Philippe Guilbaud

List of Publications by Year
in descending order

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73	2,110	218381	253896
papers	citations	26 h-index	43 g-index

77	77	77	1767
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Actinide speciation inÂrelation toÂbiological processes. Biochimie, 2006, 88, 1605-1618.	1.3	175
2	Hydration of uranyl (UO22+) cation and its nitrate ion and 18-crown-6 adducts studied by molecular dynamics simulations. The Journal of Physical Chemistry, 1993, 97, 5685-5692.	2.9	135
3	Force field representation of the UO22+ cation from free energy MD simulations in water. Tests on its 18-crown-6 and NO3â˜ adducts, and on its calix[6]arene6â˜ and CMPO complexes. Computational and Theoretical Chemistry, 1996, 366, 55-63.	1.5	128
4	Complexationâ€Induced Supramolecular Assembly Drives Metalâ€Ion Extraction. Chemistry - A European Journal, 2014, 20, 12796-12807.	1.7	86
5	Molecular dynamics study of p-tert-butylcalix[4]arenetetraamide and its complexes with neutral and cationic guests. Influence of solvation on structures and stabilities. Journal of the American Chemical Society, 1993, 115, 8298-8312.	6.6	82
6	Molecular Dynamics Studies of Concentrated Binary Aqueous Solutions of Lanthanide Salts: Structures and Exchange Dynamics. Inorganic Chemistry, 2010, 49, 519-530.	1.9	66
7	An overview of solvent extraction processes developed in Europe for advanced nuclear fuel recycling, part 1 â€" heterogeneous recycling. Separation Science and Technology, 2021, 56, 1866-1881.	1.3	55
8	Complexation of Lanthanides(III), Americium(III), and Uranium(VI) with Bitopic N,O Ligands: an Experimental and Theoretical Study. Inorganic Chemistry, 2011, 50, 6557-6566.	1.9	52
9	Elucidation of the Structure of Organic Solutions in Solvent Extraction by Combining Molecular Dynamics and Xâ€ray Scattering. Angewandte Chemie - International Edition, 2014, 53, 5346-5350.	7.2	52
10	Coordination of Tetravalent Actinides (An=Th^{IV}, U^{IV}, Np^{IV},) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 6864-6875.	1.7	52
11	Structural insights into proteinâ€"uranyl interaction: towards anÂinÂsilico detection method. Biochimie, 2006, 88, 1631-1638.	1.3	50
12	Interaction of trivalent lanthanide cations with nitrate anions: a quantum chemical investigation of monodentate/bidentate binding modes. New Journal of Chemistry, 2001, 25, 1458-1465.	1.4	44
13	New insights into the extraction of uranium(VI) by an N,N-dialkylamide. Molecular Physics, 2014, 112, 1362-1374.	0.8	44
14	Dimerization of Xanthene Dyes in Water: Experimental Studies and Molecular Dynamic Simulations. Journal of Physical Chemistry B, 2003, 107, 13803-13812.	1.2	43
15	Depletion of water-in-oil aggregates from poor solvents: Transition from weak aggregates towards reverse micelles. Current Opinion in Colloid and Interface Science, 2015, 20, 71-77.	3.4	41
16	Combining theoretical chemistry and XANES multi-edge experiments to probe actinide valence states. Comptes Rendus Chimie, 2007, 10, 859-871.	0.2	37
17	Understanding the nitrate coordination to Eu3+ ions in solution by potential of mean force calculations. Physical Chemistry Chemical Physics, 2011, 13, 5840.	1.3	37
18	Synergism in a HDEHP/TOPO Liquidâ€"Liquid Extraction System: An Intrinsic Ligands Property?. Journal of Physical Chemistry B, 2016, 120, 2814-2823.	1.2	37

