Jordi Marti Rabassa

List of Publications by Year
in descending order

77	2,550	172207	205818
papers	citations	29 h-index	48 g-index

83	83	83	2200
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hydrogen bond structure of liquid water confined in nanotubes. Chemical Physics Letters, 2000, 329, 341-345.	1.2	274
2	Molecular dynamics simulation of liquid water along the coexistence curve: Hydrogen bonds and vibrational spectra. Journal of Chemical Physics, 1996, 105, 639-649.	1.2	249
3	A molecular dynamics simulation study of hydrogen bonding in aqueous ionic solutions. Journal of Molecular Liquids, 2005, 117, 63-67.	2.3	112
4	Dynamics in hydrogen bonded liquids: water and alcohols. Journal of Molecular Liquids, 2002, 96-97, 3-17.	2.3	99
5	Hydrogen Bond Structure and Dynamics in Aqueous Electrolytes at Ambient and Supercritical Conditions. Journal of Physical Chemistry B, 2006, 110, 6332-6338.	1.2	99
6	Molecular dynamics description of a layer of water molecules on a hydrophobic surface. Journal of Chemical Physics, 2002, 117, 3425-3430.	1.2	81
7	Molecular Dynamics Simulation of Liquid Water Confined inside Graphite Channels:Â Dielectric and Dynamical Properties. Journal of Physical Chemistry B, 2006, 110, 23987-23994.	1.2	74
8	Structure of water adsorbed on a single graphene sheet. Physical Review B, 2008, 78, .	1.1	74
9	An interpretation of the low-frequency spectrum of liquid water. Journal of Chemical Physics, 2003, 118, 452-453.	1.2	72
10	Molecular simulation of liquid water confined inside graphite channels: Thermodynamics and structural properties. Journal of Chemical Physics, 2006, 124, 094703.	1.2	71
11	Molecular dynamics calculation of the infrared spectra in liquid H2O-D2O mixtures. Journal of Molecular Liquids, 1994, 62, 17-31.	2.3	59
12	Time-dependent properties of liquid water isotopes adsorbed in carbon nanotubes. Journal of Chemical Physics, 2001, 114, 10486-10492.	1.2	55
13	Molecular dynamics simulations of water confined in graphene nanochannels: From ambient to supercritical environments. Journal of Molecular Liquids, 2010, 153, 72-78.	2.3	53
14	Structure of water nanoconfined between hydrophobic surfaces. Journal of Chemical Physics, 2005, 123, 054707.	1.2	52
15	Hydrogen bonding in supercritical water confined in carbon nanotubes. Chemical Physics Letters, 2001, 341, 250-254.	1.2	51
16	Effects of concentration on structure, dielectric, and dynamic properties of aqueous NaCl solutions using a polarizable model. Journal of Chemical Physics, 2010, 132, 214505.	1.2	50
17	Protons in Supercritical Water:â€‰ A Multistate Empirical Valence Bond Study. Journal of the American Chemical Society, 2004, 126, 2125-2134.	6.6	46
18	Structure and dynamics of liquid water adsorbed on the external walls of carbon nanotubes. Journal of Chemical Physics, 2003, 119, 12540-12546.	1.2	45

