Paola D Angelo

List of Publications by Year in Descending Order

143 papers	4,358 citations	41 h-index	58 g-index
151 ext. papers	4,761 ext. citations	4.4 avg, IF	5.55 L-index

#	Paper	IF	Citations
143	Two faces of the same coin: coupling X-ray Absorption and NMR spectroscopies to investigate the exchange reaction between prototypical Cu coordination complexes. *Chemistry - A European Journal*, **2021**,	4.8	1
142	Structural and mechanistic insights into low-temperature CO oxidation over a prototypical high entropy oxide by Cu L-edge operando soft X-ray absorption spectroscopy. *Physical Chemistry Chemical Physics*, **2021**, 23, 26575-26584	3.6	2
141	Solubilization properties and structural characterization of dissociated HgO and HgCl2 in deep eutectic solvents. *Journal of Molecular Liquids*, **2021**, 329, 115505	6	6
140	Coordination of the Co and Ni Ions in TfN Based Ionic Liquids: A Combined X-ray Absorption and Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2021**, 125, 6639-6648	3.4	2
139	Hydrophobic Eutectic Solvent with Antioxidant Properties: Application for the Dispersive Liquid□liquid Microextraction of Fat-Soluble Micronutrients from Fruit Juices. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 8170-8178	8.3	7
138	Transition from molecular- to nano-scale segregation in a deep eutectic solvent - water mixture. *Journal of Molecular Liquids*, **2021**, 331, 115747	6	6
137	On the Coordination Chemistry of the lanthanum(III) Nitrate Salt in EAN/MeOH Mixtures. *Inorganic Chemistry*, **2021**, 60, 10674-10685	5.1	2
136	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
135	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
134	Application of a Low Transition Temperature Mixture for the Dispersive Liquid-Liquid Microextraction of Illicit Drugs from Urine Samples. *Molecules*, **2021**, 26,	4.8	2
133	Catching the Reversible Formation and Reactivity of Surface Defective Sites in Metal-Organic Frameworks: An Operando Ambient Pressure-NEXAFS Investigation. *Journal of Physical Chemistry Letters*, **2021**, 12, 9182-9187	6.4	4
132	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
131	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
130	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
129	Estimating a Set of Pure XANES Spectra from Multicomponent Chemical Mixtures Using a Transformation Matrix-Based Approach. *Springer Proceedings in Physics*, **2021**, 65-84	0.2	4
128	Direct Mechanistic Evidence for a Nonheme Complex Reaction through a Multivariate XAS Analysis. *Inorganic Chemistry*, **2020**, 59, 9979-9989	5.1	7
127	Deciphering Copper Coordination in the Mammalian Prion Protein Amyloidogenic Domain. *Biophysical Journal*, **2020**, 118, 676-687	2.9	8

126	Solvation of Co2+ ion in 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquid: A molecular dynamics and X-ray absorption study. *Journal of Molecular Liquids*, **2020**, 299, 112120	6	9
125	Elusive Coordination of the Ag Ion in Aqueous Solution: Evidence for a Linear Structure. *Inorganic Chemistry*, **2020**, 59, 17291-17302	5.1	7
124	Multivariate curve resolution analysis of operando XAS data for the investigation of the lithiation mechanisms in high entropy oxides. *Chemical Physics Letters*, **2020**, 760, 137968	2.5	14
123	Lithiation Mechanism in High-Entropy Oxides as Anode Materials for Li-Ion Batteries: An Operando XAS Study. *ACS Applied Materials & Interfaces*, **2020**, 12, 50344-50354	9.5	32
122	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
121	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
120	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
119	Solvation of Zn ion in 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquids: a molecular dynamics and X-ray absorption study. *Physical Chemistry Chemical Physics*, **2019**, 21, 6958-6969	3.6	11
118	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	
117	A low transition temperature mixture for the dispersive liquid-liquid microextraction of pesticides from surface waters. *Journal of Chromatography A*, **2019**, 1605, 360329	4.5	21
116	Compression of liquid Ni and Co under extreme conditions explored by x-ray absorption spectroscopy. *Physical Review B*, **2019**, 100,	3.3	6
115	Deep eutectic solvents: A structural point of view on the role of the cation. *Chemical Physics Letters: X*, **2019**, 2, 100001	2	28
114	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
113	Structure and atomic correlations in molecular systems probed by XAS reverse Monte Carlo refinement. *Journal of Chemical Physics*, **2018**, 148, 094307	3.9	8
112	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
111	Combined distribution functions: A powerful tool to identify cation coordination geometries in liquid systems. *Chemical Physics Letters*, **2018**, 691, 437-443	2.5	12
110	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
109	Ce3+ and La3+ ions in ethylammonium nitrate: A XANES and molecular dynamics investigation. *Chemical Physics Letters*, **2018**, 706, 311-316	2.5	6

