

Paola D'Angelo

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7632/publications.pdf>

Version: 2024-02-01

147
papers

5,250
citations

57631

44
h-index

110170

64
g-index

151
all docs

151
docs citations

151
times ranked

3966
citing authors

#	ARTICLE	IF	CITATIONS
1	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> , 2022, 28, .	1.7	6
2	Structural Study of a Eutectic Solvent Reveals Hydrophobic Segregation and Lack of Hydrogen Bonding between the Components. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 6337-6345.	3.2	9
3	On the Role of Water in the Formation of a Deep Eutectic Solvent Based on $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ and Urea. <i>Inorganic Chemistry</i> , 2022, 61, 8843-8853.	1.9	11
4	Following a Silent Metal Ion: A Combined X-ray Absorption and Nuclear Magnetic Resonance Spectroscopic Study of the Zn^{2+} Cation Dissipative Translocation between Two Different Ligands. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5522-5529.	2.1	10
5	Response to Comment on "Structural Study of a Eutectic Solvent Reveals Hydrophobic Segregation and Lack of Hydrogen Bonding between the Components" <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 8671-8672.	3.2	3
6	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.	1.6	10
7	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.	1.3	9
8	Solubilization properties and structural characterization of dissociated HgO and HgCl_2 in deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2021, 329, 115505.	2.3	14
9	Coordination of the Co^{2+} and Ni^{2+} Ions in Tf_2N^- Based Ionic Liquids: A Combined X-ray Absorption and Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6639-6648.	1.2	15
10	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> , 2021, 9, 8170-8178.	3.2	20
11	Transition from molecular- to nano-scale segregation in a deep eutectic solvent - water mixture. <i>Journal of Molecular Liquids</i> , 2021, 331, 115747.	2.3	21
12	On the Coordination Chemistry of the lanthanum(III) Nitrate Salt in EAN/MeOH Mixtures. <i>Inorganic Chemistry</i> , 2021, 60, 10674-10685.	1.9	10
13	Application of a Low Transition Temperature Mixture for the Dispersive Liquid-Liquid Microextraction of Illicit Drugs from Urine Samples. <i>Molecules</i> , 2021, 26, 5222.	1.7	13
14	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> , 2021, 12, 9182-9187.	2.1	15
15	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.	3.2	15
16	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.	1.3	16
17	Insights into the Structure of Reaction Intermediates Through Coupled X-ray Absorption/UV-Vis Spectroscopy. <i>Springer Proceedings in Physics</i> , 2021, , 141-154.	0.1	5
18	Estimating a Set of Pure XANES Spectra from Multicomponent Chemical Mixtures Using a Transformation Matrix-Based Approach. <i>Springer Proceedings in Physics</i> , 2021, , 65-84.	0.1	7

#	ARTICLE	IF	CITATIONS
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. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26575-26584.	1.3	17
20	Deciphering Copper Coordination in the Mammalian Prion Protein Amyloidogenic Domain. <i>Biophysical Journal</i> , 2020, 118, 676-687.	0.2	11
21	Solvation of Co ²⁺ 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> , 2020, 299, 112120.	2.3	24
22	Elusive Coordination of the Ag ⁺ Ion in Aqueous Solution: Evidence for a Linear Structure. <i>Inorganic Chemistry</i> , 2020, 59, 17291-17302.	1.9	25
23	Multivariate curve resolution analysis of operando XAS data for the investigation of the lithiation mechanisms in high entropy oxides. <i>Chemical Physics Letters</i> , 2020, 760, 137968.	1.2	26
24	Lithiation Mechanism in High-Entropy Oxides as Anode Materials for Li-Ion Batteries: An Operando XAS Study. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 50344-50354.	4.0	78
25	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.	1.3	6
26	Direct Mechanistic Evidence for a Nonheme Complex Reaction through a Multivariate XAS Analysis. <i>Inorganic Chemistry</i> , 2020, 59, 9979-9989.	1.9	13
27	A low transition temperature mixture for the dispersive liquid-liquid microextraction of pesticides from surface waters. <i>Journal of Chromatography A</i> , 2019, 1605, 360329.	1.8	35
28	Compression of liquid Ni and Co under extreme conditions explored by x-ray absorption spectroscopy. <i>Physical Review B</i> , 2019, 100, .	1.1	8
29	Unraveling the Hydration Properties of the Ba ²⁺ Aqua Ion: the Interplay of Quantum Mechanics, Molecular Dynamics, and EXAFS Spectroscopy. <i>Inorganic Chemistry</i> , 2019, 58, 14551-14559.	1.9	15
30	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.	1.3	10
31	Solvation of Zn ²⁺ 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> , 2019, 21, 6958-6969.	1.3	21
32	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> , 2019, 150, 097102.	1.2	0
33	Deep eutectic solvents: A structural point of view on the role of the cation. <i>Chemical Physics Letters: X</i> , 2019, 737, 100001.	2.1	45
34	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.	6.6	27
35	Structure and atomic correlations in molecular systems probed by XAS reverse Monte Carlo refinement. <i>Journal of Chemical Physics</i> , 2018, 148, .	1.2	13
36	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.	1.2	37

