Mario G Del PÃ³polo

List of Publications by Year
in descending order

51 papers	3,484 citations	279798 23 h-index	182427 51 g-index

51 all docs	51 docs citations	51 times ranked	3243 citing authors

#	Article	IF	Citations
1	On the Structure and Dynamics of Ionic Liquids. Journal of Physical Chemistry B, 2004, 108, 1744-1752.	2.6	649
2	Liquids with permanent porosity. Nature, 2015, 527, 216-220.	27.8	402
3	Molecular Dynamics Simulation of Ionic Liquids:â€‰ The Effect of Electronic Polarizability. Journal of Physical Chemistry B, 2004, 108, 11877-11881.	2.6	393
4	Ab Initio Molecular Dynamics Simulation of a Room Temperature Ionic Liquid. Journal of Physical Chemistry B, 2005, 109, 5895-5902.	2.6	269
5	Simulations of Ionic Liquids, Solutions, and Surfaces. Accounts of Chemical Research, 2007, 40, 1138-1145.	15.6	267
6	Structure and Dynamics of a Confined Ionic Liquid. Topics of Relevance to Dye-Sensitized Solar Cells. Journal of Physical Chemistry B, 2005, 109, 17922-17927.	2.6	202
7	Polarization Relaxation in an Ionic Liquid Confined between Electrified Wallsâ€. Journal of Physical Chemistry B, 2007, 111, 4877-4884.	2.6	138
8	Alkylated organic cages: from porous crystals to neat liquids. Chemical Science, 2012, 3, 2153.	7.4	123
9	Simulation of interfaces between room temperature ionic liquids and other liquids. Faraday Discussions, 2005, 129, 57.	3.2	118
10	Designing and understanding permanent microporosity in liquids. Physical Chemistry Chemical Physics, 2014, 16, 9422-9431.	2.8	80
11	Ion Association in [bmim][PF₆]/Naphthalene Mixtures: An Experimental and Computational Study. Journal of the American Chemical Society, 2008, 130, 7032-7041.	13.7	72
12	Development of Complex Classical Force Fields through Force Matching to ab Initio Data:Â Application to a Room-Temperature Ionic Liquid. Journal of Physical Chemistry B, 2006, 110, 5697-5707.	2.6	62
13	Solvation Structure and Transport of Acidic Protons in Ionic Liquids:Â A First-principles Simulation Study. Journal of Physical Chemistry B, 2006, 110, 8798-8803.	2.6	61
14	Neutral and Charged 1-Butyl-3-methylimidazolium Triflate Clusters:Â Equilibrium Concentration in the Vapor Phase and Thermal Properties of Nanometric Dropletsâ€. Journal of Physical Chemistry B, 2007, 111, 4938-4950.	2.6	57
15	Clusters, Liquids, and Crystals of Dialkyimidazolium Salts. A Combined Perspective from ab Initio and Classical Computer Simulations. Accounts of Chemical Research, 2007, 40, 1156-1164.	15.6	47
16	Molecular electrostatic properties of ions in an ionic liquid. Molecular Physics, 2006, 104, 2477-2483.	1.7	43
17	Dry Excess Electrons in Room-Temperature Ionic Liquids. Journal of the American Chemical Society, 2011, 133, 20186-20193.	13.7	40
18	Interaction of Room Temperature Ionic Liquid Solutions with a Cholesterol Bilayer. Journal of Physical Chemistry B, 2009, 113, 11642-11648.	2.6	39

