Paola D'Angelo

List of Publications by Year
in descending order

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147	5,250	57758	110387
papers	citations	44 h-index	64 g-index

151	151	151	3966
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Two Faces of the Same Coin: Coupling Xâ€Ray Absorption and NMR Spectroscopies to Investigate the Exchange Reaction Between Prototypical Cu Coordination Complexes. Chemistry - A European Journal, 2022, 28, .	3.3	6
2	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
3	On the Role of Water in the Formation of a Deep Eutectic Solvent Based on NiCl₂Â·6H₂O and Urea. Inorganic Chemistry, 2022, 61, 8843-8853.	4.0	11
4	Following a Silent Metal Ion: A Combined X-ray Absorption and Nuclear Magnetic Resonance Spectroscopic Study of the Zn²⁺ Cation Dissipative Translocation between Two Different Ligands. Journal of Physical Chemistry Letters, 2022, 13, 5522-5529.	4.6	10
5	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
6	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
7	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
8	Solubilization properties and structural characterization of dissociated HgO and HgCl2 in deep eutectic solvents. Journal of Molecular Liquids, 2021, 329, 115505.	4.9	14
9	Coordination of the Co²⁺ and Ni²⁺ Ions in Tf₂N^{â€“} Based Ionic Liquids: A Combined X-ray Absorption and Molecular Dynamics Study. Journal of Physical Chemistry B, 2021, 125, 6639-6648.	2.6	15
10	Hydrophobic Eutectic Solvent with Antioxidant Properties: Application for the Dispersive Liquidâ€“Liquid Microextraction of Fat-Soluble Micronutrients from Fruit Juices. ACS Sustainable Chemistry and Engineering, 2021, 9, 8170-8178.	6.7	20
11	Transition from molecular- to nano-scale segregation in a deep eutectic solvent - water mixture. Journal of Molecular Liquids, 2021, 331, 115747.	4.9	21
12	On the Coordination Chemistry of the lanthanum(III) Nitrate Salt in EAN/MeOH Mixtures. Inorganic Chemistry, 2021, 60, 10674-10685.	4.0	10
13	Application of a Low Transition Temperature Mixture for the Dispersive Liquidâ€“Liquid Microextraction of Illicit Drugs from Urine Samples. Molecules, 2021, 26, 5222.	3.8	13
14	Catching the Reversible Formation and Reactivity of Surface Defective Sites in Metalâ€“Organic Frameworks: An Operando Ambient Pressure-NEXAFS Investigation. Journal of Physical Chemistry Letters, 2021, 12, 9182-9187.	4.6	15
15	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
16	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
17	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
18	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	7

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19	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.	2.8	17
20	Deciphering Copper Coordination in the Mammalian Prion Protein Amyloidogenic Domain. Biophysical Journal, 2020, 118, 676-687.	0.5	11
21	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.	4.9	24
22	Elusive Coordination of the Ag⁺ Ion in Aqueous Solution: Evidence for a Linear Structure. Inorganic Chemistry, 2020, 59, 17291-17302.	4.0	25
23	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.	2.6	26
24	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.	8.0	78
25	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
26	Direct Mechanistic Evidence for a Nonheme Complex Reaction through a Multivariate XAS Analysis. Inorganic Chemistry, 2020, 59, 9979-9989.	4.0	13
27	A low transition temperature mixture for the dispersive liquid-liquid microextraction of pesticides from surface waters. Journal of Chromatography A, 2019, 1605, 360329.	3.7	35
28	Compression of liquid Ni and Co under extreme conditions explored by x-ray absorption spectroscopy. Physical Review B, 2019, 100, .	3.2	8
29	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
30	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
31	Solvation of Zn²⁺ 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.	2.8	21
32	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
33	Deep eutectic solvents: A structural point of view on the role of the cation. Chemical Physics Letters: X, 2019, 737, 100001.	2.1	45
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	Structure and atomic correlations in molecular systems probed by XAS reverse Monte Carlo refinement. Journal of Chemical Physics, 2018, 148, .	3.0	13
36	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

