

Jordi Marti Rabassa

List of Publications by Year in descending order

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77
papers

2,550
citations

172207

29
h-index

205818

48
g-index

83
all docs

83
docs citations

83
times ranked

2200
citing authors

#	ARTICLE	IF	CITATIONS
1	Predicting the conformational variability of oncogenic GTP-bound G12D mutated KRas-4B proteins at zwitterionic model cell membranes. <i>Nanoscale</i> , 2022, 14, 3148-3158.	2.8	10
2	In Silico Drug Design of Benzothiadiazine Derivatives Interacting with Phospholipid Cell Membranes. <i>Membranes</i> , 2022, 12, 331.	1.4	9
3	Nucleation of Helium in Liquid Lithium at 843 K and High Pressures. <i>Materials</i> , 2022, 15, 2866.	1.3	1
4	Modeling and Simulation of Lipid Membranes. <i>Membranes</i> , 2022, 12, 549.	1.4	1
5	Microscopic Interactions of Melatonin, Serotonin and Tryptophan with Zwitterionic Phospholipid Membranes. <i>International Journal of Molecular Sciences</i> , 2021, 22, 2842.	1.8	10
6	Structure of benzothiadiazine at zwitterionic phospholipid cell membranes. <i>Journal of Chemical Physics</i> , 2021, 155, 154303.	1.2	8
7	Efficient recursive Adams-Bashforth methods in molecular dynamics simulations of N-body systems interacting through pairwise potentials. <i>Molecular Simulation</i> , 2020, 46, 1248-1254.	0.9	1
8	Cellular absorption of small molecules: free energy landscapes of melatonin binding at phospholipid membranes. <i>Scientific Reports</i> , 2020, 10, 9235.	1.6	14
9	Influence of Cholesterol on the Orientation of the Farnesylated GTP-Bound KRas-4B Binding with Anionic Model Membranes. <i>Membranes</i> , 2020, 10, 364.	1.4	8
10	Long-lasting Salt Bridges Provide the Anchoring Mechanism of Oncogenic Kirsten Rat Sarcoma Proteins at Cell Membranes. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9938-9945.	2.1	17
11	Binding and dynamics of melatonin at the interface of phosphatidylcholine-cholesterol membranes. <i>PLoS ONE</i> , 2019, 14, e0224624.	1.1	16
12	Free-energy surfaces of ionic adsorption in cholesterol-free and cholesterol-rich phospholipid membranes. <i>Molecular Simulation</i> , 2018, 44, 1136-1146.	0.9	10
13	Binding free energies of small-molecules in phospholipid membranes: Aminoacids, serotonin and melatonin. <i>Chemical Physics Letters</i> , 2018, 712, 190-195.	1.2	7
14	Effects of cholesterol on the binding of the precursor neurotransmitter tryptophan to zwitterionic membranes. <i>Journal of Chemical Physics</i> , 2018, 149, 164906.	1.2	13
15	Molecular Dynamics of Di-palmitoyl-phosphatidyl-choline Biomembranes in Ionic Solution: Adsorption of the Precursor Neurotransmitter Tryptophan. <i>Procedia Computer Science</i> , 2017, 108, 1242-1250.	1.2	7
16	Surface Behavior of Aprotic Mixtures: Dimethyl Sulfoxide/Acetonitrile. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14618-14627.	1.5	3
17	Potentials of mean force in acidic proton transfer reactions in constrained geometries. <i>Molecular Simulation</i> , 2017, 43, 134-140.	0.9	0
18	Structure and Dynamics of Water at Carbon-Based Interfaces. <i>Entropy</i> , 2017, 19, 135.	1.1	16