#	Article	IF	Citations
19	Nanometric ionic-liquid films on silica: a joint experimental and computational study. Journal of Physics Condensed Matter, 2009, 21, 424118.	1.8	33
20	The interfacial electrostatic potential modulates the insertion of cell-penetrating peptides into lipid bilayers. Physical Chemistry Chemical Physics, 2018, 20, 5180-5189.	2.8	33
21	Insights into mechanochemical reactions at the molecular level: simulated indentations of aspirin and meloxicam crystals. Chemical Science, 2019, 10, 2924-2929.	7.4	29
22	Kinetic Monte Carlo Study of Electrochemical Growth in a Heteroepitaxial System. Langmuir, 2002, 18, 9087-9094.	3.5	25
23	Simulation Study of Pd Submonolayer Films on Au(hkl) and Pt(hkl) and Their Relationship to Underpotential Deposition. Langmuir, 2000, 16, 9539-9546.	3.5	24
24	On the Stability of Electrochemically Generated Nanoclusters-A Computer Simulation. Angewandte Chemie - International Edition, 2001, 40, 4674-4676.	13.8	22
25	Interaction of a Polyarginine Peptide with Membranes of Different Mechanical Properties. Biomolecules, 2019, 9, 625.	4.0	21
26	Local and semilocal density functional computations for crystals of 1-alkyl-3-methyl-imidazolium salts. Journal of Chemical Physics, 2007, 126, 144705.	3.0	20
27	Nano-indentation of a room-temperature ionic liquid film on silica: a computational experiment. Physical Chemistry Chemical Physics, 2012, 14, 2475.	2.8	17
28	Interaction of glycine, lysine, proline and histidine with dipalmitoylphosphatidylcholine lipid bilayers: a theoretical and experimental study. RSC Advances, 2015, 5, 43537-43546.	3.6	17
29	Negative Dipole Potentials and Carboxylic Polar Head Groups Foster the Insertion of Cell-Penetrating Peptides into Lipid Monolayers. Langmuir, 2018, 34, 3102-3111.	3.5	16
30	Hopanoids Like Sterols Form Compact but Fluid Films. Langmuir, 2019, 35, 9848-9857.	3.5	16
31	Nanoparticles modified with cell penetrating peptides: Assessing adsorption on membranes containing acidic lipids. Colloids and Surfaces B: Biointerfaces, 2021, 197, 111373.	5.0	15
32	Adsorption and insertion of polyarginine peptides into membrane pores: The trade-off between electrostatics, acid-base chemistry and pore formation energy. Journal of Colloid and Interface Science, 2019, 552, 701-711.	9.4	12
33	Effects of tip structure on the generation of metal clusters by an STM tip: a way to control the orientation of nanocrystallites?. Nanotechnology, 2005, 16, 974-980.	2.6	11
34	Mesophases in Nearly 2D Room-Temperature Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 15602-15609.	2.6	11
35	Noria and its derivatives as hosts for chemically and thermally robust Type II porous liquids. Chemical Science, 2021, 12, 14230-14240.	7.4	10
36	Simple models of complex aggregation: Vesicle formation by soft repulsive spheres with dipolelike interactions. Physical Review E, 2006, 73, 031404.	2.1	9

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37	On the Mechanism of the Iodideâ€“Triiodide Exchange Reaction in a Solid-State Ionic Liquid. Journal of Physical Chemistry B, 2017, 121, 6436-6441.	2.6	8
38	Molecular-level insight into the binding of arginine to a zwitterionic Langmuir monolayer. RSC Advances, 2017, 7, 30862-30869.	3.6	8
39	Thermodynamics of cell penetrating peptides on lipid membranes: sequence and membrane acidity regulate surface binding. Physical Chemistry Chemical Physics, 2020, 22, 23399-23410.	2.8	8
40	Surface charge density and fatty acids enhance the membrane permeation rate of CPPâ€“cargo complexes. Soft Matter, 2020, 16, 9890-9898.	2.7	8
41	Melting behavior of an idealized membrane model. Journal of Chemical Physics, 2008, 128, 024705.	3.0	7
42	Amphiphilic Character and Aggregation Properties of Small Cholesterol Islands on Water: A Simulation Study. Journal of Physical Chemistry B, 2009, 113, 4674-4687.	2.6	7
43	Using Intrinsic Surfaces To Calculate the Free-Energy Change When Nanoparticles Adsorb on Membranes. Journal of Physical Chemistry B, 2018, 122, 6417-6422.	2.6	7
44	Monte Carlo Simulation of Properties of Monolayers and Metal Islands Adsorbed on Metallic (111) Surfaces. Langmuir, 2004, 20, 4279-4288.	3.5	6
45	Mechanisms of Iodideâ€“Triiodide Exchange Reactions in Ionic Liquids: A Reactive Molecular-Dynamics Exploration. International Journal of Molecular Sciences, 2019, 20, 1123.	4.1	5
46	Melting of a tetrahedral network model of silica. Physical Chemistry Chemical Physics, 2009, 11, 10820.	2.8	4
47	Elucidating mysteries of phase-segregated membranes: mobile-lipid recruitment facilitates poresâ€™ passage to the fluid phase. Physical Chemistry Chemical Physics, 2018, 20, 19234-19239.	2.8	4
48	Voltage-Induced Adsorption of Cationic Nanoparticles on Lipid Membranes. Journal of Physical Chemistry B, 2022, 126, 2230-2240.	2.6	4
49	On the Reasons for Stepwise Changes in the Tunneling Current across Metallic Nanogaps. Nano Letters, 2003, 3, 1633-1637.	9.1	3
50	H-bond refinement for electron transfer membrane-bound proteinâ€“protein complexes: Cytochrome c oxidase and cytochrome c552. Computational Biology and Chemistry, 2013, 47, 31-36.	2.3	1
51	Molecular Explanation for the Abnormal Flux of Material into a Hot Spot in Ester Monolayers. Journal of Physical Chemistry B, 2017, 121, 5621-5632.	2.6	1