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19	Experimental and Molecular Dynamics Studies of Dysprosium(III) Salt Solutions for a Better Representation of the Microscopic Features Used within the Binding Mean Spherical Approximation Theory. Journal of Physical Chemistry A, 2006, 110, 11770-11779.	1.1	35
20	Solvation of UCl₆^{2â^'} Anionic Complex by MeBu₃N⁺, BuMe₂Im⁺, and BuMeIm⁺ Cations. Inorganic Chemistry, 2008, 47, 5746-5755.	1.9	34
21	Complexation of Actinide(III) and Lanthanide(III) with H₄TPAEN for a Separation of Americium from Curium and Lanthanides. Inorganic Chemistry, 2017, 56, 7861-7869.	1.9	34
22	Selective complexation of UO 2 2+ by the calix[6]arene6? anion: Structure and hydration studied by molecular dynamics simulations. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 1993, 16, 169-188.	1.6	33
23	Soluteâ€Induced Microstructural Transition from Weak Aggregates towards a Curved Film of Surfaceâ€Active Extractants. ChemPhysChem, 2012, 13, 687-691.	1.0	31
24	An overview of solvent extraction processes developed in Europe for advanced nuclear fuel recycling, Part 2 â€" homogeneous recycling. Separation Science and Technology, 2022, 57, 1724-1744.	1.3	30
25	Complexation of Ln(III) and Am(III) with the Hydrosoluble TEDGA: Speciation and Thermodynamics Studies. Procedia Chemistry, 2012, 7, 20-26.	0.7	29
26	Thermodynamics of Calcium binding to the Calmodulin N-terminal domain to evaluate site-specific affinity constants and cooperativity. Journal of Biological Inorganic Chemistry, 2015, 20, 905-919.	1.1	29
27	UO₂²⁺structure in solvent extraction phases resolved at molecular and supramolecular scales: a combined molecular dynamics, EXAFS and SWAXS approach. Physical Chemistry Chemical Physics, 2019, 21, 7894-7906.	1.3	28
28	Theoretical chemical contribution to the simulation of the LIII X-ray absorption edges of uranyl, neptunyl and osmyl hydrates and hydroxides. New Journal of Chemistry, 2004, 28, 929.	1.4	27
29	Lanthanide and alkaline-earth complexes of EDTA in water: a molecular dynamics study of structures and binding selectivitiesâ€Šâ€. Perkin Transactions II RSC, 2000, , 705-714.	1.1	26
30	First Evidence of a Water-Soluble Plutonium(IV) Hexanuclear Cluster. European Journal of Inorganic Chemistry, 2016, 2016, 3536-3540.	1.0	26
31	Aggregation in organic phases after solvent extraction of uranyl nitrate: X-ray scattering and molecular dynamic simulations. Journal of Molecular Liquids, 2019, 277, 22-35.	2.3	26
32	Stability of reverse micelles in rare-earth separation: a chemical model based on a molecular approach. Physical Chemistry Chemical Physics, 2017, 19, 7094-7100.	1.3	24
33	Behaviour of the extractant Me-TODGA upon gamma irradiation: quantification of degradation compounds and individual influences on complexation and extraction. New Journal of Chemistry, 2017, 41, 13700-13711.	1.4	24
34	Radiation chemistry of the branched-chain monoamide di-2-ethylhexyl-isobutyramide. Solvent Extraction and Ion Exchange, 2017, 35, 480-495.	0.8	23
35	The role of curvature effects in liquidâ€"liquid extraction: assessing organic phase mesoscopic properties from MD simulations. Soft Matter, 2017, 13, 5518-5526.	1.2	22
36	Radiolytic stability of N,N-dialkyl amide: effect on Pu(iv) complexes in solution. Dalton Transactions, 2018, 47, 251-263.	1.6	22

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37	How Phase Modifiers Disrupt Third-phase Formation in Solvent Extraction Solutions. Solvent Extraction and Ion Exchange, 2021, 39, 204-232.	0.8	22
38	Molecular dynamics simulations for the complexation of Ln3+ and UO22+ ions with tridentate ligand diglycolamide (DGA)Electronic supplementary information (ESI) available: Figures S1â€“S5Eu3+â€“O distances and interaction energy between Eu3+ and TMDGA as a function of time in different media.See http://www.rsc.org/suppdata/cp/b2/b205127n/. Physical Chemistry Chemical Physics, 2003, 5, 691-695.	1.3	21
39	Insight of the Metalâ€“Ligand Interaction in fâ€Element Complexes by Paramagnetic NMR Spectroscopy. Chemistry - A European Journal, 2019, 25, 4435-4451.	1.7	21
40	Probing the existence of uranyl trisulfate structures in the AMEX solvent extraction process. Chemical Communications, 2019, 55, 7583-7586.	2.2	20
41	Multi-scale modelling of uranyl chloride solutions. Journal of Chemical Physics, 2015, 142, 024501.	1.2	19
42	Perrhenate and pertechnetate complexation by an azacryptand in nitric acid medium. Dalton Transactions, 2020, 49, 1446-1455.	1.6	19
43	High-throughput computational screening of nanoporous materials in targeted applications. , 2022, 1, 355-374.		19
44	Determination of the Structures of Uranylâ€“Triâ€nâ€butylâ€Phosphate Aggregates by Coupling Experimental Results with Molecular Dynamic Simulations. Chemistry - A European Journal, 2017, 23, 16660-16670.	1.7	18
45	Structural Analysis of Uranyl Complexation by the EFâ€Hand Motif of Calmodulin: Effect of Phosphorylation. Chemistry - A European Journal, 2017, 23, 15505-15517.	1.7	18
46	The SACSESS Hydrometallurgy Domain â€" An Overview. Procedia Chemistry, 2016, 21, 218-222.	0.7	17
47	Effect of chemical environment on the radiation chemistry of N,N-di-(2-ethylhexyl)butyramide (DEHBA) and plutonium retention. Dalton Transactions, 2019, 48, 14450-14460.	1.6	16
48	Effect of metal complexation on diglycolamide radiolysis: a comparison between ex situ gamma and in situ alpha irradiation. Physical Chemistry Chemical Physics, 2022, 24, 9213-9228.	1.3	16
49	Atomistic Description of Binary Lanthanoid Salt Solutions: A Coarse-Graining Approach. Journal of Physical Chemistry B, 2011, 115, 4329-4340.	1.2	14
50	An experimental and computational look at the radiolytic degradation of TODGA and the effect on metal complexation. New Journal of Chemistry, 2021, 45, 12479-12493.	1.4	13
51	Mass spectrometry and theoretical investigation of di-alkylphosphoric acidâ€“lanthanide complexes. Radiochimica Acta, 2008, 96, .	0.5	11
52	Syntheses and evaluation of new hydrophilic azacryptands used as masking agents of technetium in solvent extraction processes. Dalton Transactions, 2021, 50, 1620-1630.	1.6	11
53	Crystal structure versus solution for two new lutetium thiocyanato complexes. New Journal of Chemistry, 2011, 35, 2755.	1.4	10
54	Molecular simulation of binary phase diagrams from the osmotic equilibrium method: vapour pressure and activity in waterâ€“ethanol mixtures. Molecular Physics, 2018, 116, 2009-2021.	0.8	9

