

Philippe Guilbaud

List of Publications by Year in descending order

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218381

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43
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77
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77
docs citations

77
times ranked

1767
citing authors

#	ARTICLE	IF	CITATIONS
1	An overview of solvent extraction processes developed in Europe for advanced nuclear fuel recycling, Part 2 " homogeneous recycling. Separation Science and Technology, 2022, 57, 1724-1744.	1.3	30
2	Effect of metal complexation on diglycolamide radiolysis: a comparison between <i>ex situ</i> gamma and <i>in situ</i> alpha irradiation. Physical Chemistry Chemical Physics, 2022, 24, 9213-9228.	1.3	16
3	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
4	High-throughput computational screening of nanoporous materials in targeted applications. , 2022, 1, 355-374.		19
5	An overview of solvent extraction processes developed in Europe for advanced nuclear fuel recycling, part 1 " heterogeneous recycling. Separation Science and Technology, 2021, 56, 1866-1881.	1.3	55
6	Liquid/liquid interface in periodic boundary condition. Physical Chemistry Chemical Physics, 2021, 23, 1178-1187.	1.3	4
7	2,2'-bipyridine as a masking agent of ruthenium in the PUREX process. Separation Science and Technology, 2021, 56, 1649-1658.	1.3	2
8	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
9	How Phase Modifiers Disrupt Third-phase Formation in Solvent Extraction Solutions. Solvent Extraction and Ion Exchange, 2021, 39, 204-232.	0.8	22
10	Thermodynamics of Malonamide Aggregation Deduced from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 3409-3418.	1.2	8
11	Aggregation of Bifunctional Extractants Used for Uranium(VI) Separation. Journal of Physical Chemistry B, 2021, 125, 10759-10771.	1.2	9
12	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
13	Perrhenate and pertechnetate complexation by an azacryptand in nitric acid medium. Dalton Transactions, 2020, 49, 1446-1455.	1.6	19
14	DEHBA (di-2-ethylhexylbutyramide) gamma radiolysis under spent nuclear fuel solvent extraction process conditions. Radiation Physics and Chemistry, 2020, 170, 108608.	1.4	7
15	Bifunctional Amidophosphonate Molecules for Uranium Extraction in Nitrate Acidic Media. Solvent Extraction and Ion Exchange, 2020, 38, 703-718.	0.8	9
16	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
17	Effect of chemical environment on the radiation chemistry of <i>N,N</i> -di-(2-ethylhexyl)butyramide (DEHBA) and plutonium retention. Dalton Transactions, 2019, 48, 14450-14460.	1.6	16
18	Probing the existence of uranyl trisulfate structures in the AMEX solvent extraction process. Chemical Communications, 2019, 55, 7583-7586.	2.2	20

