Valentina Migliorati

List of Publications by Year
in descending order

67	2,070	159585 30	254184 43
papers	citations	h-index	g-index

70	70	70	1825
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Revised Ionic Radii of Lanthanoid(III) Ions in Aqueous Solution. Inorganic Chemistry, 2011, 50, 4572-4579.	4.0	212
2	Hydration Properties of the Bromide Aqua Ion: the Interplay of First Principle and Classical Molecular Dynamics, and X-ray Absorption Spectroscopy. Inorganic Chemistry, 2010, 49, 4224-4231.	4.0	81
3	Analysis of the Detailed Configuration of Hydrated Lanthanoid(III) Ions in Aqueous Solution and Crystalline Salts by Using Kâ€•and L₃â€Edge XANES Spectroscopy. Chemistry - A European Journal, 2010, 16, 684-692.	3.3	73
4	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
5	XANES Reveals the Flexible Nature of Hydrated Strontium in Aqueous Solution. Journal of Physical Chemistry B, 2016, 120, 4114-4124.	2.6	57
6	Development of Lennard-Jones and Buckingham Potentials for Lanthanoid Ions in Water. Inorganic Chemistry, 2017, 56, 6214-6224.	4.0	57
7	Using a Combined Theoretical and Experimental Approach to Understand the Structure and Dynamics of Imidazolium-Based Ionic Liquids/Water Mixtures. 1. MD Simulations. Journal of Physical Chemistry B, 2013, 117, 12505-12515.	2.6	53
8	X-ray Absorption Spectroscopy of Hemes and Hemeproteins in Solution: Multiple Scattering Analysis. Inorganic Chemistry, 2008, 47, 9905-9918.	4.0	52
9	Unraveling halide hydration: A high dilution approach. Journal of Chemical Physics, 2014, 141, 044509.	3.0	52
10	Structural Investigation of Lanthanoid Coordination: a Combined XANES and Molecular Dynamics Study. Inorganic Chemistry, 2009, 48, 10239-10248.	4.0	51
11	A Coupled Molecular Dynamics and XANES Data Analysis Investigation of Aqueous Cadmium(II). Journal of Physical Chemistry A, 2008, 112, 11833-11841.	2.5	50
12	Integrated experimental and theoretical approach for the structural characterization of Hg2+ aqueous solutions. Journal of Chemical Physics, 2008, 128, 084502.	3.0	50
13	Using a Combined Theoretical and Experimental Approach to Understand the Structure and Dynamics of Imidazolium-Based Ionic Liquids/Water Mixtures. 2. EXAFS Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 12516-12524.	2.6	50
14	Structural and Dynamical Properties of the Hg²⁺ Aqua Ion:â€‰ A Molecular Dynamics Study. Journal of Physical Chemistry B, 2008, 112, 4694-4702.	2.6	48
15	Structural properties of geminal dicationic ionic liquid/water mixtures: a theoretical and experimental insight. Physical Chemistry Chemical Physics, 2016, 18, 16544-16554.	2.8	48
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	Solvation Structure of Zn²⁺ and Cu²⁺ Ions in Acetonitrile: A Combined EXAFS and XANES Study. Journal of Physical Chemistry B, 2015, 119, 4061-4067.	2.6	45
18	Deep eutectic solvents: A structural point of view on the role of the cation. Chemical Physics Letters: X, 2019, 737, 100001.	2.1	45