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55	Bifunctional Amidophosphonate Molecules for Uranium Extraction in Nitrate Acidic Media. Solvent Extraction and Ion Exchange, 2020, 38, 703-718.	0.8	9
56	Aggregation of Bifunctional Extractants Used for Uranium(VI) Separation. Journal of Physical Chemistry B, 2021, 125, 10759-10771.	1.2	9
57	Thermodynamics of Malonamide Aggregation Deduced from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 3409-3418.	1.2	8
58	DEHBA (di-2-ethylhexylbutyramide) gamma radiolysis under spent nuclear fuel solvent extraction process conditions. Radiation Physics and Chemistry, 2020, 170, 108608.	1.4	7
59	Coarse-grained lanthanoid chloride aqueous solutions. Journal of Molecular Liquids, 2010, 153, 107-111.	2.3	6
60	Specific Interaction between Uranium Anionic Complexes and the Cations of Bis(trifluoromethylsulfonyl)imide Based Ionic Liquids. Inorganic Chemistry, 2013, 52, 11218-11227.	1.9	6
61	Redox behavior of gas phase Pu(IV)-monodentate ligand complexes: an investigation by electrospray ionization mass spectrometry. Journal of Radioanalytical and Nuclear Chemistry, 2016, 310, 441-451.	0.7	6
62	Activity Coefficients of Aqueous Sodium, Calcium, and Europium Nitrate Solutions from Osmotic Equilibrium MD Simulations. Journal of Physical Chemistry B, 2018, 122, 7726-7736.	1.2	6
63	Evidence of Supramolecular Origin of Selectivity in Solvent Extraction of Bifunctional Amidophosphonate Extractants with Different Configurations. Solvent Extraction and Ion Exchange, 0, , 1-23.	0.8	6
64	Complexation-Induced Supramolecular Assembly Drives Metal-Ion Extraction. Chemistry - A European Journal, 2014, 20, 12685-12685.	1.7	5
65	Simulating Osmotic Equilibria: A New Tool for Calculating Activity Coefficients in Concentrated Aqueous Salt Solutions. Journal of Physical Chemistry B, 2017, 121, 9647-9658.	1.2	5
66	Liquid/liquid interface in periodic boundary condition. Physical Chemistry Chemical Physics, 2021, 23, 1178-1187.	1.3	4
67	Modeling Selectivity in Liquid/Liquid Extraction. Nuclear Science and Engineering, 2006, 153, 207-222.	0.5	3
68	Role of the Hydroxo Group in the Coordination of Citric Acid to Trivalent Americium. European Journal of Inorganic Chemistry, 2020, 2020, 1331-1344.	1.0	3
69	Force Field Parameterization of Actinyl Molecular Cations Using the 12-6-4 Model. Journal of Chemical Information and Modeling, 2022, 62, 2432-2445.	2.5	3
70	2,2â€™-bipyridine as a masking agent of ruthenium in the PUREX process. Separation Science and Technology, 2021, 56, 1649-1658.	1.3	2
71	Molecular Characterization of Actinide Oxocations from Protactinium to Plutonium. AIP Conference Proceedings, 2007, , .	0.3	1
72	Self-assembly of a bio-based extractant in methyl esters: combination of small angle X-ray scattering experiments and molecular dynamics simulations. Green Chemistry, 2017, 19, 4680-4689.	4.6	1

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73	Investigating Actinide Molecular Adducts from Absorption Edge Spectroscopy. Physica Scripta, 2005, , 891.	1.2	0