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19	UO ₂ ²⁺ structure in solvent extraction phases resolved at molecular and supramolecular scales: a combined molecular dynamics, EXAFS and SWAXS approach. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7894-7906.	1.3	28
20	Insight of the Metal-Ligand Interaction in f-Element Complexes by Paramagnetic NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2019, 25, 4435-4451.	1.7	21
21	Aggregation in organic phases after solvent extraction of uranyl nitrate: X-ray scattering and molecular dynamic simulations. <i>Journal of Molecular Liquids</i> , 2019, 277, 22-35.	2.3	26
22	Molecular simulation of binary phase diagrams from the osmotic equilibrium method: vapour pressure and activity in water-ethanol mixtures. <i>Molecular Physics</i> , 2018, 116, 2009-2021.	0.8	9
23	Radiolytic stability of N,N-dialkyl amide: effect on Pu(IV) complexes in solution. <i>Dalton Transactions</i> , 2018, 47, 251-263.	1.6	22
24	Activity Coefficients of Aqueous Sodium, Calcium, and Europium Nitrate Solutions from Osmotic Equilibrium MD Simulations. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7726-7736.	1.2	6
25	Coordination of Tetravalent Actinides (An=Th ^{IV} , U ^{IV} , Np ^{IV} ,) Tj ETQq1 1 0.784314 rgBT /Overlock 6864-6875.	1.7	52
26	Stability of reverse micelles in rare-earth separation: a chemical model based on a molecular approach. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7094-7100.	1.3	24
27	Determination of the Structures of Uranyl-Tributylphosphate Aggregates by Coupling Experimental Results with Molecular Dynamic Simulations. <i>Chemistry - A European Journal</i> , 2017, 23, 16660-16670.	1.7	18
28	Behaviour of the extractant Me-TODGA upon gamma irradiation: quantification of degradation compounds and individual influences on complexation and extraction. <i>New Journal of Chemistry</i> , 2017, 41, 13700-13711.	1.4	24
29	Self-assembly of a bio-based extractant in methyl esters: combination of small angle X-ray scattering experiments and molecular dynamics simulations. <i>Green Chemistry</i> , 2017, 19, 4680-4689.	4.6	1
30	Radiation chemistry of the branched-chain monoamide di-2-ethylhexyl-isobutyramide. <i>Solvent Extraction and Ion Exchange</i> , 2017, 35, 480-495.	0.8	23
31	Simulating Osmotic Equilibria: A New Tool for Calculating Activity Coefficients in Concentrated Aqueous Salt Solutions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9647-9658.	1.2	5
32	Structural Analysis of Uranyl Complexation by the EF-Hand Motif of Calmodulin: Effect of Phosphorylation. <i>Chemistry - A European Journal</i> , 2017, 23, 15505-15517.	1.7	18
33	The role of curvature effects in liquid-liquid extraction: assessing organic phase mesoscopic properties from MD simulations. <i>Soft Matter</i> , 2017, 13, 5518-5526.	1.2	22
34	Complexation of Actinide(III) and Lanthanide(III) with H ₄ TPAEN for a Separation of Americium from Curium and Lanthanides. <i>Inorganic Chemistry</i> , 2017, 56, 7861-7869.	1.9	34
35	The SACSESS Hydrometallurgy Domain - An Overview. <i>Procedia Chemistry</i> , 2016, 21, 218-222.	0.7	17
36	First Evidence of a Water-Soluble Plutonium(IV) Hexanuclear Cluster. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 3536-3540.	1.0	26

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37	Redox behavior of gas phase Pu(IV)-monodentate ligand complexes: an investigation by electrospray ionization mass spectrometry. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2016, 310, 441-451.	0.7	6
38	Synergism in a HDEHP/TOPO Liquid-Liquid Extraction System: An Intrinsic Ligands Property?. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2814-2823.	1.2	37
39	Depletion of water-in-oil aggregates from poor solvents: Transition from weak aggregates towards reverse micelles. <i>Current Opinion in Colloid and Interface Science</i> , 2015, 20, 71-77.	3.4	41
40	Multi-scale modelling of uranyl chloride solutions. <i>Journal of Chemical Physics</i> , 2015, 142, 024501.	1.2	19
41	Thermodynamics of Calcium binding to the Calmodulin N-terminal domain to evaluate site-specific affinity constants and cooperativity. <i>Journal of Biological Inorganic Chemistry</i> , 2015, 20, 905-919.	1.1	29
42	Complexation-Induced Supramolecular Assembly Drives Metal-Ion Extraction. <i>Chemistry - A European Journal</i> , 2014, 20, 12685-12685.	1.7	5
43	Complexation-Induced Supramolecular Assembly Drives Metal-Ion Extraction. <i>Chemistry - A European Journal</i> , 2014, 20, 12796-12807.	1.7	86
44	Elucidation of the Structure of Organic Solutions in Solvent Extraction by Combining Molecular Dynamics and X-ray Scattering. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 5346-5350.	7.2	52
45	New insights into the extraction of uranium(VI) by an N,N-dialkylamide. <i>Molecular Physics</i> , 2014, 112, 1362-1374.	0.8	44
46	Specific Interaction between Uranium Anionic Complexes and the Cations of Bis(trifluoromethylsulfonyl)imide Based Ionic Liquids. <i>Inorganic Chemistry</i> , 2013, 52, 11218-11227.	1.9	6
47	Complexation of Ln(III) and Am(III) with the Hydrosoluble TEDGA: Speciation and Thermodynamics Studies. <i>Procedia Chemistry</i> , 2012, 7, 20-26.	0.7	29
48	Solute-Induced Microstructural Transition from Weak Aggregates towards a Curved Film of Surface-Active Extractants. <i>ChemPhysChem</i> , 2012, 13, 687-691.	1.0	31
49	Crystal structure versus solution for two new lutetium thiocyanato complexes. <i>New Journal of Chemistry</i> , 2011, 35, 2755.	1.4	10
50	Understanding the nitrate coordination to Eu ³⁺ ions in solution by potential of mean force calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5840.	1.3	37
51	Atomistic Description of Binary Lanthanoid Salt Solutions: A Coarse-Graining Approach. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4329-4340.	1.2	14
52	Complexation of Lanthanides(III), Americium(III), and Uranium(VI) with Bitopic N,O Ligands: an Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2011, 50, 6557-6566.	1.9	52
53	Coarse-grained lanthanoid chloride aqueous solutions. <i>Journal of Molecular Liquids</i> , 2010, 153, 107-111.	2.3	6
54	Molecular Dynamics Studies of Concentrated Binary Aqueous Solutions of Lanthanide Salts: Structures and Exchange Dynamics. <i>Inorganic Chemistry</i> , 2010, 49, 519-530.	1.9	66