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19	On the Solvation of the Zn²⁺ Ion in Methanol: A Combined Quantum Mechanics, Molecular Dynamics, and EXAFS Approach. Inorganic Chemistry, 2011, 50, 8509-8515.	4.0	41
20	Hydration Properties of the Zn²⁺ Ion in Water at High Pressure. Inorganic Chemistry, 2013, 52, 1141-1150.	4.0	41
21	Influence of the Second Coordination Shell on the XANES Spectra of the Zn²⁺ Ion in Water and Methanol. ChemPlusChem, 2012, 77, 234-239.	2.8	40
22	The non-octarepeat copper binding site of the prion protein is a key regulator of prion conversion. Scientific Reports, 2015, 5, 15253.	3.3	39
23	Local order and long range correlations in imidazolium halide ionic liquids: a combined molecular dynamics and XAS study. Physical Chemistry Chemical Physics, 2015, 17, 16443-16453.	2.8	39
24	Influence of Counterions on the Hydration Structure of Lanthanide Ions in Dilute Aqueous Solutions. Journal of Physical Chemistry B, 2018, 122, 2779-2791.	2.6	37
25	Structural Properties and Aggregation Behavior of 1-Hexyl-3-methylimidazolium Iodide in Aqueous Solutions. Journal of Physical Chemistry B, 2015, 119, 14515-14526.	2.6	35
26	On the coordination of Zn²⁺ion in Tf₂N^{â^'}based ionic liquids: structural and dynamic properties depending on the nature of the organic cation. Physical Chemistry Chemical Physics, 2018, 20, 2662-2675.	2.8	35
27	Thermal and Structural Properties of Ethylammonium Chloride and Its Mixture with Water. Journal of Physical Chemistry B, 2011, 115, 4887-4899.	2.6	34
28	Effect of the Zn²⁺ and Hg²⁺ Ions on the Structure of Liquid Water. Journal of Physical Chemistry A, 2011, 115, 4798-4803.	2.5	34
29	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
30	Combining EXAFS spectroscopy and molecular dynamics simulations to understand the structural and dynamic properties of an imidazolium iodide ionic liquid. Physical Chemistry Chemical Physics, 2015, 17, 2464-2474.	2.8	32
31	X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts. Journal of Chemical Physics, 2011, 135, 074505.	3.0	31
32	Unraveling the Sc³⁺ Hydration Geometry: The Strange Case of the Far-Coordinated Water Molecule. Inorganic Chemistry, 2016, 55, 6703-6711.	4.0	30
33	On the development of polarizable and Lennard-Jones force fields to study hydration structure and dynamics of actinide(III) ions based on effective ionic radii. Journal of Chemical Physics, 2017, 147, 161707.	3.0	30
34	Coupled X-ray Absorption/UVâ€“vis Monitoring of Fast Oxidation Reactions Involving a Nonheme Ironâ€“Oxo Complex. Journal of the American Chemical Society, 2019, 141, 2299-2304.	13.7	27
35	Hidden Hydration Structure of Halide Ions: an Insight into the Importance of Lone Pairs. Journal of Physical Chemistry B, 2015, 119, 15729-15737.	2.6	25
36	Elusive Coordination of the Ag⁺ Ion in Aqueous Solution: Evidence for a Linear Structure. Inorganic Chemistry, 2020, 59, 17291-17302.	4.0	25

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37	A quantum mechanics, molecular dynamics and EXAFS investigation into the Hg2+ ion solvation properties in methanol solution. RSC Advances, 2013, 3, 21118.	3.6	23
38	Transition from molecular- to nano-scale segregation in a deep eutectic solvent - water mixture. Journal of Molecular Liquids, 2021, 331, 115747.	4.9	21
39	How Does Ce^{III} Nitrate Dissolve in a Protic Ionic Liquid? A Combined Molecular Dynamics and EXAFS Study. Chemistry - A European Journal, 2017, 23, 8424-8433.	3.3	19
40	Combined distribution functions: A powerful tool to identify cation coordination geometries in liquid systems. Chemical Physics Letters, 2018, 691, 437-443.	2.6	19
41	Anatomy of a deep eutectic solvent: structural properties of choline chlorideâ€‰:â€‰sesamol 1â€‰:â€‰3 compared to reline. Physical Chemistry Chemical Physics, 2021, 23, 11746-11754.	2.8	16
42	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
43	K-edge XANES investigation of octakis(DMSO)lanthanoid(iii) complexes in DMSO solution and solid iodides. Physical Chemistry Chemical Physics, 2013, 15, 8684.	2.8	15
44	Lutetium(iii) aqua ion: On the dynamical structure of the heaviest lanthanoid hydration complex. Journal of Chemical Physics, 2016, 144, 204505.	3.0	15
45	Unraveling the Hydration Properties of the Ba²⁺ Aqua Ion: the Interplay of Quantum Mechanics, Molecular Dynamics, and EXAFS Spectroscopy. Inorganic Chemistry, 2019, 58, 14551-14559.	4.0	15
46	Fate of a Deep Eutectic Solvent upon Cosolvent Addition: Choline Chlorideâ€“Sesamol 1:3 Mixtures with Methanol. ACS Sustainable Chemistry and Engineering, 2021, 9, 12252-12261.	6.7	15
47	Solubilization properties and structural characterization of dissociated HgO and HgCl2 in deep eutectic solvents. Journal of Molecular Liquids, 2021, 329, 115505.	4.9	14
48	On the possibility of using XANES to investigate bromide-based ionic liquids. Chemical Physics Letters, 2014, 591, 32-36.	2.6	12
49	Quantitative Analysis of Deconvolved X-ray Absorption Near-Edge Structure Spectra: A Tool To Push the Limits of the X-ray Absorption Spectroscopy Technique. Inorganic Chemistry, 2014, 53, 9778-9784.	4.0	11
50	Following a Chemical Reaction on the Millisecond Time Scale by Simultaneous X-ray and UV/Vis Spectroscopy. Journal of Physical Chemistry Letters, 2017, 8, 2958-2963.	4.6	11
51	Deep eutectic solvents: A structural point of view on the role of the anion. Chemical Physics Letters, 2021, 777, 138702.	2.6	11
52	Solvation structure of lanthanide(<scp>iii</scp>) bistriflimide salts in acetonitrile solution: a molecular dynamics simulation and EXAFS investigation. Physical Chemistry Chemical Physics, 2019, 21, 13058-13069.	2.8	10
53	Direct structural and mechanistic insights into fast bimolecular chemical reactions in solution through a coupled XAS/UVâ€“Vis multivariate statistical analysis. Dalton Transactions, 2021, 50, 131-142.	3.3	10
54	On the Coordination Chemistry of the lanthanum(III) Nitrate Salt in EAN/MeOH Mixtures. Inorganic Chemistry, 2021, 60, 10674-10685.	4.0	10

