Lorenzo Gontrani

List of Publications by Year
in descending order

101 papers	3,119 citations	136950 32 h-index	175258 52 g-index
105 all docs	105 docs citations	105 times ranked	2779 citing authors

#	Article	IF	Citations
1	Mesoscopic Structural Heterogeneities in Room-Temperature Ionic Liquids. Journal of Physical Chemistry Letters, 2012, 3, 27-33.	4.6	352
2	Morphology and intermolecular dynamics of 1-alkyl-3-methylimidazolium bis{(trifluoromethane)sulfonyl}amide ionic liquids: structural and dynamic evidence of nanoscale segregation. Journal of Physics Condensed Matter, 2009, 21, 424121.	1.8	236
3	Cholinium-amino acid based ionic liquids: a new method of synthesis and physico-chemical characterization. Physical Chemistry Chemical Physics, 2015, 17, 20687-20698.	2.8	131
4	Glycine and alanine: a theoretical study of solvent effects upon energetics and molecular response properties. Computational and Theoretical Chemistry, 2000, 500, 113-127.	1.5	92
5	Structural Properties of 1-Alkyl-3-methylimidazolium Bis{(trifluoromethyl)sulfonyl}amide Ionic Liquids: X-ray Diffraction Data and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 16398-16407.	2.6	92
6	Liquid Structure of Trihexyltetradecylphosphonium Chloride at Ambient Temperature: An X-ray Scattering and Simulation Study. Journal of Physical Chemistry B, 2009, 113, 9235-9240.	2.6	91
7	Liquid structure of 1-alkyl-3-methylimidazolium-hexafluorophosphates by wide angle x-ray and neutron scattering and molecular dynamics. Journal of Chemical Physics, 2011, 134, 114521.	3.0	80
8	Selected chemicalâ€“physical properties and structural heterogeneities in 1-ethyl-3-methylimidazolium alkyl-sulfate room temperature ionic liquids. Chemical Physics Letters, 2010, 493, 259-262.	2.6	79
9	Dual effect of humidity on cesium lead bromide: enhancement and degradation of perovskite films. Journal of Materials Chemistry A, 2019, 7, 12292-12302.	10.3	74
10	The Interpretation of Diffraction Patterns of Two Prototypical Protic Ionic Liquids: a Challenging Task for Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 13024-13032.	2.6	60
11	Choline-amino acid ionic liquids: past and recent achievements about the structure and properties of these really â€œgreenâ€•chemicals. Biophysical Reviews, 2018, 10, 873-880.	3.2	55
12	Amino Acid Anions in Organic Ionic Compounds. An ab Initio Study of Selected Ion Pairs. Journal of Physical Chemistry B, 2014, 118, 2471-2486.	2.6	48
13	Interaction and dynamics of ionic liquids based on choline and amino acid anions. Journal of Chemical Physics, 2015, 142, 234502.	3.0	47
14	An energy dispersive x-ray scattering and molecular dynamics study of liquid dimethyl carbonate. Journal of Chemical Physics, 2009, 131, 244503.	3.0	46
15	NMR Investigation of Imidazoliumâ€Based Ionic Liquids and Their Aqueous Mixtures. ChemPhysChem, 2012, 13, 1339-1346.	2.1	45
16	A Combined Theoretical and Experimental Study of Solid Octyl and Decylammonium Chlorides and of Their Aqueous Solutions. Journal of Physical Chemistry B, 2013, 117, 7806-7818.	2.6	45
17	Liquid Structure of 1-Ethyl-3-methylimidazolium Alkyl Sulfates by X-ray Scattering and Molecular Dynamics. Journal of Physical Chemistry B, 2012, 116, 13448-13458.	2.6	43
18	Pressure-induced mesoscopic disorder in protic ionic liquids: first computational study. Physical Chemistry Chemical Physics, 2016, 18, 2297-2302.	2.8	43

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19	UVâ"Vis Spectra of the Anticancer Campothecin Family Drugs in Aqueous Solution: Specific Spectroscopic Signatures Unraveled by a Combined Computational and Experimental Study. Journal of Physical Chemistry B, 2009, 113, 5369-5375.	2.6	42