#	ARTICLE	IF	CITATIONS
37	Combined distribution functions: A powerful tool to identify cation coordination geometries in liquid systems. <i>Chemical Physics Letters</i> , 2018, 691, 437-443.	1.2	19
38	On the coordination of Zn ²⁺ ion in Tf ₂ N ⁻ -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.	1.3	35
39	Ce ³⁺ and La ³⁺ ions in ethylammonium nitrate: A XANES and molecular dynamics investigation. <i>Chemical Physics Letters</i> , 2018, 706, 311-316.	1.2	8
40	Development of Lennard-Jones and Buckingham Potentials for Lanthanoid Ions in Water. <i>Inorganic Chemistry</i> , 2017, 56, 6214-6224.	1.9	57
41	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.	2.1	11
42	How Does Ce ^{III} Nitrate Dissolve in a Protic Ionic Liquid? A Combined Molecular Dynamics and EXAFS Study. <i>Chemistry - A European Journal</i> , 2017, 23, 8424-8433.	1.7	19
43	Structure of Water in Zn ²⁺ 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.	1.9	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. <i>Journal of Chemical Physics</i> , 2017, 147, 161707.	1.2	30
45	Hydrated and Solvated Tin(II) Ions in Solution and the Solid State, and a Coordination Chemistry Overview of the d ¹⁰ s ² Metal Ions. <i>Chemistry - A European Journal</i> , 2016, 22, 18583-18592.	1.7	17
46	Lutetium(III) aqua ion: On the dynamical structure of the heaviest lanthanoid hydration complex. <i>Journal of Chemical Physics</i> , 2016, 144, 204505.	1.2	15
47	XANES Reveals the Flexible Nature of Hydrated Strontium in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2016, 120, 4114-4124.	1.2	57
48	Structural properties of geminal dicationic ionic liquid/water mixtures: a theoretical and experimental insight. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16544-16554.	1.3	48
49	Unraveling the Sc ³⁺ Hydration Geometry: The Strange Case of the Far-Coordinated Water Molecule. <i>Inorganic Chemistry</i> , 2016, 55, 6703-6711.	1.9	30
50	The non-octarepeat copper binding site of the prion protein is a key regulator of prion conversion. <i>Scientific Reports</i> , 2015, 5, 15253.	1.6	39
51	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.	1.2	5
52	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, 16443-16453.	1.3	39
53	Hidden Hydration Structure of Halide Ions: an Insight into the Importance of Lone Pairs. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15729-15737.	1.2	25
54	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, 4061-4067.	1.2	45

#	ARTICLE	IF	CITATIONS
55	Structural Properties and Aggregation Behavior of 1-Hexyl-3-methylimidazolium Iodide in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14515-14526.	1.2	35
56	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, 2464-2474.	1.3	32
57	The Prion Switch Unravelling. <i>FASEB Journal</i> , 2015, 29, 564.13.	0.2	0
58	Structural Characterization of Ionic Liquids by X-Ray Absorption Spectroscopy. <i>Soft and Biological Matter</i> , 2014, , 149-172.	0.3	0
59	Unraveling halide hydration: A high dilution approach. <i>Journal of Chemical Physics</i> , 2014, 141, 044509.	1.2	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. <i>Inorganic Chemistry</i> , 2014, 53, 9778-9784.	1.9	11
61	Distal proximal crosstalk in the heme binding pocket of the NO sensor DNR. <i>BioMetals</i> , 2014, 27, 763-773.	1.8	13
62	On the possibility of using XANES to investigate bromide-based ionic liquids. <i>Chemical Physics Letters</i> , 2014, 591, 32-36.	1.2	12
63	Theoretical Description of Ionic Liquids. <i>Soft and Biological Matter</i> , 2014, , 127-148.	0.3	2
64	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.	1.3	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. <i>Journal of Physical Chemistry B</i> , 2013, 117, 12516-12524.	1.2	50
66	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.	1.7	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. <i>Journal of Physical Chemistry B</i> , 2013, 117, 12505-12515.	1.2	53
68	Hydration Properties and Ionic Radii of Actinide(III) Ions in Aqueous Solution. <i>Inorganic Chemistry</i> , 2013, 52, 10318-10324.	1.9	80
69	Hydration Properties of the Zn ²⁺ Ion in Water at High Pressure. <i>Inorganic Chemistry</i> , 2013, 52, 1141-1150.	1.9	41
70	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, 7806-7818.	1.2	45
71	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, 269-279.	2.0	4
72	X-ray Absorption Study of the Solvation Structure of Cu ²⁺ in Methanol and Dimethyl Sulfoxide. <i>Inorganic Chemistry</i> , 2012, 51, 8827-8833.	1.9	23

