

Valentina Migliorati

List of Publications by Year in Descending Order

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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	Solubilization properties and structural characterization of dissociated HgO and HgCl ₂ in deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2021 , 329, 115505	6	6
63	Transition from molecular- to nano-scale segregation in a deep eutectic solvent - water mixture. <i>Journal of Molecular Liquids</i> , 2021 , 331, 115747	6	6
62	On the Coordination Chemistry of the lanthanum(III) Nitrate Salt in EAN/MeOH Mixtures. <i>Inorganic Chemistry</i> , 2021 , 60, 10674-10685	5.1	2
61	Direct structural and mechanistic insights into fast bimolecular chemical reactions in solution through a coupled XAS/UV-Vis multivariate statistical analysis. <i>Dalton Transactions</i> , 2021 , 50, 131-142	4.3	5
60	Activation of C-H bonds by a nonheme iron(IV)-oxo complex: mechanistic evidence through a coupled EDXAS/UV-Vis multivariate analysis. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 1188-1196	3.6	3
59	Deep eutectic solvents: A structural point of view on the role of the anion. <i>Chemical Physics Letters</i> , 2021 , 777, 138702	2.5	4
58	Fate of a Deep Eutectic Solvent upon Cosolvent Addition: Choline Chloride-Sesamol 1:3 Mixtures with Methanol. <i>ACS Sustainable Chemistry and Engineering</i> , 2021 , 9, 12252-12261	8.3	3
57	Anatomy of a deep eutectic solvent: structural properties of choline chloride : sesamol 1 : 3 compared to reline. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 11746-11754	3.6	4
56	Insights into the Structure of Reaction Intermediates Through Coupled X-ray Absorption/UV-Vis Spectroscopy. <i>Springer Proceedings in Physics</i> , 2021 , 141-154	0.2	4
55	Elusive Coordination of the Ag Ion in Aqueous Solution: Evidence for a Linear Structure. <i>Inorganic Chemistry</i> , 2020 , 59, 17291-17302	5.1	7
54	Unraveling the solvation geometries of the lanthanum(III) bistriflimide salt in ionic liquid/acetonitrile mixtures. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 20434-20443	3.6	4
53	Unraveling the Hydration Properties of the Ba Aqua Ion: the Interplay of Quantum Mechanics, Molecular Dynamics, and EXAFS Spectroscopy. <i>Inorganic Chemistry</i> , 2019 , 58, 14551-14559	5.1	6
52	Solvation structure of lanthanide(III) bistriflimide salts in acetonitrile solution: a molecular dynamics simulation and EXAFS investigation. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 13058-13069	3.6	7
51	Response to "Comment on Qn the development of polarizable and Lennard-Jones force fields to study hydration structure and dynamics of actinide(III) ions based on effective ionic radii Q [J. Chem. Phys. 150, 097101 (2019)]. <i>Journal of Chemical Physics</i> , 2019 , 150, 097102	3.9	
50	Deep eutectic solvents: A structural point of view on the role of the cation. <i>Chemical Physics Letters: X</i> , 2019 , 2, 100001	2	28
49	Coupled X-ray Absorption/UV-vis Monitoring of Fast Oxidation Reactions Involving a Nonheme Iron-Oxo Complex. <i>Journal of the American Chemical Society</i> , 2019 , 141, 2299-2304	16.4	20
48	Influence of Counterions on the Hydration Structure of Lanthanide Ions in Dilute Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 2779-2791	3.4	24

47	Combined distribution functions: A powerful tool to identify cation coordination geometries in liquid systems. <i>Chemical Physics Letters</i> , 2018 , 691, 437-443	2.5	12
46	On the coordination of Zn ion in TfN based ionic liquids: structural and dynamic properties depending on the nature of the organic cation. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 2662-2675 ^{3,6}	3.6	21
45	Ce ³⁺ and La ³⁺ ions in ethylammonium nitrate: A XANES and molecular dynamics investigation. <i>Chemical Physics Letters</i> , 2018 , 706, 311-316	2.5	6
44	Development of Lennard-Jones and Buckingham Potentials for Lanthanoid Ions in Water. <i>Inorganic Chemistry</i> , 2017 , 56, 6214-6224	5.1	41
43	Following a Chemical Reaction on the Millisecond Time Scale by Simultaneous X-ray and UV/Vis Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 2958-2963	6.4	8
42	How Does Ce Nitrate Dissolve in a Protic Ionic Liquid? A Combined Molecular Dynamics and EXAFS Study. <i>Chemistry - A European Journal</i> , 2017 , 23, 8424-8433	4.8	17
41	Structure of Water in Zn Aqueous Solutions from Ambient Conditions up to the Gigapascal Pressure Range: A XANES and Molecular Dynamics Study. <i>Inorganic Chemistry</i> , 2017 , 56, 14013-14022	5.1	7
40	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. <i>Journal of Chemical Physics</i> , 2017 , 147, 161707 ⁹	3.9	23
39	Structural properties of geminal dicationic ionic liquid/water mixtures: a theoretical and experimental insight. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 16544-54	3.6	34
38	Unraveling the Sc(3+) Hydration Geometry: The Strange Case of the Far-Coordinated Water Molecule. <i>Inorganic Chemistry</i> , 2016 , 55, 6703-11	5.1	23
37	Lutetium(III) aqua ion: On the dynamical structure of the heaviest lanthanoid hydration complex. <i>Journal of Chemical Physics</i> , 2016 , 144, 204505	3.9	12
36	XANES Reveals the Flexible Nature of Hydrated Strontium in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 4114-24	3.4	42
35	Solvation structure of Zn(2+) and Cu(2+) ions in acetonitrile: a combined EXAFS and XANES study. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 4061-7	3.4	39
34	Structural Properties and Aggregation Behavior of 1-Hexyl-3-methylimidazolium Iodide in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 14515-26	3.4	33
33	Combining EXAFS spectroscopy and molecular dynamics simulations to understand the structural and dynamic properties of an imidazolium iodide ionic liquid. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 2464-74	3.6	29
32	The non-octarepeat copper binding site of the prion protein is a key regulator of prion conversion. <i>Scientific Reports</i> , 2015 , 5, 15253	4.9	33
31	Unraveling the perturbation induced by Zn ²⁺ and Hg ²⁺ ions on the hydrogen bond patterns of liquid methanol. <i>Chemical Physics Letters</i> , 2015 , 633, 70-75	2.5	4
30	Local order and long range correlations in imidazolium halide ionic liquids: a combined molecular dynamics and XAS study. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 16443-53	3.6	34