20	Role of ionic liquids in protein refolding: native/fibrillar versus treated lysozyme. RSC Advances, 2012, 2, 12329.	3.6	42
21	Biologically friendly room temperature ionic liquids and nanomaterials for the development of innovative enzymatic biosensors: Part II. Talanta, 2019, 194, 26-31.	5.5	37
22	Hydrogen Bonding Features in Cholinium-Based Protic Ionic Liquids from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 2635-2645.	2.6	36
23	X-Ray structure and ionic conductivity studies of anhydrous and hydrated choline chloride and oxalic acid deep eutectic solvents. Physical Chemistry Chemical Physics, 2018, 20, 30120-30124.	2.8	35
24	Hydrogen bonding in barbituric and 2-thiobarbituric acids: a theoretical and FT-IR study. Chemical Physics, 2001, 271, 293-308.	1.9	34
25	Dimerisation of urea in water solution: a quantum mechanical investigation. Physical Chemistry Chemical Physics, 2007, 9, 2206.	2.8	34
26	Thermal and Structural Properties of Ethylammonium Chloride and Its Mixture with Water. Journal of Physical Chemistry B, 2011, 115, 4887-4899.	2.6	34
27	Interaction of a long alkyl chain protic ionic liquid and water. Journal of Chemical Physics, 2014, 140, 204503.	3.0	34
28	Theoretical study of ionic liquids based on the cholinium cation. Ab initio simulations of their condensed phases. Journal of Chemical Physics, 2016, 144, 104504.	3.0	34
29	Energy dispersive X-ray diffraction and molecular dynamics meet: The structure of liquid pyrrole. Chemical Physics Letters, 2006, 417, 200-205.	2.6	33
30	Crystal Polymorphism of Hexylammonium Chloride and Structural Properties of Its Mixtures with Water. Journal of Physical Chemistry B, 2012, 116, 2104-2113.	2.6	33
31	Molecular aggregation phenomena in solution: an energy dispersive X-ray diffraction study of concentrated imidazole water solutions. Chemical Physics Letters, 1999, 301, 131-137.	2.6	32
32	Structural Determination of Ionic Liquids with Theoretical Methods: C₈mimBr and C₈mimCl. Strength and Weakness of Current Force Fields. Journal of Physical Chemistry Letters, 2010, 1, 1095-1100.	4.6	32
33	Is a medium-range order pre-peak possible for ionic liquids without an aliphatic chain?. RSC Advances, 2015, 5, 50938-50941.	3.6	32
34	Unexpected proton mobility in the bulk phase of cholinium-based ionic liquids: new insights from theoretical calculations. Physical Chemistry Chemical Physics, 2017, 19, 11869-11880.	2.8	31
35	The structural organization of N-methyl-2-pyrrolidone + water mixtures: A densitometry, x-ray diffraction, and molecular dynamics study. Journal of Chemical Physics, 2014, 140, 124503.	3.0	30
36	Low-Q peak in X-ray patterns of choline-phenylalanine and -homophenylalanine: A combined effect of chain and stacking. Chemical Physics Letters, 2016, 660, 99-101.	2.6	29

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37	Conformational isomerisms and nano-aggregation in substituted alkylammonium nitrates ionic liquids: An x-ray and computational study of 2-methoxyethylammonium nitrate. Journal of Chemical Physics, 2013, 138, 184506.	3.0	28
38	Structural studies on choline-carboxylate bio-ionic liquids by x-ray scattering and molecular dynamics. Journal of Chemical Physics, 2015, 143, 114506.	3.0	28
39	Two Different Models to Predict Ionicâ€Liquid Diffraction Patterns: Fixedâ€Charge versus Polarizable Potentials. ChemPhysChem, 2015, 16, 197-203.	2.1	28