#	ARTICLE	IF	CITATIONS
73	Unravelling the Hydration Structure of ThX ₄ (X = Br, Cl) Water Solutions by Molecular Dynamics Simulations and X-ray Absorption Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6465-6475.	1.2	28
74	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, 13024-13032.	1.2	60
75	Crystal Polymorphism of Hexylammonium Chloride and Structural Properties of Its Mixtures with Water. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2104-2113.	1.2	33
76	Effects of the Pathological Q212P Mutation on Human Prion Protein Non-Octarepeat Copper-Binding Site. <i>Biochemistry</i> , 2012, 51, 6068-6079.	1.2	32
77	Unusual Heme Binding Properties of the Dissimilative Nitrate Respiration Regulator, a Bacterial Nitric Oxide Sensor. <i>Antioxidants and Redox Signaling</i> , 2012, 17, 1178-1189.	2.5	21
78	Hydration of Lanthanoids(III) and Actinoids(III): An Experimental/Theoretical Saga. <i>Chemistry - A European Journal</i> , 2012, 18, 11162-11178.	1.7	114
79	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.	1.3	40
80	Thermal and Structural Properties of Ethylammonium Chloride and Its Mixture with Water. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4887-4899.	1.2	34
81	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, 8509-8515.	1.9	41
82	Effect of the Zn ²⁺ and Hg ²⁺ Ions on the Structure of Liquid Water. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4798-4803.	1.1	34
83	Crystal Polymorphism of Propylammonium Chloride and Structural Properties of Its Mixture with Water. <i>Journal of Physical Chemistry B</i> , 2011, 115, 11805-11815.	1.2	15
84	Revised Ionic Radii of Lanthanoid(III) Ions in Aqueous Solution. <i>Inorganic Chemistry</i> , 2011, 50, 4572-4579.	1.9	212
85	Structural Flexibility and Role of Vicinal 2-Thienyl Rings in 2,3-Dicyano-5,6-di(2-thienyl)-1,4-pyrazine, [(CN) ₂ Th ₂ Pyz], Its Palladium(II) Complex [(CN) ₂ Th ₂ Pyz(PdCl ₂) ₂], and the Related Pentametallic Pyrazinoporphyrazines [(PdCl) ₂ Th ₈ TPyzPzM] (M =) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.9	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. <i>Journal of Chemical Physics</i> , 2011, 135, 154509.	1.2	33
87	X-Ray absorption spectroscopy investigation of 1-alkyl-3-methylimidazolium bromide salts. <i>Journal of Chemical Physics</i> , 2011, 135, 074505.	1.2	31
88	Analysis of the Detailed Configuration of Hydrated Lanthanoid(III) Ions in Aqueous Solution and Crystalline Salts by Using K α and L ₃ Edge XANES Spectroscopy. <i>Chemistry - A European Journal</i> , 2010, 16, 684-692.	1.7	73
89	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> , 2010, 371, 24-29.	0.9	56
90	Unusual proximal heme pocket geometry in the deoxygenated <i>Thermobifida fusca</i> : A combined spectroscopic investigation. <i>Biophysical Chemistry</i> , 2010, 147, 1-7.	1.5	5

