

# Paola D Angelo

## List of Publications by Citations

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143  
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41  
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58  
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151  
ext. papers

4,761  
ext. citations

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L-index

#	Paper	IF	Citations
143	Hydration of lanthanoid(III) ions in aqueous solution and crystalline hydrates studied by EXAFS spectroscopy and crystallography: the myth of the "gadolinium break". <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 3056-66	4.8	219
142	Revised ionic radii of lanthanoid(III) ions in aqueous solution. <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 4572-9	5.1	170
141	Hydrogen and higher shell contributions in Zn <sup>2+</sup> , Ni <sup>2+</sup> , and Co <sup>2+</sup> aqueous solutions: an X-ray absorption fine structure and molecular dynamics study. <i>Journal of the American Chemical Society</i> , <b>2002</b> , 124, 1958-67	16.4	153
140	An extended x-ray absorption fine structure study of aqueous solutions by employing molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>1994</b> , 100, 985-994	3.9	122
139	Evidence of distorted fivefold coordination of the Cu <sup>2+</sup> aqua ion from an x-ray-absorption spectroscopy quantitative analysis. <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	118
138	The solution structure of [Cu(aq)] <sup>2+</sup> and its implications for rack-induced bonding in blue copper protein active sites. <i>Inorganic Chemistry</i> , <b>2005</b> , 44, 1922-33	5.1	116
137	Hydration of lanthanoids(III) and actinoids(III): an experimental/theoretical saga. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 11162-78	4.8	104
136	Double-electron excitation channels at the Br K edge of HBr and Br <sub>2</sub> . <i>Physical Review A</i> , <b>1993</b> , 47, 2055-2063		88
135	Development and validation of an integrated computational approach for the study of ionic species in solution by means of effective two-body potentials. The case of Zn <sup>2+</sup> , Ni <sup>2+</sup> , and Co <sup>2+</sup> in aqueous solutions. <i>Journal of the American Chemical Society</i> , <b>2002</b> , 124, 1968-76	16.4	85
134	Combined XANES and EXAFS analysis of Co <sup>2+</sup> , Ni <sup>2+</sup> , and Zn <sup>2+</sup> aqueous solutions. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	78
133	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> , <b>2010</b> , 49, 4224-31	5.1	73
132	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> , <b>2010</b> , 16, 684-92	4.8	72
131	Full quantitative multiple-scattering analysis of X-ray absorption spectra: application to potassium hexacyanoferrat(II) and -(III) complexes. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 15618-23	16.4	71
130	Hydration properties and ionic radii of actinide(III) ions in aqueous solution. <i>Inorganic Chemistry</i> , <b>2013</b> , 52, 10318-24	5.1	67
129	Evidence for sevenfold coordination in the first solvation shell of Hg(II) aqua ion. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 5430-6	16.4	66
128	Structural study of the N,NPdimethylpropyleneurea solvated lanthanoid(III) ions in solution and solid state with an analysis of the ionic radii of lanthanoid(III) ions. <i>Inorganic Chemistry</i> , <b>2010</b> , 49, 4420-32	5.1	63
127	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> , <b>2012</b> , 116, 13024-32	3.4	59