40	A study of cyclohexane, piperidine and morpholine with X-ray diffraction and molecular simulations. Journal of Molecular Liquids, 2008, 139, 23-28.	4.9	27
41	The unseen evidence of Reduced Ionicity: The elephant in (the) room temperature ionic liquids. Journal of Molecular Liquids, 2021, 324, 115069.	4.9	27
42	Microscopic Structural and Dynamic Features in Triphilic Room Temperature Ionic Liquids. Frontiers in Chemistry, 2019, 7, 285.	3.6	25
43	Excitonic Fine Structure in Emission of Linear Carbon Chains. Nano Letters, 2020, 20, 6502-6509.	9.1	25
44	Nanoscale Density Fluctuations in Ionic Liquid Binary Mixtures with Nonamphiphilic Compounds: First Experimental Evidence. Journal of Physical Chemistry B, 2016, 120, 10540-10546.	2.6	24
45	Intriguing transport dynamics of ethylammonium nitrateâ€“acetonitrile binary mixtures arising from nano-inhomogeneity. Physical Chemistry Chemical Physics, 2017, 19, 27212-27220.	2.8	24
46	Inhomogeneity in Ethylammonium Nitrateâ€“Acetonitrile Binary Mixtures: The Highest â€œLow q Excessâ€•Reported to Date. Journal of Physical Chemistry Letters, 2017, 8, 3512-3522.	4.6	24
47	NMR, Calorimetry, and Computational Studies of Aqueous Solutions of N-Methyl-2-pyrrolidone. Journal of Physical Chemistry B, 2014, 118, 10493-10502.	2.6	21
48	Micro- and mesoscopic structural features of a bio-based choline-amino acid ionic liquid. RSC Advances, 2016, 6, 34737-34743.	3.6	21
49	Effect of alkyl chain length in protic ionic liquids: an AIMD perspective. Molecular Physics, 2017, 115, 1582-1589.	1.7	20
50	The structure of liquid N-methyl pyrrolidone probed by x-ray scattering and molecular simulations. Journal of Chemical Physics, 2012, 136, 074505.	3.0	19
51	Thermo-physical properties of ammonium-based ionic liquid + N -methyl-2-pyrrolidone mixtures at 298.15 K. Fluid Phase Equilibria, 2014, 383, 49-54.	2.5	19
52	Choline salicylate ionic liquid by X-ray scattering, vibrational spectroscopy and molecular dynamics. Journal of Molecular Liquids, 2016, 218, 39-49.	4.9	19
53	Nanoscale organization in the fluorinated room temperature ionic liquid: Tetraethyl ammonium (trifluoromethanesulfonyl)(nonafluorobutylsulfonyl)imide. Journal of Chemical Physics, 2018, 148, 193816.	3.0	19
54	Synthesis, Biological Evaluation, and Molecular Modeling Studies of Rebeccamycin Analogues Modified in the Carbohydrate Moiety. ChemMedChem, 2008, 3, 266-279.	3.2	18

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55	Tautomerism in liquid 1,2,3-triazole: a combined energy-dispersive X-ray diffraction, molecular dynamics, and FTIR study. Structural Chemistry, 2013, 24, 933-943.	2.0	18
56	Heterogeneity of propyl-ammonium nitrate solid phases obtained under high pressure. Journal of Physics and Chemistry of Solids, 2015, 84, 13-16.	4.0	18
57	Structure and dynamics of propylammonium nitrate-acetonitrile mixtures: An intricate multi-scale system probed with experimental and theoretical techniques. Journal of Chemical Physics, 2018, 148, 134507.	3.0	18
58	Self-Assembly of Catecholic Moiety-Containing Cationic Random Acrylic Copolymers. Journal of Physical Chemistry B, 2015, 119, 8369-8379.	2.6	17
59	Does High Pressure Induce Structural Reorganization in Linear Alcohols? A Computational Answer. ChemPhysChem, 2016, 17, 3023-3029.	2.1	17
60	Furan and thiophene in liquid phase: An X-ray and molecular dynamics study. Chemical Physics Letters, 2006, 422, 256-261.	2.6	16
61	New pyran-based molecules as both n- and p-type sensitizers in semi-transparent Dye Sensitized Solar Cells. Dyes and Pigments, 2020, 175, 108140.	3.7	16