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19	Pair interactions among ternary DPPC/POPC/cholesterol mixtures in liquid-ordered and liquid-disordered phases. <i>Soft Matter</i> , 2016, 12, 4557-4561.	1.2	22
20	Multistate empirical valence bond study of temperature and confinement effects on proton transfer in water inside hydrophobic nanochannels. <i>Journal of Computational Chemistry</i> , 2016, 37, 1935-1946.	1.5	4
21	Free energy landscapes of sodium ions bound to DMPCâ€“cholesterol membrane surfaces at infinite dilution. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 9036-9041.	1.3	5
22	Proton transfer in liquid water confined inside graphene slabs. <i>Physical Review E</i> , 2015, 92, 032402.	0.8	6
23	¹ H Nuclear Spin Relaxation of Liquid Water from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1966-1973.	1.2	39
24	Specific Ion Binding at Phospholipid Membrane Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4495-4499.	2.3	45
25	Pattern recognition and data mining software based on artificial neural networks applied to proton transfer in aqueous environments. <i>Chinese Physics B</i> , 2014, 23, 046101.	0.7	7
26	Diffusion and spectroscopy of water and lipids in fully hydrated dimyristoylphosphatidylcholine bilayer membranes. <i>Journal of Chemical Physics</i> , 2014, 140, 104901.	1.2	34
27	Dynamical aspects of intermolecular proton transfer in liquid water and low-density amorphous ices. <i>Physical Review E</i> , 2014, 89, 052130.	0.8	7
28	Atomic Data Mining Numerical Methods, Source Code SQLite with Python. <i>Procedia, Social and Behavioral Sciences</i> , 2013, 73, 232-239.	0.5	2
29	Size effects on water adsorbed on hydrophobic probes at the nanometric scale. <i>Journal of Chemical Physics</i> , 2013, 138, 214702.	1.2	10
30	Characterization of the Methaneâ€“Graphene Hydrophobic Interaction in Aqueous Solution from <i>Ab Initio</i> Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5070-5075.	2.3	16
31	AJAC: Atomic data calculation tool in Python. <i>Chinese Physics B</i> , 2013, 22, 048901.	0.7	1
32	Fitting properties from density functional theory based molecular dynamics simulations to parameterize a rigid water force field. <i>Journal of Chemical Physics</i> , 2012, 136, 054103.	1.2	11
33	Specific ion effects in aqueous electrolyte solutions confined within graphene sheets at the nanometric scale. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10799.	1.3	43
34	Excess protons in mesoscopic water-acetone nanoclusters. <i>Journal of Chemical Physics</i> , 2012, 137, 194301.	1.2	4
35	Maintenance and Reengineering of Software: Creating a Visual C++ Graphical User Interface to Perform Specific Tasks Related to Soil Structure Interaction in Poroelastic Soil. <i>Information Technology Journal</i> , 2012, 11, 1553-1569.	0.3	1
36	Software Refactoring: Solving the Time-Dependent Schrodinger Equation via Fast Fourier Transforms and Parallel Programming. <i>Journal of Applied Sciences</i> , 2012, 12, 2115-2127.	0.1	1

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37	Aqueous electrolytes confined within functionalized silica nanopores. <i>Journal of Chemical Physics</i> , 2011, 135, 104503.	1.2	34
38	Wetting and prewetting of water on top of a single sheet of hexagonal boron nitride. <i>Physical Review E</i> , 2011, 84, 011602.	0.8	13
39	Water on graphene surfaces. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 284111.	0.7	43
40	Molecular dynamics simulations of water confined in graphene nanochannels: From ambient to supercritical environments. <i>Journal of Molecular Liquids</i> , 2010, 153, 72-78.	2.3	53
41	Effects of concentration on structure, dielectric, and dynamic properties of aqueous NaCl solutions using a polarizable model. <i>Journal of Chemical Physics</i> , 2010, 132, 214505.	1.2	50
42	Effect of Surface Roughness on the Static and Dynamic Properties of Water Adsorbed on Graphene. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4583-4589.	1.2	42
43	Molecular dynamics simulations of supercritical water confined within a carbon-slit pore. <i>Physical Review E</i> , 2009, 79, 031606.	0.8	17
44	Dynamics of water nanodroplets and aqueous protons in non-ionic reverse micelles. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1484.	1.3	13
45	Structure of water adsorbed on a single graphene sheet. <i>Physical Review B</i> , 2008, 78, .	1.1	74
46	Exploring the Picosecond Time Domain of the Solvation Dynamics of Coumarin 153 within β -Cyclodextrins. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8990-8998.	1.2	17
47	High temperature behavior of water inside flat graphite nanochannels. <i>Physical Review B</i> , 2007, 75, .	1.1	14
48	Protons in Non-ionic Aqueous Reverse Micelles. <i>Journal of Physical Chemistry B</i> , 2007, 111, 4432-4439.	1.2	18
49	Liquid Water Confined in Carbon Nanochannels at High Temperatures. <i>Journal of Physical Chemistry B</i> , 2007, 111, 12524-12530.	1.2	35
50	Molecular simulation of liquid water confined inside graphite channels: Thermodynamics and structural properties. <i>Journal of Chemical Physics</i> , 2006, 124, 094703.	1.2	71
51	Molecular Dynamics Simulation of Liquid Water Confined inside Graphite Channels: Dielectric and Dynamical Properties. <i>Journal of Physical Chemistry B</i> , 2006, 110, 23987-23994.	1.2	74
52	Hydrogen Bond Structure and Dynamics in Aqueous Electrolytes at Ambient and Supercritical Conditions. <i>Journal of Physical Chemistry B</i> , 2006, 110, 6332-6338.	1.2	99
53	Reorientational dynamics of water in aqueous ionic solutions at supercritical conditions: A computer simulation study. <i>Journal of Molecular Liquids</i> , 2006, 125, 107-114.	2.3	16
54	Ion solvation in aqueous supercritical electrolyte solutions at finite concentrations: a computer simulation study. <i>Theoretical Chemistry Accounts</i> , 2006, 115, 161-169.	0.5	9