126	Triplet correlations in the hydration shell of aquaions. <i>Chemical Physics Letters</i> , <b>1994</b> , 225, 150-155	2.5	57
125	High-energy X-ray absorption spectroscopy: a new tool for structural investigations of lanthanoids and third-row transition elements. <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 3045-55	4.8	54
124	Detection of second hydration shells in ionic solutions by XANES: computed spectra for Ni <sup>2+</sup> in water based on molecular dynamics. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 1853-8	16.4	52
123	Evidence for multielectron resonances at the Sr K edge. <i>Physical Review A</i> , <b>1996</b> , 53, 798-805	2.6	52
122	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> , <b>2013</b> , 117, 12505-15	3.4	50
121	Cuprizone neurotoxicity, copper deficiency and neurodegeneration. <i>NeuroToxicology</i> , <b>2010</b> , 31, 509-17	4.4	50
120	Structural investigation of lanthanoid coordination: a combined XANES and molecular dynamics study. <i>Inorganic Chemistry</i> , <b>2009</b> , 48, 10239-48	5.1	49
119	The solvent shell structure of aqueous iodide: X-ray absorption spectroscopy and classical, hybrid QM/MM and full quantum molecular dynamics simulations. <i>Chemical Physics</i> , <b>2010</b> , 371, 24-29	2.3	49
118	X-ray absorption spectroscopy of hemes and hemeproteins in solution: multiple scattering analysis. <i>Inorganic Chemistry</i> , <b>2008</b> , 47, 9905-18	5.1	49
117	A coupled molecular dynamics and XANES data analysis investigation of aqueous cadmium(II). <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 11833-41	2.8	48
116	Integrated experimental and theoretical approach for the structural characterization of Hg <sup>2+</sup> aqueous solutions. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 084502	3.9	48
115	Unraveling halide hydration: A high dilution approach. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 044509	3.9	46
114	Computational evidence for a variable first shell coordination of the cadmium(II) ion in aqueous solution. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 9186-93	3.4	46
113	Experimental evidence for a variable first coordination shell of the cadmium(II) ion in aqueous, dimethyl sulfoxide, and N,NPdimethylpropyleneurea solution. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 9178-85	3.4	45
112	Effect of Multielectronic Configurations on the XAFS Analysis at the Fe K Edge. <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 4505-4514	2.8	45
111	An extended x-ray absorption fine structure study by employing molecular dynamics simulations: Bromide ion in methanolic solution. <i>Journal of Chemical Physics</i> , <b>1996</b> , 104, 1779-1790	3.9	45
110	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> , <b>2013</b> , 117, 12516-24	3.4	44
109	An X-ray diffraction and X-ray absorption spectroscopy joint study of neuroglobin. <i>Archives of Biochemistry and Biophysics</i> , <b>2008</b> , 475, 7-13	4.1	44

108	Multielectron excitations at the L edges of barium in aqueous solution. <i>Physical Review B</i> , <b>1996</b> , 54, 12129-12138	3.3	44
107	A combined theoretical and experimental study of solid octyl and decylammonium chlorides and of their aqueous solutions. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 7806-18	3.4	43
106	Structural and dynamical properties of the Hg <sup>2+</sup> aqua ion: a molecular dynamics study. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 4694-702	3.4	43
105	Assessment of the validity of intermolecular potential models used in molecular dynamics simulations by extended x-ray absorption fine structure spectroscopy: A case study of Sr <sup>2+</sup> in methanol solution. <i>Journal of Chemical Physics</i> , <b>1998</b> , 108, 9487-9497	3.9	43
104	XANES Reveals the Flexible Nature of Hydrated Strontium in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 4114-24	3.4	42
103	Development of Lennard-Jones and Buckingham Potentials for Lanthanoid Ions in Water. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 6214-6224	5.1	41
102	A coupled Car-Parrinello molecular dynamics and EXAFS data analysis investigation of aqueous Co(2+). <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 13081-8	2.8	41
101	Solvation structure of Zn(2+) and Cu(2+) ions in acetonitrile: a combined EXAFS and XANES study. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 4061-7	3.4	39
100	Unusual heme iron-lipid acyl chain coordination in Escherichia coli flavohemoglobin. <i>Biophysical Journal</i> , <b>2004</b> , 86, 3882-92	2.9	39
99	Hydration properties of the Zn <sup>2+</sup> ion in water at high pressure. <i>Inorganic Chemistry</i> , <b>2013</b> , 52, 1141-50	5.1	38
98	Influence of the Second Coordination Shell on the XANES Spectra of the Zn <sup>2+</sup> Ion in Water and Methanol. <i>ChemPlusChem</i> , <b>2012</b> , 77, 234-239	2.8	37
97	On the solvation of the Zn <sup>2+</sup> ion in methanol: a combined quantum mechanics, molecular dynamics, and EXAFS approach. <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 8509-15	5.1	37
96	Structural properties of geminal dicationic ionic liquid/water mixtures: a theoretical and experimental insight. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 16544-54	3.6	34
95	Local order and long range correlations in imidazolium halide ionic liquids: a combined molecular dynamics and XAS study. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 16443-53	3.6	34
94	Structural Properties and Aggregation Behavior of 1-Hexyl-3-methylimidazolium Iodide in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 14515-26	3.4	33
93	The non-octarepeat copper binding site of the prion protein is a key regulator of prion conversion. <i>Scientific Reports</i> , <b>2015</b> , 5, 15253	4.9	33
92	Thermal and structural properties of ethylammonium chloride and its mixture with water. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 4887-99	3.4	32
91	Effect of the Zn <sup>2+</sup> and Hg <sup>2+</sup> ions on the structure of liquid water. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 4798-803	2.8	32

