Philippe Guilbaud

List of Publications by Year
in descending order

73	2,110	218662	254170
papers	citations	26 h-index	43 g-index

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

#	Article	IF	Citations
1	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.	2.5	30
2	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.	2.8	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.	5.4	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 â€" heterogeneous recycling. Separation Science and Technology, 2021, 56, 1866-1881.	2.5	55
6	Liquid/liquid interface in periodic boundary condition. Physical Chemistry Chemical Physics, 2021, 23, 1178-1187.	2.8	4
7	2,2â€™-bipyridine as a masking agent of ruthenium in the PUREX process. Separation Science and Technology, 2021, 56, 1649-1658.	2.5	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.	2.8	13
9	How Phase Modifiers Disrupt Third-phase Formation in Solvent Extraction Solutions. Solvent Extraction and Ion Exchange, 2021, 39, 204-232.	2.0	22
10	Thermodynamics of Malonamide Aggregation Deduced from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 3409-3418.	2.6	8
11	Aggregation of Bifunctional Extractants Used for Uranium(VI) Separation. Journal of Physical Chemistry B, 2021, 125, 10759-10771.	2.6	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.	3.3	11
13	Perrhenate and pertechnetate complexation by an azacryptand in nitric acid medium. Dalton Transactions, 2020, 49, 1446-1455.	3.3	19
14	DEHBA (di-2-ethylhexylbutyramide) gamma radiolysis under spent nuclear fuel solvent extraction process conditions. Radiation Physics and Chemistry, 2020, 170, 108608.	2.8	7
15	Bifunctional Amidophosphonate Molecules for Uranium Extraction in Nitrate Acidic Media. Solvent Extraction and Ion Exchange, 2020, 38, 703-718.	2.0	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.	2.0	3
17	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.	3.3	16
18	Probing the existence of uranyl trisulfate structures in the AMEX solvent extraction process. Chemical Communications, 2019, 55, 7583-7586.	4.1	20

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19	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.	2.8	28
20	Insight of the Metalâ€“Ligand Interaction in fâ€Element Complexes by Paramagnetic NMR Spectroscopy. Chemistry - A European Journal, 2019, 25, 4435-4451.	3.3	21
21	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.	4.9	26
22	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.	1.7	9
23	Radiolytic stability of N,N-dialkyl amide: effect on Pu(iv) complexes in solution. Dalton Transactions, 2018, 47, 251-263.	3.3	22
24	Activity Coefficients of Aqueous Sodium, Calcium, and Europium Nitrate Solutions from Osmotic Equilibrium MD Simulations. Journal of Physical Chemistry B, 2018, 122, 7726-7736.	2.6	6
25	Coordination of Tetravalent Actinides (An=Th^{IV}, U^{IV}, Np^{IV},) Tj ETQq1 1 0.784314 rgBT /Overlock 6864-6875.	3.3	52
26	Stability of reverse micelles in rare-earth separation: a chemical model based on a molecular approach. Physical Chemistry Chemical Physics, 2017, 19, 7094-7100.	2.8	24
27	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.	3.3	18
28	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.	2.8	24
29	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.	9.0	1
30	Radiation chemistry of the branched-chain monoamide di-2-ethylhexyl-isobutyramide. Solvent Extraction and Ion Exchange, 2017, 35, 480-495.	2.0	23
31	Simulating Osmotic Equilibria: A New Tool for Calculating Activity Coefficients in Concentrated Aqueous Salt Solutions. Journal of Physical Chemistry B, 2017, 121, 9647-9658.	2.6	5
32	Structural Analysis of Uranyl Complexation by the EFâ€Hand Motif of Calmodulin: Effect of Phosphorylation. Chemistry - A European Journal, 2017, 23, 15505-15517.	3.3	18
33	The role of curvature effects in liquidâ€“liquid extraction: assessing organic phase mesoscopic properties from MD simulations. Soft Matter, 2017, 13, 5518-5526.	2.7	22
34	Complexation of Actinide(III) and Lanthanide(III) with H₄TPAEN for a Separation of Americium from Curium and Lanthanides. Inorganic Chemistry, 2017, 56, 7861-7869.	4.0	34
35	The SACSESS Hydrometallurgy Domain â€" An Overview. Procedia Chemistry, 2016, 21, 218-222.	0.7	17
36	First Evidence of a Water-Soluble Plutonium(IV) Hexanuclear Cluster. European Journal of Inorganic Chemistry, 2016, 2016, 3536-3540.	2.0	26

