Leonardo JosÃ© Amaral de Siqueira

List of Publications by Year
in descending order

33 papers	988 citations	430874 18 h-index	434195 31 g-index
34 all docs	34 docs citations	34 times ranked	1196 citing authors

#	Article	IF	Citations
1	Alkoxy Chain Effect on the Viscosity of a Quaternary Ammonium Ionic Liquid: Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 1074-1079.	2.6	99
2	The Sulfur Dioxideâˆ'1-Butyl-3-Methylimidazolium Bromide Interaction:â€‰ Drastic Changes in Structural and Physical Properties. Journal of Physical Chemistry B, 2007, 111, 8717-8719.	2.6	95
3	Potential tuberculostatic agents. Topliss application on benzoic acid [(5-Nitro-thiophen-2-yl)-methylene]-hydrazide series. Bioorganic and Medicinal Chemistry, 2002, 10, 557-560.	3.0	81
4	Molecular Dynamics Simulation of the Ionic LiquidN-Ethyl-N,N-dimethyl-N-(2-methoxyethyl)ammonium Bis(trifluoromethanesulfonyl)imide. Journal of Physical Chemistry B, 2007, 111, 11776-11785.	2.6	71
5	From molten salts to room temperature ionic liquids: Simulation studies on chloroaluminate systems. Faraday Discussions, 2012, 154, 171-188.	3.2	59
6	Molecular dynamics simulation of the polymer electrolyte poly(ethyleneoxide)âˆ•LiClO4. I. Structural properties. Journal of Chemical Physics, 2005, 122, 194911.	3.0	58
7	Molecular dynamics simulation of the polymer electrolyte poly(ethylene oxide)/LiClO4. II. Dynamical properties. Journal of Chemical Physics, 2006, 125, 214903.	3.0	56
8	Charge ordering and intermediate range order in ammonium ionic liquids. Journal of Chemical Physics, 2011, 135, 204506.	3.0	56
9	Shielding of Ionic Interactions by Sulfur Dioxide in an Ionic Liquid. Journal of Physical Chemistry B, 2008, 112, 6430-6435.	2.6	52
10	Mechanism of Action of Thymol on Cell Membranes Investigated through Lipid Langmuir Monolayers at the Airâ€“Water Interface and Molecular Simulation. Langmuir, 2016, 32, 3234-3241.	3.5	47
11	Molecular Dynamics Simulations of Acidic Gases at Interface of Quaternary Ammonium Ionic Liquids. Journal of Physical Chemistry C, 2014, 118, 22012-22020.	3.1	27
12	Molecular Dynamics Simulations of Ether-Modified Phosphonium Ionic Liquid Confined in between Planar and Porous Graphene Electrode Models. Journal of Physical Chemistry C, 2019, 123, 10816-10825.	3.1	24
13	Comparing the performance of sulfonium and phosphonium ionic liquids as electrolytes for supercapacitors by molecular dynamics simulations. Electrochimica Acta, 2020, 364, 137181.	5.2	24
14	Molecular Dynamics Simulations of Polymerâ€“Ionic Liquid (1-Ethyl-3-methylimidazolium) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 227 Td (Information and Modeling, 2020, 60, 485-499.	5.4	23
15	Probing the local environment of hybrid materials designed from ionic liquids and synthetic clay by Raman spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 469-475.	3.9	20
16	Ether-Functionalized Sulfonium Ionic Liquid and Its Binary Mixtures with Acetonitrile as Electrolyte for Electrochemical Double Layer Capacitors: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2020, 124, 6679-6689.	2.6	20
17	Raman spectra of polymer electrolytes based on poly(ethylene glycol) dimethyl ether, lithium perchlorate, and the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate. Vibrational Spectroscopy, 2010, 54, 155-158.	2.2	19
18	Atomistic study of the physical properties of sulfonium-based ionic liquids as electrolyte for supercapacitors. Journal of Molecular Liquids, 2019, 296, 112065.	4.9	19

#	Article	IF	Citations
19	Molecular dynamics simulation of molten sodium chlorate. Journal of Chemical Physics, 2003, 119, 8002-8012.	3.0	18
20	Effect of SO₂ on the Transport Properties of an Imidazolium Ionic Liquid and Its Lithium Solution. Journal of Physical Chemistry B, 2011, 115, 9662-9670.	2.6	18
21	The Equilibrium Structure of Lithium Salt Solutions in Ether-Functionalized Ammonium Ionic Liquids. Journal of Physical Chemistry B, 2012, 116, 12319-12324.	2.6	16
22	Molecular dynamics simulations of polyethers and a quaternary ammonium ionic liquid as CO2 absorbers. Journal of Chemical Physics, 2018, 148, 134908.	3.0	13
23	Comparing Graphite and Graphene Oxide Supercapacitors with a Constant Potential Model. Journal of Physical Chemistry C, 2021, 125, 2318-2326.	3.1	13
24	Molecular dynamics and a spectroscopic study of sulfur dioxide absorption by an ionic liquid and its mixtures with PEO. Physical Chemistry Chemical Physics, 2016, 18, 28901-28910.	2.8	11
25	Vibrational characterization of poly(1-methylpyrrole-co-squaric acid) and poly(1-dodecylpyrrole-co-squaric acid) by enhanced Raman spectroscopy. Journal of Raman Spectroscopy, 2006, 37, 1346-1353.	2.5	10
26	Energy and power performances of binary mixtures of ionic liquids in planar and porous electrodes by molecular dynamics simulations. Electrochimica Acta, 2022, 410, 139982.	5.2	8
27	Monitoring the 1160cmâ˜1 band of pyridazine to investigate complexes with formamide. Vibrational Spectroscopy, 2011, 55, 273-278.	2.2	6
28	Structure of tetraalkylammonium ionic liquids in the interlayer of modified montmorillonite. Journal of Physics Condensed Matter, 2014, 26, 284107.	1.8	6
29	Development of coarse-grained force field to investigate sodium-ion transport mechanisms in cyanoborate-based ionic liquid. Journal of Molecular Liquids, 2021, 338, 116648.	4.9	6
30	Understanding the Influence of the Electrochemical Behavior of Potassium Hexacyanoferrate(II/III) on Acetonitrile/Water Binary Mixtures: An Experimental and Molecular Dynamics Study. Journal of Physical Chemistry C, 2018, 122, 2717-2725.	3.1	5
31	Synthesis of Furan Derivatives Condensed with Carbohydrates. Molecules, 2001, 6, 728-735.	3.8	4
32	Poly(p-phenylene vinylene-b-ethylene glycol) dispersed in butyltrimethylammonium bis(trifluoromethanesulfonyl)imide as luminescent ionic liquids. Materials Chemistry and Physics, 2022, 284, 126021.	4.0	3
33	Solvent effects and energy transfer processes in luminescent composite. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 397, 112581.	3.9	1