90	Lithiation Mechanism in High-Entropy Oxides as Anode Materials for Li-Ion Batteries: An Operando XAS Study. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 50344-50354	9.5	32
89	Structural characterization of zinc(II) chloride in aqueous solution and in the protic ionic liquid ethyl ammonium nitrate by x-ray absorption spectroscopy. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 154509	3.9	31
88	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> , <b>2015</b> , 17, 2464-74	3.6	29
87	Crystal polymorphism of hexylammonium chloride and structural properties of its mixtures with water. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 2104-13	3.4	29
86	X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts. <i>Journal of Chemical Physics</i> , <b>2011</b> , 135, 074505	3.9	29
85	Structure of the hydrated and dimethyl sulfoxide solvated rubidium ions in solution. <i>Inorganic Chemistry</i> , <b>2004</b> , 43, 3543-9	5.1	29
84	Deep eutectic solvents: A structural point of view on the role of the cation. <i>Chemical Physics Letters: X</i> , <b>2019</b> , 2, 100001	2	28
83	Ion hydration under pressure. <i>Physical Review Letters</i> , <b>2003</b> , 91, 165505	7.4	27
82	Effects of the pathological Q212P mutation on human prion protein non-octarepeat copper-binding site. <i>Biochemistry</i> , <b>2012</b> , 51, 6068-79	3.2	26
81	Influence of Counterions on the Hydration Structure of Lanthanide Ions in Dilute Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 2779-2791	3.4	24
80	X-ray absorption fine structure spectroscopic studies of Octakis(DMSO)lanthanoid(III) complexes in solution and in the solid iodides. <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 7742-8	5.1	24
79	Unraveling the Sc(3+) Hydration Geometry: The Strange Case of the Far-Coordinated Water Molecule. <i>Inorganic Chemistry</i> , <b>2016</b> , 55, 6703-11	5.1	23
78	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> , <b>2017</b> , 147, 161707	3.9	23
77	Unravelling the hydration structure of ThX <sub>4</sub> (X = Br, Cl) water solutions by molecular dynamics simulations and X-ray absorption spectroscopy. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 6465-75	3.4	23
76	Double-Electron Excitation Channels at the Ca <sup>2+</sup> K-Edge of Hydrated Calcium Ion. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 11857-11865	3.4	23
75	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> , <b>2018</b> , 20, 2662-2675	3.6	21
74	A low transition temperature mixture for the dispersive liquid-liquid microextraction of pesticides from surface waters. <i>Journal of Chromatography A</i> , <b>2019</b> , 1605, 360329	4.5	21
73	Hidden Hydration Structure of Halide Ions: an Insight into the Importance of Lone Pairs. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 15729-37	3.4	21

