# 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 | A general purpose model for the condensed phases of water: TIP4P/2005. Journal of Chemical Physics, 2005, 123, 234505. | 1.2 | 2,907 |
| 2 | A potential model for the study of ices and amorphous water: TIP4P/Ice. Journal of Chemical Physics, 2005, 122, 234511. | 1.2 | 1,041 |
| 3 | Simulating water with rigid non-polarizable models: a general perspective. Physical Chemistry Chemical Physics, 2011, 13, 19663. | 1.3 | 749 |
| 4 | 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 |
| 5 | 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 |
| 6 | The melting temperature of the most common models of water. Journal of Chemical Physics, 2005, 122, 114507. | 1.2 | 338 |
| 7 | The shear viscosity of rigid water models. Journal of Chemical Physics, 2010, 132, 096101. | 1.2 | 276 |
| 8 | Widom line and the liquidâ€“liquid critical point for the TIP4P/2005 water model. Journal of Chemical Physics, 2010, 133, 234502. | 1.2 | 267 |
| 9 | Phase Diagram of Water from Computer Simulation. Physical Review Letters, 2004, 92, 255701. | 2.9 | 264 |
| 10 | Homogeneous Ice Nucleation at Moderate Supercooling from Molecular Simulation. Journal of the American Chemical Society, 2013, 135, 15008-15017. | 6.6 | 256 |
| 11 | 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 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | A flexible model for water based on TIP4P/2005. Journal of Chemical Physics, 2011, 135, 224516. | 1.2 | 153 |
| 16 | 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 |
| 17 | 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 |
| 18 | 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 |

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| 19 | 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 |
| 20 | 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 |
| 21 | The Voronoi polyhedra as tools for structure determination in simple disordered systems. The Journal of Physical Chemistry, 1993, 97, 4211-4215. | 2.9 | 97 |
| 22 | Heat capacity of water: A signature of nuclear quantum effects. Journal of Chemical Physics, 2010, 132, 046101. | 1.2 | 90 |
| 23 | A potential model for sodium chloride solutions based on the TIP4P/2005 water model. Journal of Chemical Physics, 2017, 147, 104501. | 1.2 | 82 |
| 24 | Ionic distribution around simple DNA models. I. Cylindrically averaged properties. Journal of Chemical Physics, 1995, 103, 8273-8284. | 1.2 | 80 |
| 25 | The melting temperature of the six site potential model of water. Journal of Chemical Physics, 2006, 125, 166101. | 1.2 | 74 |
| 26 | Tracing the phase diagram of the four-site water potential (TIP4P). Journal of Chemical Physics, 2004, 121, 1165-1166. | 1.2 | 73 |
| 27 | Can simple models describe the phase diagram of water?. Journal of Physics Condensed Matter, 2005, 17, S3283-S3288. | 0.7 | 72 |
| 28 | 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 |
| 29 | 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 |
| 30 | 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 |
| 31 | The fluidâ€“solid equilibrium for a charged hard sphere model revisited. Journal of Chemical Physics, 2003, 119, 964-971. | 1.2 | 59 |
| 32 | Combinatorial entropy and phase diagram of partially ordered ice phases. Journal of Chemical Physics, 2004, 121, 10145-10158. | 1.2 | 54 |
| 33 | The range of meta stability of ice-water melting for two simple models of water. Molecular Physics, 2005, 103, 1-5. | 0.8 | 54 |
| 34 | The Water Forcefield:â€‰ Importance of Dipolar and Quadrupolar Interactions. Journal of Physical Chemistry C, 2007, 111, 15811-15822. | 1.5 | 54 |
| 35 | Note: Equation of state and compressibility of supercooled water: Simulations and experiment. Journal of Chemical Physics, 2011, 134, 186101. | 1.2 | 52 |
| 36 | Order-Disorder Transition in the Solid Phase of a Charged Hard Sphere Model. Physical Review Letters, 2000, 85, 3217-3220. | 2.9 | 49 |

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| 37 | Fluid-solid equilibrium of a charged hard-sphere model. Physical Review E, 1996, 54, 2746-2760. | 0.8 | 48 |
| 38 | A comprehensive scenario of the thermodynamic anomalies of water using the TIP4P/2005 model. Journal of Chemical Physics, 2016, 145, 054505. | 1.2 | 48 |
| 39 | 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 |
| 40 | Perturbation theory for polyatomic fluids. Molecular Physics, 1981, 42, 999-1008. | 0.8 | 36 |
| 41 | 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 |
| 42 | Extension of the optimized RHNC equation to multicomponent liquids. Journal of Chemical Physics, 1987, 87, 2249-2256. | 1.2 | 35 |
| 43 | Homogeneous bubble nucleation in water at negative pressure: A Voronoi polyhedra analysis. Journal of Chemical Physics, 2013, 138, 084508. | 1.2 | 35 |
| 44 | 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 |
| 45 | Ionic distribution around simple B-DNA models II. Deviations from cylindrical symmetry. Journal of Chemical Physics, 1998, 109, 6200-6210. | 1.2 | 33 |
| 46 | 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 |
| 47 | Properties of ices at 0 K: A test of water models. Journal of Chemical Physics, 2007, 127, 154518. | 1.2 | 32 |
| 48 | 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 |
| 49 | Ionic distribution around simple B-DNA models. III. The effect of ionic charge. Journal of Chemical Physics, 2001, 114, 4277-4284. | 1.2 | 29 |
| 50 | Ionic association in electrolyte solutions: A Voronoi polyhedra analysis. Journal of Chemical Physics, 1994, 101, 10892-10898. | 1.2 | 27 |
| 51 | 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 |
| 52 | 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 |
| 53 | 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 |
| 54 | Estimating the solubility of 1:1 electrolyte aqueous solutions: the chemical potential difference rule. Molecular Physics, 2017, 115, 1301-1308. | 0.8 | 21 |