29	Hidden Hydration Structure of Halide Ions: an Insight into the Importance of Lone Pairs. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 15729-37	3.4	21
28	Unraveling halide hydration: A high dilution approach. <i>Journal of Chemical Physics</i> , 2014 , 141, 044509	3.9	46
27	Quantitative analysis of deconvolved X-ray absorption near-edge structure spectra: a tool to push the limits of the X-ray absorption spectroscopy technique. <i>Inorganic Chemistry</i> , 2014 , 53, 9778-84	5.1	8
26	On the possibility of using XANES to investigate bromide-based ionic liquids. <i>Chemical Physics Letters</i> , 2014 , 591, 32-36	2.5	12
25	Theoretical Description of Ionic Liquids. <i>Soft and Biological Matter</i> , 2014 , 127-148	0.8	1
24	K-edge XANES investigation of octakis(DMSO)lanthanoid(III) complexes in DMSO solution and solid iodides. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 8684-91	3.6	15
23	Using a combined theoretical and experimental approach to understand the structure and dynamics of imidazolium-based ionic liquids/water mixtures. 2. EXAFS spectroscopy. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 12516-24	3.4	44
22	A quantum mechanics, molecular dynamics and EXAFS investigation into the Hg ²⁺ ion solvation properties in methanol solution. <i>RSC Advances</i> , 2013 , 3, 21118	3.7	20
21	Using a combined theoretical and experimental approach to understand the structure and dynamics of imidazolium-based ionic liquids/water mixtures. 1. MD simulations. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 12505-15	3.4	50
20	Hydration properties of the Zn ²⁺ ion in water at high pressure. <i>Inorganic Chemistry</i> , 2013 , 52, 1141-50	5.1	38
19	A combined theoretical and experimental study of solid octyl and decylammonium chlorides and of their aqueous solutions. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 7806-18	3.4	43
18	The interpretation of diffraction patterns of two prototypical protic ionic liquids: a challenging task for classical molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 13024-32	3.4	59
17	Crystal polymorphism of hexylammonium chloride and structural properties of its mixtures with water. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 2104-13	3.4	29
16	Influence of the Second Coordination Shell on the XANES Spectra of the Zn ²⁺ Ion in Water and Methanol. <i>ChemPlusChem</i> , 2012 , 77, 234-239	2.8	37
15	Carbon monoxide binding to the heme group at the dimeric interface modulates structure and copper accessibility in the Cu,Zn superoxide dismutase from <i>Haemophilus ducreyi</i> : in silico and in vitro evidences. <i>Journal of Biomolecular Structure and Dynamics</i> , 2012 , 30, 269-79	3.6	4
14	Revised ionic radii of lanthanoid(III) ions in aqueous solution. <i>Inorganic Chemistry</i> , 2011 , 50, 4572-9	5.1	170
13	Thermal and structural properties of ethylammonium chloride and its mixture with water. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 4887-99	3.4	32
12	On the solvation of the Zn ²⁺ ion in methanol: a combined quantum mechanics, molecular dynamics, and EXAFS approach. <i>Inorganic Chemistry</i> , 2011 , 50, 8509-15	5.1	37

11	Effect of the Zn ²⁺ and Hg ²⁺ ions on the structure of liquid water. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 4798-803	2.8	32
10	Crystal polymorphism of propylammonium chloride and structural properties of its mixture with water. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 11805-15	3.4	15
9	X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts. <i>Journal of Chemical Physics</i> , 2011 , 135, 074505	3.9	29
8	Hydration properties of the bromide aqua ion: the interplay of first principle and classical molecular dynamics, and X-ray absorption spectroscopy. <i>Inorganic Chemistry</i> , 2010 , 49, 4224-31	5.1	73
7	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. <i>Chemistry - A European Journal</i> , 2010 , 16, 684-92	4.8	72
6	Structural investigation of lanthanoid coordination: a combined XANES and molecular dynamics study. <i>Inorganic Chemistry</i> , 2009 , 48, 10239-48	5.1	49
5	Measurement of x-ray multielectron photoexcitations at the L _{IIK} edge. <i>Physical Review B</i> , 2008 , 78,	3.3	8
4	X-ray absorption spectroscopy of hemes and hemeproteins in solution: multiple scattering analysis. <i>Inorganic Chemistry</i> , 2008 , 47, 9905-18	5.1	49
3	A coupled molecular dynamics and XANES data analysis investigation of aqueous cadmium(II). <i>Journal of Physical Chemistry A</i> , 2008 , 112, 11833-41	2.8	48
2	Structural and dynamical properties of the Hg ²⁺ aqua ion: a molecular dynamics study. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 4694-702	3.4	43
1	Integrated experimental and theoretical approach for the structural characterization of Hg ²⁺ aqueous solutions. <i>Journal of Chemical Physics</i> , 2008 , 128, 084502	3.9	48