72	X-ray absorption investigation of a unique protein domain able to bind both copper(I) and copper(II) at adjacent sites of the N-terminus of Haemophilus ducreyi Cu,Zn superoxide dismutase. <i>Biochemistry</i> , <b>2005</b> , 44, 13144-50	3.2	21
71	A quantum mechanics, molecular dynamics and EXAFS investigation into the Hg <sup>2+</sup> ion solvation properties in methanol solution. <i>RSC Advances</i> , <b>2013</b> , 3, 21118	3.7	20
70	Unusual heme binding properties of the dissimilative nitrate respiration regulator, a bacterial nitric oxide sensor. <i>Antioxidants and Redox Signaling</i> , <b>2012</b> , 17, 1178-89	8.4	20
69	Evidence of three-body correlation functions in Rb <sup>+</sup> and Sr <sup>2+</sup> acetonitrile solutions. <i>Journal of Chemical Physics</i> , <b>1999</b> , 111, 5107-5115	3.9	20
68	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> , <b>2019</b> , 141, 2299-2304	16.4	20
67	X-ray absorption study of the solvation structure of Cu <sup>2+</sup> in methanol and dimethyl sulfoxide. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 8827-33	5.1	19
66	A structural study of the hydrated and the dimethylsulfoxide, N,N'-dimethylpropyleneurea, and N,N-dimethylthioformamide solvated iron(II) and iron(III) ions in solution and solid state. <i>Inorganica Chimica Acta</i> , <b>2007</b> , 360, 1809-1818	2.7	19
65	Dynamic investigation of protein metal active sites: interplay of XANES and molecular dynamics simulations. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 14901-9	16.4	18
64	What first principles molecular dynamics can tell us about EXAFS spectroscopy of radioactive heavy metal cations in water. <i>Radiochimica Acta</i> , <b>2009</b> , 97,	1.9	18
63	How Does Ce Nitrate Dissolve in a Protic Ionic Liquid? A Combined Molecular Dynamics and EXAFS Study. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 8424-8433	4.8	17
62	K-edge XANES investigation of octakis(DMSO)lanthanoid(III) complexes in DMSO solution and solid iodides. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 8684-91	3.6	15
61	Crystal polymorphism of propylammonium chloride and structural properties of its mixture with water. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 11805-15	3.4	15
60	K- and L-edge XAFS determination of the local structure of aqueous Nd(III) and Eu(III). <i>Journal of Synchrotron Radiation</i> , <b>2001</b> , 8, 666-8	2.4	15
59	Quantitative analysis of XANES spectra of disordered systems based on molecular dynamics. <i>Journal of Synchrotron Radiation</i> , <b>2005</b> , 12, 75-9	2.4	14
58	Multivariate curve resolution analysis of operando XAS data for the investigation of the lithiation mechanisms in high entropy oxides. <i>Chemical Physics Letters</i> , <b>2020</b> , 760, 137968	2.5	14
57	Distal-proximal crosstalk in the heme binding pocket of the NO sensor DNR. <i>BioMetals</i> , <b>2014</b> , 27, 763-733.4	3.4	13
56	Combined distribution functions: A powerful tool to identify cation coordination geometries in liquid systems. <i>Chemical Physics Letters</i> , <b>2018</b> , 691, 437-443	2.5	12
55	On the possibility of using XANES to investigate bromide-based ionic liquids. <i>Chemical Physics Letters</i> , <b>2014</b> , 591, 32-36	2.5	12



