Valentina Migliorati

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

64 papers	1,683 citations	28 h-index	39 g-index
70 ext. papers	1,876 ext. citations	4.1 avg, IF	4.93 L-index

#	Paper	IF	Citations
64	Revised ionic radii of lanthanoid(III) ions in aqueous solution. *Inorganic Chemistry*, **2011**, 50, 4572-9	5.1	170
63	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, 4224-31	5.1	73
62	Analysis of the detailed configuration of hydrated lanthanoid(III) ions in aqueous solution and crystalline salts by using K- and L(3)-edge XANES spectroscopy. *Chemistry - A European Journal*, **2010**, 16, 684-92	4.8	72
61	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, 13024-32	3.4	59
60	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, 12505-15	3.4	50
59	Structural investigation of lanthanoid coordination: a combined XANES and molecular dynamics study. *Inorganic Chemistry*, **2009**, 48, 10239-48	5.1	49
58	X-ray absorption spectroscopy of hemes and hemeproteins in solution: multiple scattering analysis. *Inorganic Chemistry*, **2008**, 47, 9905-18	5.1	49
57	A coupled molecular dynamics and XANES data analysis investigation of aqueous cadmium(II). *Journal of Physical Chemistry A*, **2008**, 112, 11833-41	2.8	48
56	Integrated experimental and theoretical approach for the structural characterization of Hg2+ aqueous solutions. *Journal of Chemical Physics*, **2008**, 128, 084502	3.9	48
55	Unraveling halide hydration: A high dilution approach. *Journal of Chemical Physics*, **2014**, 141, 044509	3.9	46
54	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, 12516-24	3.4	44
53	A combined theoretical and experimental study of solid octyl and decylammonium chlorides and of their aqueous solutions. *Journal of Physical Chemistry B*, **2013**, 117, 7806-18	3.4	43
52	Structural and dynamical properties of the Hg2+ aqua ion: a molecular dynamics study. *Journal of Physical Chemistry B*, **2008**, 112, 4694-702	3.4	43
51	XANES Reveals the Flexible Nature of Hydrated Strontium in Aqueous Solution. *Journal of Physical Chemistry B*, **2016**, 120, 4114-24	3.4	42
50	Development of Lennard-Jones and Buckingham Potentials for Lanthanoid Ions in Water. *Inorganic Chemistry*, **2017**, 56, 6214-6224	5.1	41
49	Solvation structure of Zn(2+) and Cu(2+) ions in acetonitrile: a combined EXAFS and XANES study. *Journal of Physical Chemistry B*, **2015**, 119, 4061-7	3.4	39
48	Hydration properties of the Zn2+ ion in water at high pressure. *Inorganic Chemistry*, **2013**, 52, 1141-50	5.1	38

47	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	37
46	On the solvation of the Zn2+ ion in methanol: a combined quantum mechanics, molecular dynamics, and EXAFS approach. *Inorganic Chemistry*, **2011**, 50, 8509-15	5.1	37
45	Structural properties of geminal dicationic ionic liquid/water mixtures: a theoretical and experimental insight. *Physical Chemistry Chemical Physics*, **2016**, 18, 16544-54	3.6	34
44	Local order and long range correlations in imidazolium halide ionic liquids: a combined molecular dynamics and XAS study. *Physical Chemistry Chemical Physics*, **2015**, 17, 16443-53	3.6	34
43	Structural Properties and Aggregation Behavior of 1-Hexyl-3-methylimidazolium Iodide in Aqueous Solutions. *Journal of Physical Chemistry B*, **2015**, 119, 14515-26	3.4	33
42	The non-octarepeat copper binding site of the prion protein is a key regulator of prion conversion. *Scientific Reports*, **2015**, 5, 15253	4.9	33
41	Thermal and structural properties of ethylammonium chloride and its mixture with water. *Journal of Physical Chemistry B*, **2011**, 115, 4887-99	3.4	32
40	Effect of the Zn2+ and Hg2+ ions on the structure of liquid water. *Journal of Physical Chemistry A*, **2011**, 115, 4798-803	2.8	32
39	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, 2464-74	3.6	29
38	Crystal polymorphism of hexylammonium chloride and structural properties of its mixtures with water. *Journal of Physical Chemistry B*, **2012**, 116, 2104-13	3.4	29
37	X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts. *Journal of Chemical Physics*, **2011**, 135, 074505	3.9	29
36	Deep eutectic solvents: A structural point of view on the role of the cation. *Chemical Physics Letters: X*, **2019**, 2, 100001	2	28
35	Influence of Counterions on the Hydration Structure of Lanthanide Ions in Dilute Aqueous Solutions. *Journal of Physical Chemistry B*, **2018**, 122, 2779-2791	3.4	24
34	Unraveling the Sc(3+) Hydration Geometry: The Strange Case of the Far-Coordinated Water Molecule. *Inorganic Chemistry*, **2016**, 55, 6703-11	5.1	23
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	3.9	23
32	On the coordination of Zn ion in TfN based ionic liquids: structural and dynamic properties depending on the nature of the organic cation. *Physical Chemistry Chemical Physics*, **2018**, 20, 2662-2675	3.6	21
31	Hidden Hydration Structure of Halide Ions: an Insight into the Importance of Lone Pairs. *Journal of Physical Chemistry B*, **2015**, 119, 15729-37	3.4	21
30	A quantum mechanics, molecular dynamics and EXAFS investigation into the Hg2+ ion solvation properties in methanol solution. *RSC Advances*, **2013**, 3, 21118	3.7	20