62	Crystal Polymorphism of Propylammonium Chloride and Structural Properties of Its Mixture with Water. Journal of Physical Chemistry B, 2011, 115, 11805-11815.	2.6	15
63	Bio ionic liquids and water mixtures: a structural study. RSC Advances, 2017, 7, 19338-19344.	3.6	15
64	A joint experimental and computational study on ethylammonium nitrate-ethylene glycol 1:1 mixture. Structural, kinetic, dynamic and spectroscopic properties. Journal of Molecular Liquids, 2017, 226, 2-8.	4.9	15
65	Novel Thienyl DPP derivatives Functionalized with Terminal Electronâ€Acceptor Groups: Synthesis, Optical Properties and OFET Performance. Chemistry - A European Journal, 2022, 28, .	3.3	15
66	A new insight into the nanostructure of alkylammonium alkanoates based ionic liquids in water. Physical Chemistry Chemical Physics, 2016, 18, 11497-11502.	2.8	14
67	Mesoscopic structural organization in fluorinated pyrrolidinium-based room temperature ionic liquids. Journal of Molecular Liquids, 2019, 289, 111110.	4.9	14
68	A combined electrochemical, infrared and EDXD tool to disclose Deep Eutectic Solvents formation when one precursor is liquid: Glyceline as case study. Journal of Molecular Liquids, 2020, 319, 114292.	4.9	14
69	X-ray and molecular dynamics studies of butylammonium butanoateâ€“water binary mixtures. Physical Chemistry Chemical Physics, 2017, 19, 1975-1981.	2.8	13
70	How do arenediazonium salts behave in deep eutectic solvents? A combined experimental and computational approach. Journal of Molecular Liquids, 2021, 339, 116743.	4.9	13
71	Mesoscopic structural organization in fluorinated room temperature ionic liquids. Comptes Rendus Chimie, 2018, 21, 757-770.	0.5	12
72	In-Depth Physico-Chemical and Structural Investigation of a Dicarboxylic Acid/Choline Chloride Natural Deep Eutectic Solvent (NADES): A Spotlight on the Importance of a Rigorous Preparation Procedure. ACS Sustainable Chemistry and Engineering, 2019, , .	6.7	12

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73	Room Temperature Syntheses of ZnO and Their Structures. Symmetry, 2021, 13, 733.	2.2	11
74	Choline Hydrogen Dicarboxylate Ionic Liquids by X-ray Scattering, Vibrational Spectroscopy and Molecular Dynamics: H-Fumarate and H-Maleate and Their Conformations. Molecules, 2020, 25, 4990.	3.8	10
75	FTIR spectra and density functional theory P.E.D. assignments of oxiranes in Ar matrix at 12K. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 558-567.	3.9	9
76	Structural and vibrational study of 2-MethoxyEthylAmmonium Nitrate (2-OMeEAN): Interpretation of experimental results with ab initio molecular dynamics. Journal of Chemical Physics, 2016, 145, 024507.	3.0	9
77	Hydration of diazoles in water solution: pyrazole. A theoretical and X-ray diffraction study. Physical Chemistry Chemical Physics, 2009, 11, 9431.	2.8	8
78	Chloromethyl-oxirane and chloromethyl-thiirane in liquid phase: A joint experimental and quantum chemical study. Chemical Physics, 2016, 473, 24-31.	1.9	8
79	First Evidence of Electrode Reconstruction in Mesoporous NiO After Operation as Photocathode of Dyeâ€Sensitized Solar Cells. ChemistrySelect, 2018, 3, 6729-6736.	1.5	8
80	Dendrimer crown-ether tethered multi-wall carbon nanotubes support methyltrioxorhenium in the selective oxidation of olefins to epoxides. RSC Advances, 2020, 10, 17185-17194.	3.6	8
81	Overcoming the Inadequacy of X-ray Powder Diffraction in Reliable Hydrogen Location with the Aid of First Principles Calculations: Crystal Structure Determination of Orotaldehyde Monohydrate. Journal of Physical Chemistry A, 2009, 113, 353-359.	2.5	7