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55	A molecular dynamics simulation study of hydrogen bonding in aqueous ionic solutions. <i>Journal of Molecular Liquids</i> , 2005, 117, 63-67.	2.3	112
56	Temperature dependence of the generalized frequency distribution of water molecules: comparison of experiments and molecular dynamics simulations. <i>Molecular Simulation</i> , 2005, 31, 1019-1025.	0.9	4
57	Structure of water nanoconfined between hydrophobic surfaces. <i>Journal of Chemical Physics</i> , 2005, 123, 054707.	1.2	52
58	A molecular dynamics transition path sampling study of model lipid bilayer membranes in aqueous environments. <i>Journal of Physics Condensed Matter</i> , 2004, 16, 5669-5678.	0.7	11
59	Transition path sampling study of flip-flop transitions in model lipid bilayer membranes. <i>Physical Review E</i> , 2004, 69, 061918.	0.8	40
60	Comment on "An interpretation of the low-frequency spectrum of liquid water" [J. Chem. Phys. 118, 452 (2003)]. <i>Journal of Chemical Physics</i> , 2004, 120, 1657-1658.	1.2	30
61	Protons in Supercritical Water: A Multistate Empirical Valence Bond Study. <i>Journal of the American Chemical Society</i> , 2004, 126, 2125-2134.	6.6	46
62	Structure and dynamics of liquid water adsorbed on the external walls of carbon nanotubes. <i>Journal of Chemical Physics</i> , 2003, 119, 12540-12546.	1.2	45
63	An interpretation of the low-frequency spectrum of liquid water. <i>Journal of Chemical Physics</i> , 2003, 118, 452-453.	1.2	72
64	Flip-flop dynamics in a model lipid bilayer membrane. <i>Europhysics Letters</i> , 2003, 61, 409-414.	0.7	17
65	Molecular dynamics description of a layer of water molecules on a hydrophobic surface. <i>Journal of Chemical Physics</i> , 2002, 117, 3425-3430.	1.2	81
66	Dynamics in hydrogen bonded liquids: water and alcohols. <i>Journal of Molecular Liquids</i> , 2002, 96-97, 3-17.	2.3	99
67	Density dependence of reorientational dynamics in supercritical water. <i>Journal of Molecular Liquids</i> , 2002, 101, 137-147.	2.3	15
68	Microscopic dynamics of confined supercritical water. <i>Chemical Physics Letters</i> , 2002, 354, 227-232.	1.2	33
69	Reorientational motions in sub- and supercritical water under extreme confinement. <i>Chemical Physics Letters</i> , 2002, 365, 536-541.	1.2	21
70	Hydrogen bonding in supercritical water confined in carbon nanotubes. <i>Chemical Physics Letters</i> , 2001, 341, 250-254.	1.2	51
71	Time-dependent properties of liquid water isotopes adsorbed in carbon nanotubes. <i>Journal of Chemical Physics</i> , 2001, 114, 10486-10492.	1.2	55
72	Hydrogen bond structure of liquid water confined in nanotubes. <i>Chemical Physics Letters</i> , 2000, 329, 341-345.	1.2	274

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73	Molecular dynamics simulation of liquid water along the coexistence curve: Hydrogen bonds and vibrational spectra. <i>Journal of Chemical Physics</i> , 1996, 105, 639-649.	1.2	249
74	A molecular dynamics study of heavy water steam. <i>Molecular Physics</i> , 1995, 86, 263-271.	0.8	9
75	Molecular dynamics simulation of liquid water at 523 K. <i>Journal of Physics Condensed Matter</i> , 1994, 6, 2283-2290.	0.7	32
76	Molecular dynamics calculation of the infrared spectra in liquid H ₂ O-D ₂ O mixtures. <i>Journal of Molecular Liquids</i> , 1994, 62, 17-31.	2.3	59
77	Computer Simulation of Molecular Motions in Liquids: Infrared Spectra of Water and Heavy Water. <i>Molecular Simulation</i> , 1993, 11, 321-336.	0.9	41