole-Quadrupole Force Ratios Determine the Ability of Potential Models to Describe the Phase Diagram of Water. Physical Review Letters, 2007, 98, 237801.	2.9	69
31	Properties of ices at 0 K: A test of water models. Journal of Chemical Physics, 2007, 127, 154518.	1.2	32
32	The Water Forcefield:â€‰ Importance of Dipolar and Quadrupolar Interactions. Journal of Physical Chemistry C, 2007, 111, 15811-15822.	1.5	54
33	The melting point of hexagonal ice (Ih) is strongly dependent on the quadrupole of the water models. Physical Chemistry Chemical Physics, 2007, 9, 2775.	1.3	30
34	Ice: A fruitful source of information about liquid water. Journal of Molecular Liquids, 2007, 136, 214-220.	2.3	15
35	Vapor-liquid equilibria from the triple point up to the critical point for the new generation of TIP4P-like models: TIP4P/Ew, TIP4P/2005, and TIP4P/ice. Journal of Chemical Physics, 2006, 125, 034503.	1.2	210
36	The melting temperature of the six site potential model of water. Journal of Chemical Physics, 2006, 125, 166101.	1.2	74

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37	The melting point of ice Ih for common water models calculated from direct coexistence of the solid-liquid interface. Journal of Chemical Physics, 2006, 124, 144506.	1.2	386
38	Computer Simulation of the Ionic Atmosphere around Z-DNA. Journal of Physical Chemistry B, 2006, 110, 25080-25090.	1.2	4
39	Radial distribution functions and densities for the SPC/E, TIP4P and TIP5P models for liquid water and ices Ih, Ic, II, III, IV, V, VI, VII, VIII, IX, XI and XII. Physical Chemistry Chemical Physics, 2005, 7, 1450.	1.3	111
40	Relation between the melting temperature and the temperature of maximum density for the most common models of water. Journal of Chemical Physics, 2005, 123, 144504.	1.2	117
41	Can simple models describe the phase diagram of water?. Journal of Physics Condensed Matter, 2005, 17, S3283-S3288.	0.7	72
42	The range of meta stability of ice-water melting for two simple models of water. Molecular Physics, 2005, 103, 1-5.	0.8	54
43	A potential model for the study of ices and amorphous water: TIP4P/Ice. Journal of Chemical Physics, 2005, 122, 234511.	1.2	1,041
44	The melting temperature of the most common models of water. Journal of Chemical Physics, 2005, 122, 114507.	1.2	338
45	A general purpose model for the condensed phases of water: TIP4P/2005. Journal of Chemical Physics, 2005, 123, 234505.	1.2	2,907
46	Tracing the phase diagram of the four-site water potential (TIP4P). Journal of Chemical Physics, 2004, 121, 1165-1166.	1.2	73
47	Combinatorial entropy and phase diagram of partially ordered ice phases. Journal of Chemical Physics, 2004, 121, 10145-10158.	1.2	54
48	Formation of high density amorphous ice by decompression of ice VII and ice VIII at 135 K. Journal of Chemical Physics, 2004, 121, 11907-11911.	1.2	24
49	Computer simulation of the thermodynamics of the Bâ€‰â†'â€‰Z-DNA transition: effect of the ionic size and charge. Molecular Physics, 2004, 102, 2141-2148.	0.8	4
50	Phase Diagram of Water from Computer Simulation. Physical Review Letters, 2004, 92, 255701.	2.9	264
51	The fluidâ€“solid equilibrium for a charged hard sphere model revisited. Journal of Chemical Physics, 2003, 119, 964-971.	1.2	59
52	Characterization of the order-disorder transition of a charged hard-sphere model. Physical Review E, 2003, 68, 052501.	0.8	8
53	Theory and simulation of the triplet structure factor and triplet direct correlation functions in binary mixtures. Journal of Chemical Physics, 2002, 116, 730-736.	1.2	19
54	Study of the triplet and pair structure of strong electrolytes modeled via truncated Coulomb interactions. Journal of Chemical Physics, 2002, 117, 3763-3771.	1.2	6