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19	Specific Ion Binding at Phospholipid Membrane Surfaces. Journal of Chemical Theory and Computation, 2015, 11, 4495-4499.	2.3	45
20	Water on graphene surfaces. Journal of Physics Condensed Matter, 2010, 22, 284111.	0.7	43
21	Specific ion effects in aqueous eletrolyte solutions confined within graphene sheets at the nanometric scale. Physical Chemistry Chemical Physics, 2012, 14, 10799.	1.3	43
22	Effect of Surface Roughness on the Static and Dynamic Properties of Water Adsorbed on Graphene. Journal of Physical Chemistry B, 2010, 114, 4583-4589.	1.2	42
23	Computer Simulation of Molecular Motions in Liquids: Infrared Spectra of Water and Heavy Water. Molecular Simulation, 1993, 11, 321-336.	0.9	41
24	Transition path sampling study of flip-flop transitions in model lipid bilayer membranes. Physical Review E, 2004, 69, 061918.	0.8	40
25	¹H Nuclear Spin Relaxation of Liquid Water from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 1966-1973.	1.2	39
26	Liquid Water Confined in Carbon Nanochannels at High Temperatures. Journal of Physical Chemistry B, 2007, 111, 12524-12530.	1.2	35
27	Aqueous electrolytes confined within functionalized silica nanopores. Journal of Chemical Physics, 2011, 135, 104503.	1.2	34
28	Diffusion and spectroscopy of water and lipids in fully hydrated dimyristoylphosphatidylcholine bilayer membranes. Journal of Chemical Physics, 2014, 140, 104901.	1.2	34
29	Microscopic dynamics of confined supercritical water. Chemical Physics Letters, 2002, 354, 227-232.	1.2	33
30	Molecular dynamics simulation of liquid water at 523 K. Journal of Physics Condensed Matter, 1994, 6, 2283-2290.	0.7	32
31	Comment on â€œAn interpretation of the low-frequency spectrum of liquid waterâ€•[J. Chem. Phys. 118, 452 (2003)]. Journal of Chemical Physics, 2004, 120, 1657-1658.	1.2	30
32	Pair interactions among ternary DPPC/POPC/cholesterol mixtures in liquid-ordered and liquid-disordered phases. Soft Matter, 2016, 12, 4557-4561.	1.2	22
33	Reorientational motions in sub- and supercritical water under extreme confinement. Chemical Physics Letters, 2002, 365, 536-541.	1.2	21
34	Protons in Non-ionic Aqueous Reverse Micelles. Journal of Physical Chemistry B, 2007, 111, 4432-4439.	1.2	18
35	Flip-flop dynamics in a model lipid bilayer membrane. Europhysics Letters, 2003, 61, 409-414.	0.7	17
36	Exploring the Picosecond Time Domain of the Solvation Dynamics of Coumarin 153 within Î²-Cyclodextrins. Journal of Physical Chemistry B, 2008, 112, 8990-8998.	1.2	17

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37	Molecular dynamics simulations of supercritical water confined within a carbon-slit pore. Physical Review E, 2009, 79, 031606.	0.8	17
38	Long-lasting Salt Bridges Provide the Anchoring Mechanism of Oncogenic Kirsten Rat Sarcoma Proteins at Cell Membranes. Journal of Physical Chemistry Letters, 2020, 11, 9938-9945.	2.1	17
39	Reorientational dynamics of water in aqueous ionic solutions at supercritical conditions: A computer simulation study. Journal of Molecular Liquids, 2006, 125, 107-114.	2.3	16
40	Characterization of the Methaneâ€“Graphene Hydrophobic Interaction in Aqueous Solution from Ab Initio Simulations. Journal of Chemical Theory and Computation, 2013, 9, 5070-5075.	2.3	16
41	Structure and Dynamics of Water at Carbon-Based Interfaces. Entropy, 2017, 19, 135.	1.1	16
42	Binding and dynamics of melatonin at the interface of phosphatidylcholine-cholesterol membranes. PLoS ONE, 2019, 14, e0224624.	1.1	16
43	Density dependence of reorientational dynamics in supercritical water. Journal of Molecular Liquids, 2002, 101, 137-147.	2.3	15
44	High temperature behavior of water inside flat graphite nanochannels. Physical Review B, 2007, 75, .	1.1	14
45	Cellular absorption of small molecules: free energy landscapes of melatonin binding at phospholipid membranes. Scientific Reports, 2020, 10, 9235.	1.6	14
46	Dynamics of water nanodroplets and aqueous protons in non-ionic reverse micelles. Physical Chemistry Chemical Physics, 2009, 11, 1484.	1.3	13
47	Wetting and prewetting of water on top of a single sheet of hexagonal boron nitride. Physical Review E, 2011, 84, 011602.	0.8	13
48	Effects of cholesterol on the binding of the precursor neurotransmitter tryptophan to zwitterionic membranes. Journal of Chemical Physics, 2018, 149, 164906.	1.2	13
49	A molecular dynamics transition path sampling study of model lipid bilayer membranes in aqueous environments. Journal of Physics Condensed Matter, 2004, 16, 5669-5678.	0.7	11
50	Fitting properties from density functional theory based molecular dynamics simulations to parameterize a rigid water force field. Journal of Chemical Physics, 2012, 136, 054103.	1.2	11
51	Size effects on water adsorbed on hydrophobic probes at the nanometric scale. Journal of Chemical Physics, 2013, 138, 214702.	1.2	10
52	Free-energy surfaces of ionic adsorption in cholesterol-free and cholesterol-rich phospholipid membranes. Molecular Simulation, 2018, 44, 1136-1146.	0.9	10
53	Microscopic Interactions of Melatonin, Serotonin and Tryptophan with Zwitterionic Phospholipid Membranes. International Journal of Molecular Sciences, 2021, 22, 2842.	1.8	10
54	Predicting the conformational variability of oncogenic GTP-bound G12D mutated KRas-4B proteins at zwitterionic model cell membranes. Nanoscale, 2022, 14, 3148-3158.	2.8	10