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37	Combined distribution functions: A powerful tool to identify cation coordination geometries in liquid systems. Chemical Physics Letters, 2018, 691, 437-443.	2.6	19
38	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
39	Ce3+ and La3+ ions in ethylammonium nitrate: A XANES and molecular dynamics investigation. Chemical Physics Letters, 2018, 706, 311-316.	2.6	8
40	Development of Lennard-Jones and Buckingham Potentials for Lanthanoid Ions in Water. Inorganic Chemistry, 2017, 56, 6214-6224.	4.0	57
41	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
42	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
43	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
44	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
45	Hydrated and Solvated Tin(II) Ions in Solution and the Solid State, and a Coordination Chemistry Overview of the d¹⁰s² Metal Ions. Chemistry - A European Journal, 2016, 22, 18583-18592.	3.3	17
46	Lutetium(iii) aqua ion: On the dynamical structure of the heaviest lanthanoid hydration complex. Journal of Chemical Physics, 2016, 144, 204505.	3.0	15
47	XANES Reveals the Flexible Nature of Hydrated Strontium in Aqueous Solution. Journal of Physical Chemistry B, 2016, 120, 4114-4124.	2.6	57
48	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
49	Unraveling the Sc³⁺ Hydration Geometry: The Strange Case of the Far-Coordinated Water Molecule. Inorganic Chemistry, 2016, 55, 6703-6711.	4.0	30
50	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
51	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
52	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
53	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
54	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

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55	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
56	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
57	The Prion Switch Unravelled. FASEB Journal, 2015, 29, 564.13.	0.5	0
58	Structural Characterization of Ionic Liquids by X-Ray Absorption Spectroscopy. Soft and Biological Matter, 2014, , 149-172.	0.3	0
59	Unraveling halide hydration: A high dilution approach. Journal of Chemical Physics, 2014, 141, 044509.	3.0	52
60	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
61	Distalâ€“proximal crosstalk in the heme binding pocket of the NO sensor DNR. BioMetals, 2014, 27, 763-773.	4.1	13
62	On the possibility of using XANES to investigate bromide-based ionic liquids. Chemical Physics Letters, 2014, 591, 32-36.	2.6	12
63	Theoretical Description of Ionic Liquids. Soft and Biological Matter, 2014, , 127-148.	0.3	2
64	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
65	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
66	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
67	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
68	Hydration Properties and Ionic Radii of Actinide(III) Ions in Aqueous Solution. Inorganic Chemistry, 2013, 52, 10318-10324.	4.0	80
69	Hydration Properties of the Zn²⁺ Ion in Water at High Pressure. Inorganic Chemistry, 2013, 52, 1141-1150.	4.0	41
70	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
71	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
72	X-ray Absorption Study of the Solvation Structure of Cu²⁺ in Methanol and Dimethyl Sulfoxide. Inorganic Chemistry, 2012, 51, 8827-8833.	4.0	23

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73	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, 6465-6475.	2.6	28
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, 13024-13032.	2.6	60
75	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
76	Effects of the Pathological Q212P Mutation on Human Prion Protein Non-Octarepeat Copper-Binding Site. Biochemistry, 2012, 51, 6068-6079.	2.5	32
77	Unusual Heme Binding Properties of the Dissimilative Nitrate Respiration Regulator, a Bacterial Nitric Oxide Sensor. Antioxidants and Redox Signaling, 2012, 17, 1178-1189.	5.4	21
78	Hydration of Lanthanoids(III) and Actinoids(III): An Experimental/Theoretical Saga. Chemistry - A European Journal, 2012, 18, 11162-11178.	3.3	114
79	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
80	Thermal and Structural Properties of Ethylammonium Chloride and Its Mixture with Water. Journal of Physical Chemistry B, 2011, 115, 4887-4899.	2.6	34
81	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
82	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
83	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
84	Revised Ionic Radii of Lanthanoid(III) Ions in Aqueous Solution. Inorganic Chemistry, 2011, 50, 4572-4579.	4.0	212
85	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 =) Tj ETQq1 1 0.784314 rgBT /Overlock 10	4.0	7
86	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.	3.0	33
87	X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts. Journal of Chemical Physics, 2011, 135, 074505.	3.0	31
88	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
89	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.	1.9	56
90	Unusual proximal heme pocket geometry in the deoxygenated Thermobifida fusca: A combined spectroscopic investigation. Biophysical Chemistry, 2010, 147, 1-7.	2.8	5