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55	An inhomogeneous integral equation for the triplet structure of binary liquids. Journal of Chemical Physics, 2001, 114, 3562-3569.	1.2	8
56	Ionic distribution around simple B-DNA models. III. The effect of ionic charge. Journal of Chemical Physics, 2001, 114, 4277-4284.	1.2	29
57	Computer simulation results for the free-energy difference between B-DNA and Z-DNA. Journal of Physics Condensed Matter, 2000, 12, A327-A332.	0.7	5
58	On the triplet structure of binary liquids. Journal of Chemical Physics, 2000, 113, 3302-3309.	1.2	9
59	Order-Disorder Transition in the Solid Phase of a Charged Hard Sphere Model. Physical Review Letters, 2000, 85, 3217-3220.	2.9	49
60	The role of the molecular shape on the conformational transition from B-to Z-DNA. Journal of Chemical Physics, 1999, 110, 11094-11095.	1.2	7
61	The Radial Boundary of Polyelectrolyte Solutions Containing Asymmetrical Salts. Molecular Simulation, 1999, 21, 249-255.	0.9	2
62	Ionic distribution around simple B-DNA models II. Deviations from cylindrical symmetry. Journal of Chemical Physics, 1998, 109, 6200-6210.	1.2	33
63	The free energy difference between simple models of B- and Z-DNA: Computer simulation and theoretical predictions. Journal of Chemical Physics, 1997, 106, 8239-8253.	1.2	13
64	Influence of association on the liquidâ€“vapor phase coexistence of simple systems. Journal of Chemical Physics, 1997, 106, 1569-1575.	1.2	12
65	Fluid-solid equilibrium of a charged hard-sphere model. Physical Review E, 1996, 54, 2746-2760.	0.8	48
66	Theory and simulation of central force model potentials: Application to homonuclear diatomic molecules. Journal of Chemical Physics, 1996, 105, 10008-10021.	1.2	7
67	A method for the computer simulation of the free-energy difference in conformational changes of polyelectrolytes. Application to the B- to Z-DNA transition. Europhysics Letters, 1996, 34, 471-476.	0.7	7
68	Monte Carlo simulation and integral-equation studies of a fluid of charged hard spheres near the critical region. Physical Review E, 1995, 51, 289-296.	0.8	59
69	Ionic distribution around simple DNA models. I. Cylindrically averaged properties. Journal of Chemical Physics, 1995, 103, 8273-8284.	1.2	80
70	A Modulated Bulk as a Fuzzy Boundary for the Simulation of Long-Ranged Inhomogeneous Systems. Molecular Simulation, 1995, 14, 313-329.	0.9	10
71	The influence of concentration and ionic strength on the cluster structure of highly charged electrolyte solutions. Molecular Physics, 1994, 81, 143-156.	0.8	24
72	Connectivity in a binary mixture of randomly centered spheres with selective particle clustering. Journal of Chemical Physics, 1994, 100, 1769-1770.	1.2	0

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73	Ionic association in electrolyte solutions: A Voronoi polyhedra analysis. Journal of Chemical Physics, 1994, 101, 10892-10898.	1.2	27
74	The Voronoi polyhedra as tools for structure determination in simple disordered systems. The Journal of Physical Chemistry, 1993, 97, 4211-4215.	2.9	97
75	Pair connectedness functions and percolation in highly charged electrolyte solutions. Journal of Chemical Physics, 1993, 99, 9037-9046.	1.2	15
76	Monte Carlo simulations of a hydrophobic weak polyelectrolyte. Charge distribution as a function of conformation. Journal of Chemical Physics, 1993, 99, 4231-4232.	1.2	2
77	Monte Carlo simulation of the equation of state of hard tetrahedral molecules. Molecular Physics, 1992, 76, 1411-1421.	0.8	7
78	Cluster structure in model electrolyte solutions. Chemical Physics, 1991, 153, 79-89.	0.9	16
79	Fractal analysis of ionic trajectories in electrolyte solutions. Chemical Physics Letters, 1991, 183, 125-128.	1.2	1
80	Background and bridge functions for the homonuclear hard diatomic fluid. Journal of Chemical Physics, 1989, 90, 7330-7337.	1.2	10
81	New aspects in the simulation and behaviour of polar molecular fluids. Molecular Physics, 1989, 68, 1067-1078.	0.8	12
82	The solution of the reference hypernetted chain equation for the dipolar hard diatomic fluid. Journal of Chemical Physics, 1989, 91, 2581-2586.	1.2	19
83	Thermodynamics of a quadrupolar hard diatomic fluid using a perturbation theory with nonspherical reference system. The Journal of Physical Chemistry, 1989, 93, 4636-4642.	2.9	8
84	Extension of the optimized RHNC equation to multicomponent liquids. Journal of Chemical Physics, 1987, 87, 2249-2256.	1.2	35
85	An improved integral equation for linear polyatomic fluids. Chemical Physics Letters, 1987, 135, 133-136.	1.2	4
86	Structure and thermodynamics of the dipolar hard sphere fluid from the referenceâ€hypernetted chain equation with minimized free energy. Journal of Chemical Physics, 1986, 85, 2916-2921.	1.2	33
87	A unified treatment of the equation of state of hard linear bodies. Journal of Molecular Liquids, 1985, 30, 133-137.	2.3	20
88	MC test of perturbation theories based on siteâ€“site potentials. Journal of Chemical Physics, 1985, 82, 2445-2452.	1.2	16
89	Generalized boublick equation: an accurate expression for the equation of state of hard fused spheres. Physics and Chemistry of Liquids, 1983, 12, 183-189.	0.4	5
90	The structure of liquid neon: an anomaly resolved. Journal of Physics C: Solid State Physics, 1983, 16, L441-L444.	1.5	8

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91	Thermodynamic properties of halogens from a perturbation theory for interaction site model fluids. Journal of the Chemical Society, Faraday Transactions 2, 1982, 78, 965.	1.1	5
92	Thermodynamic properties of nitrogen from a perturbation theory for ISM fluids. Chemical Physics Letters, 1982, 85, 117-119.	1.2	2
93	Perturbation theory for polyatomic fluids. Molecular Physics, 1981, 42, 999-1008.	0.8	36