#	ARTICLE	IF	CITATIONS
91	X-ray absorption spectroscopy study of the solvation structure of zinc(II) in dimethyl sulfoxide solution. <i>Chemical Physics Letters</i> , 2010, 499, 113-116.	1.2	10
92	Polarized X-ray Absorption Near-Edge Structure Spectroscopy of Neuroglobin and Myoglobin Single Crystals. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13223-13231.	1.2	12
93	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, 4224-4231.	1.9	81
94	Cuprizone neurotoxicity, copper deficiency and neurodegeneration. <i>NeuroToxicology</i> , 2010, 31, 509-517.	1.4	59
95	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> , 2010, 498, 43-49.	1.4	3
96	Structural Study of the N,N -Dimethylpropyleneurea Solvated Lanthanoid(III) Ions in Solution and Solid State with an Analysis of the Ionic Radii of Lanthanoid(III) Ions. <i>Inorganic Chemistry</i> , 2010, 49, 4420-4432.	1.9	74
97	Dynamic Investigation of Protein Metal Active Sites: Interplay of XANES and Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2010, 132, 14901-14909.	6.6	18
98	What first principles molecular dynamics can tell us about EXAFS spectroscopy of radioactive heavy metal cations in water. <i>Radiochimica Acta</i> , 2009, 97, 339-346.	0.5	22
99	Structural Investigation of Lanthanoid Coordination: a Combined XANES and Molecular Dynamics Study. <i>Inorganic Chemistry</i> , 2009, 48, 10239-10248.	1.9	51
100	Structure and dynamics of hemeproteins using X-ray Absorption Spectroscopy. <i>Journal of Physics: Conference Series</i> , 2009, 190, 012195.	0.3	1
101	Molecular dynamics to rationalize EXAFS experiments: A dynamical model explaining hydration behaviour across the lanthanoid(III) series. <i>Journal of Physics: Conference Series</i> , 2009, 190, 012056.	0.3	11
102	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> , 2008, 14, 3056-3066.	1.7	248
103	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> , 2008, 14, 3045-3055.	1.7	55
104	Measurement of x-ray multielectron photoexcitations at the $\text{L}_{2,3}$ edges of lanthanoid(III) ions. <i>Physical Review B</i> , 2008, 78, .	1.1	8
105	An X-ray diffraction and X-ray absorption spectroscopy joint study of neuroglobin. <i>Archives of Biochemistry and Biophysics</i> , 2008, 475, 7-13.	1.4	50
106	X-ray Absorption Spectroscopy of Hemes and Hemeproteins in Solution: Multiple Scattering Analysis. <i>Inorganic Chemistry</i> , 2008, 47, 9905-9918.	1.9	52
107	A Coupled Molecular Dynamics and XANES Data Analysis Investigation of Aqueous Cadmium(II). <i>Journal of Physical Chemistry A</i> , 2008, 112, 11833-11841.	1.1	50
108	Structural and Dynamical Properties of the Hg^{2+} Aqua Ion: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4694-4702.	1.2	48

#	ARTICLE	IF	CITATIONS
109	Integrated experimental and theoretical approach for the structural characterization of Hg ²⁺ aqueous solutions. <i>Journal of Chemical Physics</i> , 2008, 128, 084502.	1.2	50
110	Progresses in the MXAN Fitting Procedure. <i>AIP Conference Proceedings</i> , 2007, , .	0.3	10
111	Evidence for Sevenfold Coordination in the First Solvation Shell of Hg(II) Aqua Ion. <i>Journal of the American Chemical Society</i> , 2007, 129, 5430-5436.	6.6	78
112	X-ray Absorption Fine Structure Spectroscopic Studies of Octakis(DMSO)lanthanoid(III) Complexes in Solution and in the Solid Iodides. <i>Inorganic Chemistry</i> , 2007, 46, 7742-7748.	1.9	26
113	Hemeproteins: Recent Advances in Quantitative XANES Analysis. <i>AIP Conference Proceedings</i> , 2007, , .	0.3	2
114	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> , 2007, 360, 1809-1818.	1.2	23
115	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> , 2007, 360, 2744-2750.	1.2	17
116	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> , 2007, 131-132, 105-112.	2.3	9
117	A Coupled Car-Parrinello Molecular Dynamics and EXAFS Data Analysis Investigation of Aqueous Co ²⁺ . <i>Journal of Physical Chemistry A</i> , 2006, 110, 13081-13088.	1.1	46
118	Detection of Second Hydration Shells in Ionic Solutions by XANES: Computed Spectra for Ni ²⁺ in Water Based on Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2006, 128, 1853-1858.	6.6	59
119	The Solution Structure of [Cu(aq)] ²⁺ and Its Implications for Rack-Induced Bonding in Blue Copper Protein Active Sites. <i>Inorganic Chemistry</i> , 2005, 44, 1922-1933.	1.9	134
120	Quantitative analysis of XANES spectra of disordered systems based on molecular dynamics. <i>Journal of Synchrotron Radiation</i> , 2005, 12, 75-79.	1.0	16
121	Computational Evidence for a Variable First Shell Coordination of the Cadmium(II) Ion in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2005, 109, 9186-9193.	1.2	49
122	Experimental Evidence for a Variable First Coordination Shell of the Cadmium(II) Ion in Aqueous, Dimethyl Sulfoxide, and N,N-Dimethylpropyleneurea Solution. <i>Journal of Physical Chemistry B</i> , 2005, 109, 9178-9185.	1.2	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. <i>Biochemistry</i> , 2005, 44, 13144-13150.	1.2	22
124	A Quantitative Structural Investigation of the XANES Spectra of Potassium Ferrocyanide III at the Iron KEdge. <i>Physica Scripta</i> , 2005, , 152.	1.2	1
125	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> , 2004, 126, 15618-15623.	6.6	73
126	Structure of the Hydrated and Dimethyl Sulfoxide Solvated Rubidium Ions in Solution. <i>Inorganic Chemistry</i> , 2004, 43, 3543-3549.	1.9	33