108	Development of Lennard-Jones and Buckingham Potentials for Lanthanoid Ions in Water. *Inorganic Chemistry*, **2017**, 56, 6214-6224	5.1	41
107	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
106	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
105	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
104	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
103	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
102	Unraveling the Sc(3+) Hydration Geometry: The Strange Case of the Far-Coordinated Water Molecule. *Inorganic Chemistry*, **2016**, 55, 6703-11	5.1	23
101	Hydrated and Solvated Tin(II) Ions in Solution and the Solid State, and a Coordination Chemistry Overview of the d s Metal Ions. *Chemistry - A European Journal*, **2016**, 22, 18583-18592	4.8	10
100	Lutetium(iii) aqua ion: On the dynamical structure of the heaviest lanthanoid hydration complex. *Journal of Chemical Physics*, **2016**, 144, 204505	3.9	12
99	XANES Reveals the Flexible Nature of Hydrated Strontium in Aqueous Solution. *Journal of Physical Chemistry B*, **2016**, 120, 4114-24	3.4	42
98	XAS in Liquid Systems **2016**, 745-771		5
97	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
96	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
95	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
94	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
93	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
92	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
91	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

90	The Prion Switch Unravelled. *FASEB Journal*, **2015**, 29, 564.13	0.9	
89	Unraveling halide hydration: A high dilution approach. *Journal of Chemical Physics*, **2014**, 141, 044509	3.9	46
88	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
87	Distal-proximal crosstalk in the heme binding pocket of the NO sensor DNR. *BioMetals*, **2014**, 27, 763-73	3.4	13
86	On the possibility of using XANES to investigate bromide-based ionic liquids. *Chemical Physics Letters*, **2014**, 591, 32-36	2.5	12
85	Structural Characterization of Ionic Liquids by X-Ray Absorption Spectroscopy. *Soft and Biological Matter*, **2014**, 149-172	0.8	
84	Theoretical Description of Ionic Liquids. *Soft and Biological Matter*, **2014**, 127-148	0.8	1
83	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
82	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
81	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
80	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
79	Hydration properties and ionic radii of actinide(III) ions in aqueous solution. *Inorganic Chemistry*, **2013**, 52, 10318-24	5.1	67
78	Hydration properties of the Zn2+ ion in water at high pressure. *Inorganic Chemistry*, **2013**, 52, 1141-50	5.1	38
77	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
76	X-ray absorption study of the solvation structure of Cu2+ in methanol and dimethyl sulfoxide. *Inorganic Chemistry*, **2012**, 51, 8827-33	5.1	19
75	Unravelling the hydration structure of ThX4 (X = Br, Cl) water solutions by molecular dynamics simulations and X-ray absorption spectroscopy. *Journal of Physical Chemistry B*, **2012**, 116, 6465-75	3.4	23
74	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
73	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

72	Effects of the pathological Q212P mutation on human prion protein non-octarepeat copper-binding site. *Biochemistry*, **2012**, 51, 6068-79	3.2	26
71	Unusual heme binding properties of the dissimilative nitrate respiration regulator, a bacterial nitric oxide sensor. *Antioxidants and Redox Signaling*, **2012**, 17, 1178-89	8.4	20
70	Hydration of lanthanoids(III) and actinoids(III): an experimental/theoretical saga. *Chemistry - A European Journal*, **2012**, 18, 11162-78	4.8	104
69	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
68	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
67	Revised ionic radii of lanthanoid(III) ions in aqueous solution. *Inorganic Chemistry*, **2011**, 50, 4572-9	5.1	170
66	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 = Mg(II)(H2O), Zn(II)). *Inorganic Chemistry*, **2011**, 50, 12116-25	5.1	7
65	Structural characterization of zinc(II) chloride in aqueous solution and in the protic ionic liquid ethyl ammonium nitrate by x-ray absorption spectroscopy. *Journal of Chemical Physics*, **2011**, 135, 154509	3.9	31
64	Thermal and structural properties of ethylammonium chloride and its mixture with water. *Journal of Physical Chemistry B*, **2011**, 115, 4887-99	3.4	32
63	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
62	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
61	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
60	X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts. *Journal of Chemical Physics*, **2011**, 135, 074505	3.9	29
59	Polarized X-ray absorption near-edge structure spectroscopy of neuroglobin and myoglobin single crystals. *Journal of Physical Chemistry B*, **2010**, 114, 13223-31	3.4	12
58	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
57	Cuprizone neurotoxicity, copper deficiency and neurodegeneration. *NeuroToxicology*, **2010**, 31, 509-17	4.4	50
56	Fe-heme structure in Cu, Zn superoxide dismutase from Haemophilus ducreyi by X-ray absorption spectroscopy. *Archives of Biochemistry and Biophysics*, **2010**, 498, 43-9	4.1	3
55	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. *Inorganic Chemistry*, **2010**, 49, 4420-32	5.1	63