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| 55 | A unified treatment of the equation of state of hard linear bodies. Journal of Molecular Liquids, 1985, 30, 133-137. | 2.3 | 20 |
| 56 | â€œIn Silicoâ€•Seawater. Journal of Chemical Theory and Computation, 2021, 17, 1715-1725. | 2.3 | 20 |
| 57 | 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 |
| 58 | 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 |
| 59 | Detecting vapour bubbles in simulations of metastable water. Journal of Chemical Physics, 2014, 141, 18C511. | 1.2 | 19 |
| 60 | MC test of perturbation theories based on siteâ€“site potentials. Journal of Chemical Physics, 1985, 82, 2445-2452. | 1.2 | 16 |
| 61 | Cluster structure in model electrolyte solutions. Chemical Physics, 1991, 153, 79-89. | 0.9 | 16 |
| 62 | Pair connectedness functions and percolation in highly charged electrolyte solutions. Journal of Chemical Physics, 1993, 99, 9037-9046. | 1.2 | 15 |
| 63 | Ice: A fruitful source of information about liquid water. Journal of Molecular Liquids, 2007, 136, 214-220. | 2.3 | 15 |
| 64 | Bubble nucleation in simple and molecular liquids via the largest spherical cavity method. Journal of Chemical Physics, 2015, 142, 154903. | 1.2 | 15 |
| 65 | 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 |
| 66 | Nucleation free-energy barriers with Hybrid Monte-Carlo/Umbrella Sampling. Physical Chemistry Chemical Physics, 2014, 16, 24913-24919. | 1.3 | 13 |
| 67 | New aspects in the simulation and behaviour of polar molecular fluids. Molecular Physics, 1989, 68, 1067-1078. | 0.8 | 12 |
| 68 | Influence of association on the liquidâ€“vapor phase coexistence of simple systems. Journal of Chemical Physics, 1997, 106, 1569-1575. | 1.2 | 12 |
| 69 | Physics and chemistry of water and ice. Physical Chemistry Chemical Physics, 2011, 13, 19660. | 1.3 | 12 |
| 70 | Background and bridge functions for the homonuclear hard diatomic fluid. Journal of Chemical Physics, 1989, 90, 7330-7337. | 1.2 | 10 |
| 71 | A Modulated Bulk as a Fuzzy Boundary for the Simulation of Long-Ranged Inhomogeneous Systems. Molecular Simulation, 1995, 14, 313-329. | 0.9 | 10 |
| 72 | On the triplet structure of binary liquids. Journal of Chemical Physics, 2000, 113, 3302-3309. | 1.2 | 9 |

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| 75 | An inhomogeneous integral equation for the triplet structure of binary liquids. Journal of Chemical Physics, 2001, 114, 3562-3569. | 1.2 | 8 |
| 76 | Characterization of the order-disorder transition of a charged hard-sphere model. Physical Review E, 2003, 68, 052501. | 0.8 | 8 |
| 77 | Monte Carlo simulation of the equation of state of hard tetrahedral molecules. Molecular Physics, 1992, 76, 1411-1421. | 0.8 | 7 |
| 78 | Theory and simulation of central force model potentials: Application to homonuclear diatomic molecules. Journal of Chemical Physics, 1996, 105, 10008-10021. | 1.2 | 7 |
| 79 | 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 |
| 80 | 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 |
| 81 | 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 |
| 82 | 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 |
| 83 | 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 |
| 84 | 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 |
| 85 | An improved integral equation for linear polyatomic fluids. Chemical Physics Letters, 1987, 135, 133-136. | 1.2 | 4 |
| 86 | 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 |
| 87 | Computer Simulation of the Ionic Atmosphere around Z-DNA. Journal of Physical Chemistry B, 2006, 110, 25080-25090. | 1.2 | 4 |
| 88 | Effect of dissolved salt on the anomalies of water at negative pressure. Journal of Chemical Physics, 2020, 152, 194501. | 1.2 | 4 |
| 89 | Thermodynamic properties of nitrogen from a perturbation theory for ISM fluids. Chemical Physics Letters, 1982, 85, 117-119. | 1.2 | 2 |
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| 91 | The Radial Boundary of Polyelectrolyte Solutions Containing Asymmetrical Salts. Molecular Simulation, 1999, 21, 249-255. | 0.9 | 2 |
| 92 | Fractal analysis of ionic trajectories in electrolyte solutions. Chemical Physics Letters, 1991, 183, 125-128. | 1.2 | 1 |
| 93 | Connectivity in a binary mixture of randomly centered spheres with selective particle clustering. Journal of Chemical Physics, 1994, 100, 1769-1770. | 1.2 | 0 |