#	ARTICLE	IF	CITATIONS
127	Effect of Multielectronic Configurations on the XAFS Analysis at the Fe K Edge. Journal of Physical Chemistry A, 2004, 108, 4505-4514.	1.1	49
128	Double-Electron Excitation Channels at the Ca ²⁺ K-Edge of Hydrated Calcium Ion. Journal of Physical Chemistry B, 2004, 108, 11857-11865.	1.2	28
129	Unusual Heme Iron-Lipid Acyl Chain Coordination in Escherichia coli Flavohemoglobin. Biophysical Journal, 2004, 86, 3882-3892.	0.2	40
130	Ion Hydration under Pressure. Physical Review Letters, 2003, 91, 165505.	2.9	31
131	The MXAN procedure: a new method of modeling the XANES spectra to obtain structural quantitative information. AIP Conference Proceedings, 2003, , .	0.3	4
132	Hydrogen and Higher Shell Contributions in Zn ²⁺ , Ni ²⁺ , and Co ²⁺ +Aqueous Solutions: An X-ray Absorption Fine Structure and Molecular Dynamics Study. Journal of the American Chemical Society, 2002, 124, 1958-1967.	6.6	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 Zn ²⁺ , Ni ²⁺ , and Co ²⁺ in Aqueous Solutions. Journal of the American Chemical Society, 2002, 124, 1968-1976.	6.6	92
134	Combined XANES and EXAFS analysis of Co ²⁺ , Ni ²⁺ , and Zn ²⁺ aqueous solutions. Physical Review B, 2002, 66, .	1.1	88
135	Evidence of distorted fivefold coordination of the Cu ²⁺ aqua ion from an x-ray-absorption spectroscopy quantitative analysis. Physical Review B, 2002, 65, .	1.1	131
136	EXAFS and molecular dynamics studies of ionic solutions. Journal of Synchrotron Radiation, 2001, 8, 173-177.	1.0	10
137	K- and L-edge XAFS determination of the local structure of aqueous Nd(III) and Eu(III). Journal of Synchrotron Radiation, 2001, 8, 666-668.	1.0	17
138	Complete spectrum of multielectron excitations at the Br K edge x-ray absorption spectra. Physical Review B, 2001, 64, .	1.1	10
139	Fourier transform infrared and dielectric study of water in C12E4 liquid crystals. Journal of Chemical Physics, 2000, 113, 8783-8790.	1.2	5
140	Evidence of three-body correlation functions in Rb ⁺ and Sr ²⁺ acetonitrile solutions. Journal of Chemical Physics, 1999, 111, 5107-5115.	1.2	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 Sr ²⁺ in methanol solution. Journal of Chemical Physics, 1998, 108, 9487-9497.	1.2	45
142	Evidence for multielectron resonances at the Sr K edge. Physical Review A, 1996, 53, 798-805.	1.0	57
143	Multielectron excitations at the L edges of barium in aqueous solution. Physical Review B, 1996, 54, 12129-12138.	1.1	48
144	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.	1.2	48

#	ARTICLE	IF	CITATIONS
145	Triplet correlations in the hydration shell of aquaions. <i>Chemical Physics Letters</i> , 1994, 225, 150-155.	1.2	59
146	An extended x-ray absorption fine structure study of aqueous solutions by employing molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1994, 100, 985-994.	1.2	133
147	Double-electron excitation channels at the BrKedge of HBr and Br ₂ . <i>Physical Review A</i> , 1993, 47, 2055-2063.	1.0	101