82	Structural Flexibility and Role of Vicinal 2-Thienyl Rings in 2,3-Dicyano-5,6-di(2-thienyl)-1,4-pyrazine, [(CN)₂Th₂Pyz], Its Palladium(II) Complex [(CN)₂Th₂Pyz(PdCl₂)₂], and the Related Pentametallic Pyrazinoporphyrazines [(PdCl₂)₄Th₈TPyzPzM] (M =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 367 T	4.0	7
83	Water and hexane in an ionic liquid: computational evidence of association under high pressure. Physical Chemistry Chemical Physics, 2017, 19, 8661-8666.	2.8	7
84	A structural and theoretical study of the alkylammonium nitrates forefather: Liquid methylammonium nitrate. Chemical Physics Letters, 2017, 684, 304-309.	2.6	7
85	Detection of Heavy Metals in Water Using Graphene Oxide Quantum Dots: An Experimental and Theoretical Study. Molecules, 2021, 26, 5519.	3.8	7
86	Recent Advances in the Synthesis of Inorganic Materials Using Environmentally Friendly Media. Molecules, 2022, 27, 2045.	3.8	7
87	A new electrochemical sensor for extra-virgin olive oils classification. Food Control, 2020, 109, 106903.	5.5	6
88	An X-ray and computational study of liquid pentylammonium nitrate. Chemical Physics Letters, 2017, 687, 38-43.	2.6	5
89	New Experimental Evidences Regarding Conformational Equilibrium in Ammoniumâ^'Bis(trifluoromethanesulfonyl)imide Ionic Liquids. ChemPhysChem, 2018, 19, 2776-2781.	2.1	5
90	Communication: Anion-specific response of mesoscopic organization in ionic liquids upon pressurization. Journal of Chemical Physics, 2018, 148, 211102.	3.0	5

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91	New Insights into the Structure of Glycols and Derivatives: A Comparative X-Ray Diffraction, Raman and Molecular Dynamics Study of Ethane-1,2-Diol, 2-Methoxyethan-1-ol and 1,2-Dimethoxy Ethane. Crystals, 2020, 10, 1011.	2.2	5
92	The Opposite Effect of Water and N-Methyl-2-Pyrrolidone Cosolvents on the Nanostructural Organization of Ethylammonium Butanoate Ionic Liquid: A Small- and Wide-Angle X-Ray Scattering and Molecular Dynamics Simulations Study. Journal of Physical Chemistry B, 2017, 121, 6399-6407.	2.6	3
93	Medium range interactions evidences in compounds with aliphatic lateral chain: 1-pentanoic acid, 1-pentanol and pentylammonium nitrate as test cases. Chemical Physics Letters, 2019, 734, 136738.	2.6	3
94	Coupled hydroxyl and ether functionalisation in EAN derivatives: the effect of hydrogen bond donor/acceptor groups on the structural heterogeneity studied with X-ray diffractions and fixed charge/polarizable simulations. Physical Chemistry Chemical Physics, 2019, 21, 11464-11475.	2.8	3
95	X-Ray Diffraction Studies of Ionic Liquids: From Spectra to Structure and Back. Soft and Biological Matter, 2014, , 1-37.	0.3	3
96	Laser vs. thermal treatments of green pigment PG36: coincidence and toxicity of processes. Archives of Toxicology, 2021, 95, 2367-2383.	4.2	2
97	Computational methods applied to the discovery of stem cell factor ligands. Theoretical Chemistry Accounts, 2008, 120, 523-531.	1.4	1
98	New insights into chloromethyl-oxirane and chloromethyl-thiirane in liquid and solid phase from low-temperature infrared spectroscopy and ab initio modeling. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 247, 119061.	3.9	1
99	Higher fullerenes: Compositional analysis by EDXD and molecular dynamics. , 2014, , .		0
100	Brominated carbon black: An EDXD study. , 2014, , .		0
101	Physical-chemical studies on putrescine (butane-1,4-diamine) and its solutions: Experimental and computational investigations. Journal of Molecular Liquids, 2021, 322, 114568.	4.9	0