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91	X-ray absorption spectroscopy study of the solvation structure of zinc(II) in dimethyl sulfoxide solution. Chemical Physics Letters, 2010, 499, 113-116.	2.6	10
92	Polarized X-ray Absorption Near-Edge Structure Spectroscopy of Neuroglobin and Myoglobin Single Crystals. Journal of Physical Chemistry B, 2010, 114, 13223-13231.	2.6	12
93	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
94	Cuprizone neurotoxicity, copper deficiency and neurodegeneration. NeuroToxicology, 2010, 31, 509-517.	3.0	59
95	Fe-heme structure in Cu,Zn superoxide dismutase from Haemophilus ducreyi by X-ray Absorption Spectroscopy. Archives of Biochemistry and Biophysics, 2010, 498, 43-49.	3.0	3
96	Structural Study of the N,Nâ€²-Dimethylpropyleneurea Solvated Lanthanoid(III) Ions in Solution and Solid State with an Analysis of the Ionic Radii of Lanthanoid(III) Ions. Inorganic Chemistry, 2010, 49, 4420-4432.	4.0	74
97	Dynamic Investigation of Protein Metal Active Sites: Interplay of XANES and Molecular Dynamics Simulations. Journal of the American Chemical Society, 2010, 132, 14901-14909.	13.7	18
98	What first principles molecular dynamics can tell us about EXAFS spectroscopy of radioactive heavy metal cations in water. Radiochimica Acta, 2009, 97, 339-346.	1.2	22
99	Structural Investigation of Lanthanoid Coordination: a Combined XANES and Molecular Dynamics Study. Inorganic Chemistry, 2009, 48, 10239-10248.	4.0	51
100	Structure and dynamics of hemeproteins using X-ray Absorption Spectroscopy. Journal of Physics: Conference Series, 2009, 190, 012195.	0.4	1
101	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.	0.4	11
102	Hydration of Lanthanoid(III) Ions in Aqueous Solution and Crystalline Hydrates Studied by EXAFS Spectroscopy and Crystallography: The Myth of the â€œGadolinium Breakâ€• Chemistry - A European Journal, 2008, 14, 3056-3066.	3.3	248
103	Highâ€Energy Xâ€ray Absorption Spectroscopy: A New Tool for Structural Investigations of Lanthanoids and Thirdâ€Row Transition Elements. Chemistry - A European Journal, 2008, 14, 3045-3055.	3.3	55
104	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
105	An X-ray diffraction and X-ray absorption spectroscopy joint study of neuroglobin. Archives of Biochemistry and Biophysics, 2008, 475, 7-13.	3.0	50
106	X-ray Absorption Spectroscopy of Hemes and Hemeproteins in Solution: Multiple Scattering Analysis. Inorganic Chemistry, 2008, 47, 9905-9918.	4.0	52
107	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
108	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

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109	Integrated experimental and theoretical approach for the structural characterization of Hg2+ aqueous solutions. Journal of Chemical Physics, 2008, 128, 084502.	3.0	50
110	Progresses in the MXAN Fitting Procedure. AIP Conference Proceedings, 2007, , .	0.4	10
111	Evidence for Sevenfold Coordination in the First Solvation Shell of Hg(II) Aqua Ion. Journal of the American Chemical Society, 2007, 129, 5430-5436.	13.7	78
112	X-ray Absorption Fine Structure Spectroscopic Studies of Octakis(DMSO)lanthanoid(III) Complexes in Solution and in the Solid Iodides. Inorganic Chemistry, 2007, 46, 7742-7748.	4.0	26
113	Hemeproteins: Recent Advances in Quantitative XANES Analysis. AIP Conference Proceedings, 2007, , .	0.4	2
114	A structural study of the hydrated and the dimethylsulfoxide, N,Nâ€²-dimethylpropyleneurea, and N,N-dimethylthioformamide solvated iron(II) and iron(III) ions in solution and solid state. Inorganica Chimica Acta, 2007, 360, 1809-1818.	2.4	23
115	On the complex formation of iron(III) bromide in the space-demanding solvent N,Nâ€²-dimethylpropyleneurea and the structure of the trisbromoiron(III) complex in solution and crystalline state. Inorganica Chimica Acta, 2007, 360, 2744-2750.	2.4	17
116	A structural study of the N,Nâ€²-dimethylpropyleneurea solvated zinc(II) and cadmium(II) ions in solution and crystalline state. Journal of Molecular Liquids, 2007, 131-132, 105-112.	4.9	9
117	A Coupled Car-Parrinello Molecular Dynamics and EXAFS Data Analysis Investigation of Aqueous Co2+. Journal of Physical Chemistry A, 2006, 110, 13081-13088.	2.5	46
118	Detection of Second Hydration Shells in Ionic Solutions by XANES:Â Computed Spectra for Ni2+in Water Based on Molecular Dynamics. Journal of the American Chemical Society, 2006, 128, 1853-1858.	13.7	59
119	The Solution Structure of [Cu(aq)]2+and Its Implications for Rack-Induced Bonding in Blue Copper Protein Active Sites. Inorganic Chemistry, 2005, 44, 1922-1933.	4.0	134
120	Quantitative analysis of XANES spectra of disordered systems based on molecular dynamics. Journal of Synchrotron Radiation, 2005, 12, 75-79.	2.4	16
121	Computational Evidence for a Variable First Shell Coordination of the Cadmium(II) Ion in Aqueous Solution. Journal of Physical Chemistry B, 2005, 109, 9186-9193.	2.6	49
122	Experimental Evidence for a Variable First Coordination Shell of the Cadmium(II) Ion in Aqueous, Dimethyl Sulfoxide, andN,Nâ€˜-Dimethylpropyleneurea Solution. Journal of Physical Chemistry B, 2005, 109, 9178-9185.	2.6	53
123	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, 13144-13150.	2.5	22
124	A Quantitative Structural Investigation of the XANES Spectra of Potassium Ferrocyanide III at the Iron KEdge. Physica Scripta, 2005, , 152.	2.5	1
125	Full Quantitative Multiple-Scattering Analysis of X-ray Absorption Spectra:Â Application to Potassium Hexacyanoferrat(II) and -(III) Complexes. Journal of the American Chemical Society, 2004, 126, 15618-15623.	13.7	73
126	Structure of the Hydrated and Dimethyl Sulfoxide Solvated Rubidium Ions in Solution. Inorganic Chemistry, 2004, 43, 3543-3549.	4.0	33

