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	Voltage-Induced Adsorption of Cationic Nanoparticles on Lipid Membranes. Journal of Physical Chemistry B, 2022, 126, 2230-2240.	2.6	4
2	Nanoparticles modified with cell penetrating peptides: Assessing adsorption on membranes containing acidic lipids. Colloids and Surfaces B: Biointerfaces, 2021, 197, 111373.	5.0	15
3	Noria and its derivatives as hosts for chemically and thermally robust Type II porous liquids. Chemical Science, 2021, 12, 14230-14240.	7.4	10
4	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
5	Surface charge density and fatty acids enhance the membrane permeation rate of CPPâ€“cargo complexes. Soft Matter, 2020, 16, 9890-9898.	2.7	8
6	Hopanoids Like Sterols Form Compact but Fluid Films. Langmuir, 2019, 35, 9848-9857.	3.5	16
7	Interaction of a Polyarginine Peptide with Membranes of Different Mechanical Properties. Biomolecules, 2019, 9, 625.	4.0	21
8	Insights into mechanochemical reactions at the molecular level: simulated indentations of aspirin and meloxicam crystals. Chemical Science, 2019, 10, 2924-2929.	7.4	29
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	Molecular-level insight into the binding of arginine to a zwitterionic Langmuir monolayer. RSC Advances, 2017, 7, 30862-30869.	3.6	8
18	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

#	Article	IF	Citations
19	Liquids with permanent porosity. Nature, 2015, 527, 216-220.	27.8	402
20	Designing and understanding permanent microporosity in liquids. Physical Chemistry Chemical Physics, 2014, 16, 9422-9431.	2.8	80
21	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
22	Nano-indentation of a room-temperature ionic liquid film on silica: a computational experiment. Physical Chemistry Chemical Physics, 2012, 14, 2475.	2.8	17
23	Alkylated organic cages: from porous crystals to neat liquids. Chemical Science, 2012, 3, 2153.	7.4	123
24	Dry Excess Electrons in Room-Temperature Ionic Liquids. Journal of the American Chemical Society, 2011, 133, 20186-20193.	13.7	40
25	Nanometric ionic-liquid films on silica: a joint experimental and computational study. Journal of Physics Condensed Matter, 2009, 21, 424118.	1.8	33
26	Interaction of Room Temperature Ionic Liquid Solutions with a Cholesterol Bilayer. Journal of Physical Chemistry B, 2009, 113, 11642-11648.	2.6	39
27	Mesophases in Nearly 2D Room-Temperature Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 15602-15609.	2.6	11
28	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
29	Melting of a tetrahedral network model of silica. Physical Chemistry Chemical Physics, 2009, 11, 10820.	2.8	4
30	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
31	Melting behavior of an idealized membrane model. Journal of Chemical Physics, 2008, 128, 024705.	3.0	7
32	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
33	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
34	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
35	Simulations of Ionic Liquids, Solutions, and Surfaces. Accounts of Chemical Research, 2007, 40, 1138-1145.	15.6	267
36	Polarization Relaxation in an Ionic Liquid Confined between Electrified Wallsâ€. Journal of Physical Chemistry B, 2007, 111, 4877-4884.	2.6	138

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37	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
38	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
39	Molecular electrostatic properties of ions in an ionic liquid. Molecular Physics, 2006, 104, 2477-2483.	1.7	43
40	Simple models of complex aggregation: Vesicle formation by soft repulsive spheres with dipolelike interactions. Physical Review E, 2006, 73, 031404.	2.1	9
41	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
42	Simulation of interfaces between room temperature ionic liquids and other liquids. Faraday Discussions, 2005, 129, 57.	3.2	118
43	Ab Initio Molecular Dynamics Simulation of a Room Temperature Ionic Liquid. Journal of Physical Chemistry B, 2005, 109, 5895-5902.	2.6	269
44	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
45	Molecular Dynamics Simulation of Ionic Liquids:â€‰ The Effect of Electronic Polarizability. Journal of Physical Chemistry B, 2004, 108, 11877-11881.	2.6	393
46	Monte Carlo Simulation of Properties of Monolayers and Metal Islands Adsorbed on Metallic (111) Surfaces. Langmuir, 2004, 20, 4279-4288.	3.5	6
47	On the Structure and Dynamics of Ionic Liquids. Journal of Physical Chemistry B, 2004, 108, 1744-1752.	2.6	649
48	On the Reasons for Stepwise Changes in the Tunneling Current across Metallic Nanogaps. Nano Letters, 2003, 3, 1633-1637.	9.1	3
49	Kinetic Monte Carlo Study of Electrochemical Growth in a Heteroepitaxial System. Langmuir, 2002, 18, 9087-9094.	3.5	25
50	On the Stability of Electrochemically Generated Nanoclusters-A Computer Simulation. Angewandte Chemie - International Edition, 2001, 40, 4674-4676.	13.8	22
51	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