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55	A molecular dynamics study of heavy water steam. Molecular Physics, 1995, 86, 263-271.	0.8	9
56	Ion solvation in aqueous supercritical electrolyte solutions at finite concentrations: a computer simulation study. Theoretical Chemistry Accounts, 2006, 115, 161-169.	0.5	9
57	In Silico Drug Design of Benzothiadiazine Derivatives Interacting with Phospholipid Cell Membranes. Membranes, 2022, 12, 331.	1.4	9
58	Influence of Cholesterol on the Orientation of the Farnesylated GTP-Bound KRas-4B Binding with Anionic Model Membranes. Membranes, 2020, 10, 364.	1.4	8
59	Structure of benzothiadiazine at zwitterionic phospholipid cell membranes. Journal of Chemical Physics, 2021, 155, 154303.	1.2	8
60	Pattern recognition and data mining software based on artificial neural networks applied to proton transfer in aqueous environments. Chinese Physics B, 2014, 23, 046101.	0.7	7
61	Dynamical aspects of intermolecular proton transfer in liquid water and low-density amorphous ices. Physical Review E, 2014, 89, 052130.	0.8	7
62	Molecular Dynamics of Di-palmitoyl-phosphatidyl-choline Biomembranes in Ionic Solution: Adsorption of the Precursor Neurotransmitter Tryptophan. Procedia Computer Science, 2017, 108, 1242-1250.	1.2	7
63	Binding free energies of small-molecules in phospholipid membranes: Aminoacids, serotonin and melatonin. Chemical Physics Letters, 2018, 712, 190-195.	1.2	7
64	Proton transfer in liquid water confined inside graphene slabs. Physical Review E, 2015, 92, 032402.	0.8	6
65	Free energy landscapes of sodium ions bound to DMPCâ€“cholesterol membrane surfaces at infinite dilution. Physical Chemistry Chemical Physics, 2016, 18, 9036-9041.	1.3	5
66	Temperature dependence of the generalized frequency distribution of water molecules: comparison of experiments and molecular dynamics simulations. Molecular Simulation, 2005, 31, 1019-1025.	0.9	4
67	Excess protons in mesoscopic water-acetone nanoclusters. Journal of Chemical Physics, 2012, 137, 194301.	1.2	4
68	Multistate empirical valence bond study of temperature and confinement effects on proton transfer in water inside hydrophobic nanochannels. Journal of Computational Chemistry, 2016, 37, 1935-1946.	1.5	4
69	Surface Behavior of Aprotic Mixtures: Dimethyl Sulfoxide/Acetonitrile. Journal of Physical Chemistry C, 2017, 121, 14618-14627.	1.5	3
70	Atomic Data Mining Numerical Methods, Source Code SQlite with Python. Procedia, Social and Behavioral Sciences, 2013, 73, 232-239.	0.5	2
71	AJAC: Atomic data calculation tool in Python. Chinese Physics B, 2013, 22, 048901.	0.7	1
72	Efficient recursive Adamsâ€“Bashforth methods in molecular dynamics simulations of N-body systems interacting through pairwise potentials. Molecular Simulation, 2020, 46, 1248-1254.	0.9	1

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73	Maintenance and Reengineering of Software: Creating a Visual C++ Graphical User Interface to Perform Specific Tasks Related to Soil Structure Interaction in Poroelastic Soil. Information Technology Journal, 2012, 11, 1553-1569.	0.3	1
74	Software Refactoring: Solving the Time-Dependent Schrodinger Equation via Fast Fourier Transforms and Parallel Programming. Journal of Applied Sciences, 2012, 12, 2115-2127.	0.1	1
75	Nucleation of Helium in Liquid Lithium at 843 K and High Pressures. Materials, 2022, 15, 2866.	1.3	1
76	Modeling and Simulation of Lipid Membranes. Membranes, 2022, 12, 549.	1.4	1
77	Potentials of mean force in acidic proton transfer reactions in constrained geometries. Molecular Simulation, 2017, 43, 134-140.	0.9	0