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37	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.	1.5	6
38	Synergism in a HDEHP/TOPO Liquidâ€“Liquid Extraction System: An Intrinsic Ligands Property?. Journal of Physical Chemistry B, 2016, 120, 2814-2823.	2.6	37
39	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.	7.4	41
40	Multi-scale modelling of uranyl chloride solutions. Journal of Chemical Physics, 2015, 142, 024501.	3.0	19
41	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.	2.6	29
42	Complexation-Induced Supramolecular Assembly Drives Metal-Ion Extraction. Chemistry - A European Journal, 2014, 20, 12685-12685.	3.3	5
43	Complexationâ€Induced Supramolecular Assembly Drives Metalâ€Ion Extraction. Chemistry - A European Journal, 2014, 20, 12796-12807.	3.3	86
44	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.	13.8	52
45	New insights into the extraction of uranium(VI) by an N,N-dialkylamide. Molecular Physics, 2014, 112, 1362-1374.	1.7	44
46	Specific Interaction between Uranium Anionic Complexes and the Cations of Bis(trifluoromethylsulfonyl)imide Based Ionic Liquids. Inorganic Chemistry, 2013, 52, 11218-11227.	4.0	6
47	Complexation of Ln(III) and Am(III) with the Hydrosoluble TEDGA: Speciation and Thermodynamics Studies. Procedia Chemistry, 2012, 7, 20-26.	0.7	29
48	Soluteâ€Induced Microstructural Transition from Weak Aggregates towards a Curved Film of Surfaceâ€Active Extractants. ChemPhysChem, 2012, 13, 687-691.	2.1	31
49	Crystal structure versus solution for two new lutetium thiocyanato complexes. New Journal of Chemistry, 2011, 35, 2755.	2.8	10
50	Understanding the nitrate coordination to Eu3+ ions in solution by potential of mean force calculations. Physical Chemistry Chemical Physics, 2011, 13, 5840.	2.8	37
51	Atomistic Description of Binary Lanthanoid Salt Solutions: A Coarse-Graining Approach. Journal of Physical Chemistry B, 2011, 115, 4329-4340.	2.6	14
52	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.	4.0	52
53	Coarse-grained lanthanoid chloride aqueous solutions. Journal of Molecular Liquids, 2010, 153, 107-111.	4.9	6
54	Molecular Dynamics Studies of Concentrated Binary Aqueous Solutions of Lanthanide Salts: Structures and Exchange Dynamics. Inorganic Chemistry, 2010, 49, 519-530.	4.0	66

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55	Solvation of UCl₆^{2â”} Anionic Complex by MeBu₃N⁺, BuMe₂Im⁺, and BuMeIm⁺ Cations. Inorganic Chemistry, 2008, 47, 5746-5755.	4.0	34
56	Mass spectrometry and theoretical investigation of di-alkylphosphoric acidâ€“lanthanide complexes. Radiochimica Acta, 2008, 96, .	1.2	11
57	Molecular Characterization of Actinide Oxocations from Protactinium to Plutonium. AIP Conference Proceedings, 2007, , .	0.4	1
58	Combining theoretical chemistry and XANES multi-edge experiments to probe actinide valence states. Comptes Rendus Chimie, 2007, 10, 859-871.	0.5	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. Journal of Physical Chemistry A, 2006, 110, 11770-11779.	2.5	35
60	Structural insights into proteinâ€“uranyl interaction: towards anÂinÂsilico detection method. Biochimie, 2006, 88, 1631-1638.	2.6	50
61	Actinide speciation inÂrelation toÂbiological processes. Biochimie, 2006, 88, 1605-1618.	2.6	175
62	Modeling Selectivity in Liquid/Liquid Extraction. Nuclear Science and Engineering, 2006, 153, 207-222.	1.1	3
63	Investigating Actinide Molecular Adducts from Absorption Edge Spectroscopy. Physica Scripta, 2005, , 891.	2.5	0
64	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.	2.8	27
65	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.	2.8	21
66	Dimerization of Xanthene Dyes in Water: Experimental Studies and Molecular Dynamic Simulations. Journal of Physical Chemistry B, 2003, 107, 13803-13812.	2.6	43
67	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.	2.8	44
68	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
69	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
70	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
71	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.	13.7	82
72	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

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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.	2.0	6