54	Polarized X-ray absorption near-edge structure spectroscopy of neuroglobin and myoglobin single crystals. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 13223-31	3.4	12
53	On the complex formation of iron(III) bromide in the space-demanding solvent N,N'-dimethylpropyleneurea and the structure of the trisbromoiron(III) complex in solution and crystalline state. <i>Inorganica Chimica Acta</i> , <b>2007</b> , 360, 2744-2750	2.7	12
52	Lutetium(III) aqua ion: On the dynamical structure of the heaviest lanthanoid hydration complex. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 204505	3.9	12
51	Solvation of Zn ion in 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquids: a molecular dynamics and X-ray absorption study. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 6958-6969 <sup>3.6</sup>	3.6	11
50	Molecular dynamics to rationalize EXAFS experiments: A dynamical model explaining hydration behaviour across the lanthanoid(III) series. <i>Journal of Physics: Conference Series</i> , <b>2009</b> , 190, 012056	0.3	10
49	X-ray absorption spectroscopy study of the solvation structure of zinc(II) in dimethyl sulfoxide solution. <i>Chemical Physics Letters</i> , <b>2010</b> , 499, 113-116	2.5	10
48	Complete spectrum of multielectron excitations at the Br L edge x-ray absorption spectra. <i>Physical Review B</i> , <b>2001</b> , 64,	3.3	10
47	Hydrated and Solvated Tin(II) Ions in Solution and the Solid State, and a Coordination Chemistry Overview of the d s Metal Ions. <i>Chemistry - A European Journal</i> , <b>2016</b> , 22, 18583-18592	4.8	10
46	Solvation of Co <sup>2+</sup> ion in 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquid: A molecular dynamics and X-ray absorption study. <i>Journal of Molecular Liquids</i> , <b>2020</b> , 299, 112120	6	9
45	Following a Chemical Reaction on the Millisecond Time Scale by Simultaneous X-ray and UV/Vis Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 2958-2963	6.4	8
44	Structure and atomic correlations in molecular systems probed by XAS reverse Monte Carlo refinement. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 094307	3.9	8
43	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> , <b>2014</b> , 53, 9778-84	5.1	8
42	Measurement of x-ray multielectron photoexcitations at the L edge. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	8
41	Progresses in the MXAN Fitting Procedure. <i>AIP Conference Proceedings</i> , <b>2007</b> ,	0	8
40	EXAFS and molecular dynamics studies of ionic solutions. <i>Journal of Synchrotron Radiation</i> , <b>2001</b> , 8, 173-174	2.4	8
39	Deciphering Copper Coordination in the Mammalian Prion Protein Amyloidogenic Domain. <i>Biophysical Journal</i> , <b>2020</b> , 118, 676-687	2.9	8
38	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> , <b>2017</b> , 56, 14013-14022	5.1	7
37	Solvation structure of lanthanide(III) bistriflimide salts in acetonitrile solution: a molecular dynamics simulation and EXAFS investigation. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 13058-13069 <sup>3.6</sup>	3.6	7

36	Direct Mechanistic Evidence for a Nonheme Complex Reaction through a Multivariate XAS Analysis. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 9979-9989	5.1	7
35	Structural flexibility and role of vicinal 2-thienyl rings in 2,3-dicyano-5,6-di(2-thienyl)-1,4-pyrazine, [(CN) <sub>2</sub> Th <sub>2</sub> Pyz], its palladium(II) complex [(CN) <sub>2</sub> Th <sub>2</sub> Pyz(PdCl <sub>2</sub> ) <sub>2</sub> ], and the related pentametallic pyrazinoporphyrazines [(PdCl <sub>2</sub> ) <sub>4</sub> Th <sub>8</sub> TPyzPz <sub>4</sub> M] (M = Mg(II)(H <sub>2</sub> O), Zn(II)). <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 12116-25	5.1	7
34	A structural study of the N,N'-dimethylpropyleneurea solvated zinc(II) and cadmium(II) ions in solution and crystalline state. <i>Journal of Molecular Liquids</i> , <b>2007</b> , 131-132, 105-112	6	7
33	Elusive Coordination of the Ag Ion in Aqueous Solution: Evidence for a Linear Structure. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 17291-17302	5.1	7
32	Hydrophobic Eutectic Solvent with Antioxidant Properties: Application for the Dispersive Liquid-Liquid Microextraction of Fat-Soluble Micronutrients from Fruit Juices. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2021</b> , 9, 8170-8178	8.3	7
31	Unraveling the Hydration Properties of the Ba Aqua Ion: the Interplay of Quantum Mechanics, Molecular Dynamics, and EXAFS Spectroscopy. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 14551-14559	5.1	6
30	Ce <sup>3+</sup> and La <sup>3+</sup> ions in ethylammonium nitrate: A XANES and molecular dynamics investigation. <i>Chemical Physics Letters</i> , <b>2018</b> , 706, 311-316	2.5	6
29	Compression of liquid Ni and Co under extreme conditions explored by x-ray absorption spectroscopy. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	6
28	Solubilization properties and structural characterization of dissociated HgO and HgCl <sub>2</sub> in deep eutectic solvents. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 329, 115505	6	6
27	Transition from molecular- to nano-scale segregation in a deep eutectic solvent - water mixture. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 331, 115747	6	6
26	XAS in Liquid Systems <b>2016</b> , 745-771		5
25	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> , <b>2021</b> , 50, 131-142	4.3	5
24	Unraveling the perturbation induced by Zn <sup>2+</sup> and Hg <sup>2+</sup> ions on the hydrogen bond patterns of liquid methanol. <i>Chemical Physics Letters</i> , <b>2015</b> , 633, 70-75	2.5	4
23	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> , <b>2012</b> , 30, 269-79	3.6	4
22	Unusual proximal heme pocket geometry in the deoxygenated <i>Thermobifida fusca</i> : A combined spectroscopic investigation. <i>Biophysical Chemistry</i> , <b>2010</b> , 147, 1-7	3.5	4
21	Unraveling the solvation geometries of the lanthanum(III) bistriflimide salt in ionic liquid/acetone nitrile mixtures. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 20434-20443	3.6	4
20	Catching the Reversible Formation and Reactivity of Surface Defective Sites in Metal-Organic Frameworks: An Operando Ambient Pressure-NEXAFS Investigation. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 9182-9187	6.4	4
19	Anatomy of a deep eutectic solvent: structural properties of choline chloride : sesamol 1 : 3 compared to reline. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 11746-11754	3.6	4