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55	Activation of Câ€“H bonds by a nonheme iron(iv)â€“oxo complex: mechanistic evidence through a coupled EDXAS/UV-Vis multivariate analysis. Physical Chemistry Chemical Physics, 2021, 23, 1188-1196.	2.8	9
56	Structural Study of a Eutectic Solvent Reveals Hydrophobic Segregation and Lack of Hydrogen Bonding between the Components. ACS Sustainable Chemistry and Engineering, 2022, 10, 6337-6345.	6.7	9
57	Measurement of x-ray multielectron photoexcitations at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mtext>I</mml:mtext><mml:mo>â^’</mml:mo></mml:msup><mml:mtext>â€‰</mml:mtext></mml:mrow></mml:math> Physical Review B, 2008, 78, .	3.2	8
58	Structure of Water in Zn²⁺ Aqueous Solutions from Ambient Conditions up to the Gigapascal Pressure Range: A XANES and Molecular Dynamics Study. Inorganic Chemistry, 2017, 56, 14013-14022.	4.0	8
59	Ce3+ and La3+ ions in ethylammonium nitrate: A XANES and molecular dynamics investigation. Chemical Physics Letters, 2018, 706, 311-316.	2.6	8
60	Unraveling the solvation geometries of the lanthanum(<scp>iii</scp>) bistriflimide salt in ionic liquid/acetonitrile mixtures. Physical Chemistry Chemical Physics, 2020, 22, 20434-20443.	2.8	6
61	Unraveling the perturbation induced by Zn2+ and Hg2+ ions on the hydrogen bond patterns of liquid methanol. Chemical Physics Letters, 2015, 633, 70-75.	2.6	5
62	Insights into the Structure of Reaction Intermediates Through Coupled X-ray Absorption/UV-Vis Spectroscopy. Springer Proceedings in Physics, 2021, , 141-154.	0.2	5
63	Carbon monoxide binding to the heme group at the dimeric interface modulates structure and copper accessibility in the Cu,Zn superoxide dismutase fromHaemophilus ducreyi: in silico andin vitroevidences. Journal of Biomolecular Structure and Dynamics, 2012, 30, 269-279.	3.5	4
64	Solvation structure of the Hg(NO3)2 and Hg(TfO)2 salts in dilute aqueous and methanol solutions: An insight into the Hg2+ coordination chemistry. Journal of Molecular Liquids, 2022, 363, 119801.	4.9	4
65	Response to Comment on â€œStructural Study of a Eutectic Solvent Reveals Hydrophobic Segregation and Lack of Hydrogen Bonding between the Componentsâ€• ACS Sustainable Chemistry and Engineering, 2022, 10, 8671-8672.	6.7	3
66	Theoretical Description of Ionic Liquids. Soft and Biological Matter, 2014, , 127-148.	0.3	2
67	Response to â€œComment on â€˜On the development of polarizable and Lennard-Jones force fields to study hydration structure and dynamics of actinide(III) ions based on effective ionic radiiâ€™â€•[J. Chem. Phys. 150, 097101 (2019)]. Journal of Chemical Physics, 2019, 150, 097102.	3.0	0