54	Dynamic investigation of protein metal active sites: interplay of XANES and molecular dynamics simulations. *Journal of the American Chemical Society*, **2010**, 132, 14901-9	16.4	18
53	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
52	The solvent shell structure of aqueous iodide: X-ray absorption spectroscopy and classical, hybrid QM/MM and full quantum molecular dynamics simulations. *Chemical Physics*, **2010**, 371, 24-29	2.3	49
51	Unusual proximal heme pocket geometry in the deoxygenated Thermobifida fusca: A combined spectroscopic investigation. *Biophysical Chemistry*, **2010**, 147, 1-7	3.5	4
50	X-ray absorption spectroscopy study of the solvation structure of zinc(II) in dimethyl sulfoxide solution. *Chemical Physics Letters*, **2010**, 499, 113-116	2.5	10
49	What first principles molecular dynamics can tell us about EXAFS spectroscopy of radioactive heavy metal cations in water. *Radiochimica Acta*, **2009**, 97,	1.9	18
48	Structural investigation of lanthanoid coordination: a combined XANES and molecular dynamics study. *Inorganic Chemistry*, **2009**, 48, 10239-48	5.1	49
47	Structure and dynamics of hemeproteins using X-ray Absorption Spectroscopy. *Journal of Physics: Conference Series*, **2009**, 190, 012195	0.3	
46	Molecular dynamics to rationalize EXAFS experiments: A dynamical model explaining hydration behaviour across the lanthanoid(III) series. *Journal of Physics: Conference Series*, **2009**, 190, 012056	0.3	10
45	Measurement of x-ray multielectron photoexcitations at the I K edge. *Physical Review B*, **2008**, 78,	3.3	8
44	An X-ray diffraction and X-ray absorption spectroscopy joint study of neuroglobin. *Archives of Biochemistry and Biophysics*, **2008**, 475, 7-13	4.1	44
43	X-ray absorption spectroscopy of hemes and hemeproteins in solution: multiple scattering analysis. *Inorganic Chemistry*, **2008**, 47, 9905-18	5.1	49
42	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
41	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
40	Integrated experimental and theoretical approach for the structural characterization of Hg2+ aqueous solutions. *Journal of Chemical Physics*, **2008**, 128, 084502	3.9	48
39	Hydration of lanthanoid(III) ions in aqueous solution and crystalline hydrates studied by EXAFS spectroscopy and crystallography: the myth of the "gadolinium break". *Chemistry - A European Journal*, **2008**, 14, 3056-66	4.8	219
38	High-energy X-ray absorption spectroscopy: a new tool for structural investigations of lanthanoids and third-row transition elements. *Chemistry - A European Journal*, **2008**, 14, 3045-55	4.8	54
37	X-ray absorption fine structure spectroscopic studies of Octakis(DMSO)lanthanoid(III) complexes in solution and in the solid iodides. *Inorganic Chemistry*, **2007**, 46, 7742-8	5.1	24