18	Insights into the Structure of Reaction Intermediates Through Coupled X-ray Absorption/UV-Vis Spectroscopy. <i>Springer Proceedings in Physics</i> , <b>2021</b> , 141-154	0.2	4
17	Estimating a Set of Pure XANES Spectra from Multicomponent Chemical Mixtures Using a Transformation Matrix-Based Approach. <i>Springer Proceedings in Physics</i> , <b>2021</b> , 65-84	0.2	4
16	Fe-heme structure in Cu, Zn superoxide dismutase from <i>Haemophilus ducreyi</i> by X-ray absorption spectroscopy. <i>Archives of Biochemistry and Biophysics</i> , <b>2010</b> , 498, 43-9	4.1	3
15	The MXAN procedure: a new method of modeling the XANES spectra to obtain structural quantitative information. <i>AIP Conference Proceedings</i> , <b>2003</b> ,	0	3
14	Fourier transform infrared and dielectric study of water in 12E4 liquid crystals. <i>Journal of Chemical Physics</i> , <b>2000</b> , 113, 8783-8790	3.9	3
13	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> , <b>2021</b> , 23, 1188-1196	3.6	3
12	Fate of a Deep Eutectic Solvent upon Cosolvent Addition: Choline Chloride-Sesamol 1:3 Mixtures with Methanol. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2021</b> , 9, 12252-12261	8.3	3
11	Hemeproteins: Recent Advances in Quantitative XANES Analysis. <i>AIP Conference Proceedings</i> , <b>2007</b> ,	0	2
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8	On the Coordination Chemistry of the lanthanum(III) Nitrate Salt in EAN/MeOH Mixtures. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 10674-10685	5.1	2
7	Application of a Low Transition Temperature Mixture for the Dispersive Liquid-Liquid Microextraction of Illicit Drugs from Urine Samples. <i>Molecules</i> , <b>2021</b> , 26,	4.8	2
6	Two faces of the same coin: coupling X-ray Absorption and NMR spectroscopies to investigate the exchange reaction between prototypical Cu coordination complexes. <i>Chemistry - A European Journal</i> , <b>2021</b> ,	4.8	1
5	Theoretical Description of Ionic Liquids. <i>Soft and Biological Matter</i> , <b>2014</b> , 127-148	0.8	1
4	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)]. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 097102	3.9	
3	Structural Characterization of Ionic Liquids by X-Ray Absorption Spectroscopy. <i>Soft and Biological Matter</i> , <b>2014</b> , 149-172	0.8	
2	Structure and dynamics of hemeproteins using X-ray Absorption Spectroscopy. <i>Journal of Physics: Conference Series</i> , <b>2009</b> , 190, 012195	0.3	
1	The Prion Switch Unravalled. <i>FASEB Journal</i> , <b>2015</b> , 29, 564.13	0.9	