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127	Effect of Multielectronic Configurations on the XAFS Analysis at the Fe K Edge. Journal of Physical Chemistry A, 2004, 108, 4505-4514.	2.5	49
128	Double-Electron Excitation Channels at the Ca2+ K-Edge of Hydrated Calcium Ion. Journal of Physical Chemistry B, 2004, 108, 11857-11865.	2.6	28
129	Unusual Heme Iron-Lipid Acyl Chain Coordination in Escherichia coli Flavohemoglobin. Biophysical Journal, 2004, 86, 3882-3892.	0.5	40
130	Ion Hydration under Pressure. Physical Review Letters, 2003, 91, 165505.	7.8	31
131	The MXAN procedure: a new method of modeling the XANES spectra to obtain structural quantitative information. AIP Conference Proceedings, 2003, , .	0.4	4
132	Hydrogen and Higher Shell Contributions in Zn2+, Ni2+, and Co2+Aqueous Solutions:Â An X-ray Absorption Fine Structure and Molecular Dynamics Study. Journal of the American Chemical Society, 2002, 124, 1958-1967.	13.7	175
133	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, 1968-1976.	13.7	92
134	Combined XANES and EXAFS analysis ofCo2+,Ni2+,andZn2+aqueous solutions. Physical Review B, 2002, 66, .	3.2	88
135	Evidence of distorted fivefold coordination of theCu2+aqua ion from an x-ray-absorption spectroscopy quantitative analysis. Physical Review B, 2002, 65, .	3.2	131
136	EXAFS and molecular dynamics studies of ionic solutions. Journal of Synchrotron Radiation, 2001, 8, 173-177.	2.4	10
137	K- andL-edge XAFS determination of the local structure of aqueous Nd(III) and Eu(III). Journal of Synchrotron Radiation, 2001, 8, 666-668.	2.4	17
138	Complete spectrum of multielectron excitations at the Br- K edge x-ray absorption spectra. Physical Review B, 2001, 64, .	3.2	10
139	Fourier transform infrared and dielectric study of waterâ€“C12E4 liquid crystals. Journal of Chemical Physics, 2000, 113, 8783-8790.	3.0	5
140	Evidence of three-body correlation functions in Rb+ and Sr2+ acetonitrile solutions. Journal of Chemical Physics, 1999, 111, 5107-5115.	3.0	24
141	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.	3.0	45
142	Evidence for multielectron resonances at the SrKedge. Physical Review A, 1996, 53, 798-805.	2.5	57
143	Multielectron excitations at theLedges of barium in aqueous solution. Physical Review B, 1996, 54, 12129-12138.	3.2	48
144	An extended xâ€ray absorption fine structure study by employing molecular dynamics simulations: Bromide ion in methanolic solution. Journal of Chemical Physics, 1996, 104, 1779-1790.	3.0	48

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145	Triplet correlations in the hydration shell of aquaions. Chemical Physics Letters, 1994, 225, 150-155.	2.6	59
146	An extended xâ€ray absorption fine structure study of aqueous solutions by employing molecular dynamics simulations. Journal of Chemical Physics, 1994, 100, 985-994.	3.0	133
147	Double-electron excitation channels at the BrKedge of HBr andBr2. Physical Review A, 1993, 47, 2055-2063.	2.5	101