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55	Solvation of UCl_6^{2+} Anionic Complex by $MeBu_3N^+$, $BuMe_2Im^+$, and $BuMelm^+$ Cations. <i>Inorganic Chemistry</i> , 2008, 47, 5746-5755.	1.9	34
56	Mass spectrometry and theoretical investigation of di-alkylphosphoric acid-lanthanide complexes. <i>Radiochimica Acta</i> , 2008, 96, .	0.5	11
57	Molecular Characterization of Actinide Oxocations from Protactinium to Plutonium. <i>AIP Conference Proceedings</i> , 2007, , .	0.3	1
58	Combining theoretical chemistry and XANES multi-edge experiments to probe actinide valence states. <i>Comptes Rendus Chimie</i> , 2007, 10, 859-871.	0.2	37
59	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. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11770-11779.	1.1	35
60	Structural insights into protein-uranyl interaction: towards an in situ detection method. <i>Biochimie</i> , 2006, 88, 1631-1638.	1.3	50
61	Actinide speciation in relation to biological processes. <i>Biochimie</i> , 2006, 88, 1605-1618.	1.3	175
62	Modeling Selectivity in Liquid/Liquid Extraction. <i>Nuclear Science and Engineering</i> , 2006, 153, 207-222.	0.5	3
63	Investigating Actinide Molecular Adducts from Absorption Edge Spectroscopy. <i>Physica Scripta</i> , 2005, , 891.	1.2	0
64	Theoretical chemical contribution to the simulation of the LIII X-ray absorption edges of uranyl, neptunyl and osmyl hydrates and hydroxides. <i>New Journal of Chemistry</i> , 2004, 28, 929.	1.4	27
65	Molecular dynamics simulations for the complexation of Ln^{3+} and UO_2^{2+} ions with tridentate ligand diglycolamide (DGA) Electronic supplementary information (ESI) available: Figures S1-S5 Eu^{3+} -O distances and interaction energy between Eu^{3+} and TMDGA as a function of time in different media. See http://www.rsc.org/suppdata/cp/b2/b205127n/ . <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 691-695.	1.3	21
66	Dimerization of Xanthene Dyes in Water: Experimental Studies and Molecular Dynamic Simulations. <i>Journal of Physical Chemistry B</i> , 2003, 107, 13803-13812.	1.2	43
67	Interaction of trivalent lanthanide cations with nitrate anions: a quantum chemical investigation of monodentate/bidentate binding modes. <i>New Journal of Chemistry</i> , 2001, 25, 1458-1465.	1.4	44
68	Lanthanide and alkaline-earth complexes of EDTA in water: a molecular dynamics study of structures and binding selectivities. <i>Perkin Transactions II RSC</i> , 2000, , 705-714.	1.1	26
69	Force field representation of the UO_2^{2+} cation from free energy MD simulations in water. Tests on its 18-crown-6 and NO_3^- adducts, and on its calix[6]arene 6^- and CMPO complexes. <i>Computational and Theoretical Chemistry</i> , 1996, 366, 55-63.	1.5	128
70	Selective complexation of UO_2^{2+} by the calix[6]arene 6^- anion: Structure and hydration studied by molecular dynamics simulations. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 1993, 16, 169-188.	1.6	33
71	Molecular dynamics study of p-tert-butylcalix[4]arene tetraamide and its complexes with neutral and cationic guests. Influence of solvation on structures and stabilities. <i>Journal of the American Chemical Society</i> , 1993, 115, 8298-8312.	6.6	82
72	Hydration of uranyl (UO_2^{2+}) cation and its nitrate ion and 18-crown-6 adducts studied by molecular dynamics simulations. <i>The Journal of Physical Chemistry</i> , 1993, 97, 5685-5692.	2.9	135

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73	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