29	Coupled X-ray Absorption/UV-vis Monitoring of Fast Oxidation Reactions Involving a Nonheme Iron-Oxo Complex. *Journal of the American Chemical Society*, **2019**, 141, 2299-2304	16.4	20
28	How Does Ce Nitrate Dissolve in a Protic Ionic Liquid? A Combined Molecular Dynamics and EXAFS Study. *Chemistry - A European Journal*, **2017**, 23, 8424-8433	4.8	17
27	K-edge XANES investigation of octakis(DMSO)lanthanoid(III) complexes in DMSO solution and solid iodides. *Physical Chemistry Chemical Physics*, **2013**, 15, 8684-91	3.6	15
26	Crystal polymorphism of propylammonium chloride and structural properties of its mixture with water. *Journal of Physical Chemistry B*, **2011**, 115, 11805-15	3.4	15
25	Combined distribution functions: A powerful tool to identify cation coordination geometries in liquid systems. *Chemical Physics Letters*, **2018**, 691, 437-443	2.5	12
24	On the possibility of using XANES to investigate bromide-based ionic liquids. *Chemical Physics Letters*, **2014**, 591, 32-36	2.5	12
23	Lutetium(iii) aqua ion: On the dynamical structure of the heaviest lanthanoid hydration complex. *Journal of Chemical Physics*, **2016**, 144, 204505	3.9	12
22	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	6.4	8
21	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, 9778-84	5.1	8
20	Measurement of x-ray multielectron photoexcitations at the I K edge. *Physical Review B*, **2008**, 78,	3.3	8
19	Structure of Water in Zn Aqueous Solutions from Ambient Conditions up to the Gigapascal Pressure Range: A XANES and Molecular Dynamics Study. *Inorganic Chemistry*, **2017**, 56, 14013-14022	5.1	7
18	Solvation structure of lanthanide(iii) bistriflimide salts in acetonitrile solution: a molecular dynamics simulation and EXAFS investigation. *Physical Chemistry Chemical Physics*, **2019**, 21, 13058-13069	3.6	7
17	Elusive Coordination of the Ag Ion in Aqueous Solution: Evidence for a Linear Structure. *Inorganic Chemistry*, **2020**, 59, 17291-17302	5.1	7
16	Unraveling the Hydration Properties of the Ba Aqua Ion: the Interplay of Quantum Mechanics, Molecular Dynamics, and EXAFS Spectroscopy. *Inorganic Chemistry*, **2019**, 58, 14551-14559	5.1	6
15	Ce3+ and La3+ ions in ethylammonium nitrate: A XANES and molecular dynamics investigation. *Chemical Physics Letters*, **2018**, 706, 311-316	2.5	6
14	Solubilization properties and structural characterization of dissociated HgO and HgCl2 in deep eutectic solvents. *Journal of Molecular Liquids*, **2021**, 329, 115505	6	6
13	Transition from molecular- to nano-scale segregation in a deep eutectic solvent - water mixture. *Journal of Molecular Liquids*, **2021**, 331, 115747	6	6
12	Direct structural and mechanistic insights into fast bimolecular chemical reactions in solution through a coupled XAS/UV-Vis multivariate statistical analysis. *Dalton Transactions*, **2021**, 50, 131-142	4.3	5

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11	Unraveling the perturbation induced by Zn2+ and Hg2+ ions on the hydrogen bond patterns of liquid methanol. *Chemical Physics Letters*, **2015**, 633, 70-75	2.5	4
10	Carbon monoxide binding to the heme group at the dimeric interface modulates structure and copper accessibility in the Cu,Zn superoxide dismutase from Haemophilus ducreyi: in silico and in vitro evidences. *Journal of Biomolecular Structure and Dynamics*, **2012**, 30, 269-79	3.6	4
9	Unraveling the solvation geometries of the lanthanum(III) bistriflimide salt in ionic liquid/acetonitrile mixtures. *Physical Chemistry Chemical Physics*, **2020**, 22, 20434-20443	3.6	4
8	Deep eutectic solvents: A structural point of view on the role of the anion. *Chemical Physics Letters*, **2021**, 777, 138702	2.5	4
7	Anatomy of a deep eutectic solvent: structural properties of choline chloride : sesamol 1 : 3 compared to reline. *Physical Chemistry Chemical Physics*, **2021**, 23, 11746-11754	3.6	4
6	Insights into the Structure of Reaction Intermediates Through Coupled X-ray Absorption/UV-Vis Spectroscopy. *Springer Proceedings in Physics*, **2021**, 141-154	0.2	4
5	Activation of C-H bonds by a nonheme iron(IV)-oxo complex: mechanistic evidence through a coupled EDXAS/UV-Vis multivariate analysis. *Physical Chemistry Chemical Physics*, **2021**, 23, 1188-1196	3.6	3
4	Fate of a Deep Eutectic Solvent upon Cosolvent Addition: Choline Chloride-Sesamol 1:3 Mixtures with Methanol. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 12252-12261	8.3	3
3	On the Coordination Chemistry of the lanthanum(III) Nitrate Salt in EAN/MeOH Mixtures. *Inorganic Chemistry*, **2021**, 60, 10674-10685	5.1	2
2	Theoretical Description of Ionic Liquids. *Soft and Biological Matter*, **2014**, 127-148	0.8	1
1	Response to "Comment on ‘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’ [J. Chem. Phys. 150, 097101 (2019)]. *Journal of Chemical Physics*, **2019**, 150, 097102	3.9	