36	Hemeproteins: Recent Advances in Quantitative XANES Analysis. *AIP Conference Proceedings*, **2007**,	0	2
35	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. *Inorganica Chimica Acta*, **2007**, 360, 1809-1818	2.7	19
34	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. *Inorganica Chimica Acta*, **2007**, 360, 2744-2750	2.7	12
33	A structural study of the N,N?-dimethylpropyleneurea solvated zinc(II) and cadmium(II) ions in solution and crystalline state. *Journal of Molecular Liquids*, **2007**, 131-132, 105-112	6	7
32	Progresses in the MXAN Fitting Procedure. *AIP Conference Proceedings*, **2007**,	0	8
31	Evidence for sevenfold coordination in the first solvation shell of Hg(II) aqua ion. *Journal of the American Chemical Society*, **2007**, 129, 5430-6	16.4	66
30	A coupled Car-Parrinello molecular dynamics and EXAFS data analysis investigation of aqueous Co(2+). *Journal of Physical Chemistry A*, **2006**, 110, 13081-8	2.8	41
29	Detection of second hydration shells in ionic solutions by XANES: computed spectra for Ni2+ in water based on molecular dynamics. *Journal of the American Chemical Society*, **2006**, 128, 1853-8	16.4	52
28	Computational evidence for a variable first shell coordination of the cadmium(II) ion in aqueous solution. *Journal of Physical Chemistry B*, **2005**, 109, 9186-93	3.4	46
27	Experimental evidence for a variable first coordination shell of the cadmium(II) ion in aqueous, dimethyl sulfoxide, and N,NPdimethylpropyleneurea solution. *Journal of Physical Chemistry B*, **2005**, 109, 9178-85	3.4	45
26	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. *Biochemistry*, **2005**, 44, 13144-50	3.2	21
25	The solution structure of [Cu(aq)]2+ and its implications for rack-induced bonding in blue copper protein active sites. *Inorganic Chemistry*, **2005**, 44, 1922-33	5.1	116
24	Quantitative analysis of XANES spectra of disordered systems based on molecular dynamics. *Journal of Synchrotron Radiation*, **2005**, 12, 75-9	2.4	14
23	Full quantitative multiple-scattering analysis of X-ray absorption spectra: application to potassium hexacyanoferrat(II) and -(III) complexes. *Journal of the American Chemical Society*, **2004**, 126, 15618-23	16.4	71
22	Structure of the hydrated and dimethyl sulfoxide solvated rubidium ions in solution. *Inorganic Chemistry*, **2004**, 43, 3543-9	5.1	29
21	Effect of Multielectronic Configurations on the XAFS Analysis at the Fe K Edge. *Journal of Physical Chemistry A*, **2004**, 108, 4505-4514	2.8	45
20	Double-Electron Excitation Channels at the Ca2+ K-Edge of Hydrated Calcium Ion. *Journal of Physical Chemistry B*, **2004**, 108, 11857-11865	3.4	23
19	Unusual heme iron-lipid acyl chain coordination in Escherichia coli flavohemoglobin. *Biophysical Journal*, **2004**, 86, 3882-92	2.9	39

18	The MXAN procedure: a new method of modeling the XANES spectra to obtain structural quantitative information. *AIP Conference Proceedings*, **2003**,	0	3
17	Ion hydration under pressure. *Physical Review Letters*, **2003**, 91, 165505	7.4	27
16	Hydrogen and higher shell contributions in Zn2+, Ni2+, and Co2+ aqueous solutions: an X-ray absorption fine structure and molecular dynamics study. *Journal of the American Chemical Society*, **2002**, 124, 1958-67	16.4	153
15	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 Zn2+, Ni2+, and Co2+ in aqueous solutions. *Journal of the American Chemical Society*, **2002**, 124, 1968-76	16.4	85
14	Combined XANES and EXAFS analysis of Co2+, Ni2+, and Zn2+ aqueous solutions. *Physical Review B*, **2002**, 66,	3.3	78
13	Evidence of distorted fivefold coordination of the Cu2+ aqua ion from an x-ray-absorption spectroscopy quantitative analysis. *Physical Review B*, **2002**, 65,	3.3	118
12	EXAFS and molecular dynamics studies of ionic solutions. *Journal of Synchrotron Radiation*, **2001**, 8, 173-7	2.4	8
11	K- and L-edge XAFS determination of the local structure of aqueous Nd(III) and Eu(III). *Journal of Synchrotron Radiation*, **2001**, 8, 666-8	2.4	15
10	Complete spectrum of multielectron excitations at the Br K edge x-ray absorption spectra. *Physical Review B*, **2001**, 64,	3.3	10
9	Fourier transform infrared and dielectric study of water–12E4 liquid crystals. *Journal of Chemical Physics*, **2000**, 113, 8783-8790	3.9	3
8	Evidence of three-body correlation functions in Rb+ and Sr2+ acetonitrile solutions. *Journal of Chemical Physics*, **1999**, 111, 5107-5115	3.9	20
7	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 Sr2+ in methanol solution. *Journal of Chemical Physics*, **1998**, 108, 9487-9497	3.9	43
6	Evidence for multielectron resonances at the Sr K edge. *Physical Review A*, **1996**, 53, 798-805	2.6	52
5	Multielectron excitations at the L edges of barium in aqueous solution. *Physical Review B*, **1996**, 54, 12129-12138	3.3	44
4	An extended x-ray absorption fine structure study by employing molecular dynamics simulations: Bromide ion in methanolic solution. *Journal of Chemical Physics*, **1996**, 104, 1779-1790	3.9	45
3	Triplet correlations in the hydration shell of aquaions. *Chemical Physics Letters*, **1994**, 225, 150-155	2.5	57
2	An extended x-ray absorption fine structure study of aqueous solutions by employing molecular dynamics simulations. *Journal of Chemical Physics*, **1994**, 100, 985-994	3.9	122
1	Double-electron excitation channels at the Br K edge of HBr and Br2. *Physical Review A*, **1993**, 47, 2055-2063	2.6	88