

# Dominique Guillaumont

## List of Publications by Year in descending order

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77  
papers

2,288  
citations

186265

28  
h-index

223800

46  
g-index

80  
all docs

80  
docs citations

80  
times ranked

2192  
citing authors

#	ARTICLE	IF	CITATIONS
1	Calculation of the absorption wavelength of dyes using time-dependent density-functional theory (TD-DFT). <i>Dyes and Pigments</i> , 2000, 46, 85-92.	3.7	236
2	Thermodynamic Study of the Complexation of Trivalent Actinide and Lanthanide Cations by ADPTZ, a Tridentate N-Donor Ligand. <i>Inorganic Chemistry</i> , 2005, 44, 1404-1412.	4.0	119
3	An ab Initio MO Study of the Photochromic Reaction of Dithienylethenes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7222-7227.	2.5	117
4	Theoretical Study on the Photochromic Cycloreversion Reactions of Dithienylethenes; on the Role of the Conical Intersections. <i>Journal of the American Chemical Society</i> , 2004, 126, 12112-12120.	13.7	114
5	Quantum Chemistry Study of Actinide(III) and Lanthanide(III) Complexes with Tridentate Nitrogen Ligands. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6893-6900.	2.5	106
6	Multiphoton Gated Photochromic Reaction in a Diarylethene Derivative. <i>Journal of the American Chemical Society</i> , 2001, 123, 753-754.	13.7	95
7	Solving the Hydration Structure of the Heaviest Actinide Aqua Ion Known: The Californium(III) Case. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 3811-3815.	13.8	64
8	Computational modeling of actinide materials and complexes. <i>MRS Bulletin</i> , 2010, 35, 883-888.	3.5	64
9	Quantum yields and potential energy surfaces: a theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 821-829.	1.9	57
10	Theoretical study of an intermediate, a factor determining the quantum yield in photochromism of diarylethene derivatives. <i>Computational and Theoretical Chemistry</i> , 2002, 579, 115-120.	1.5	55
11	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.	4.0	52
12	Luminescent Eu(III) and Gd(III) Trisbipyridine Cryptates: Experimental and Theoretical Study of the Substituent Effects. <i>ChemPhysChem</i> , 2007, 8, 480-488.	2.1	48
13	Actinide(III) and lanthanide(III) complexes with nitrogen ligands: Counterions and ligand substituent effects on the metal-ligand bond. <i>Computational and Theoretical Chemistry</i> , 2006, 771, 105-110.	1.5	45
14	Structures of Plutonium(IV) and Uranium(VI) with <i>N,N</i> -Dialkyl Amides from Crystallography, X-ray Absorption Spectra, and Theoretical Calculations. <i>Inorganic Chemistry</i> , 2016, 55, 5558-5569.	4.0	43
15	Density Functional Theory Calculations of the Redox Potentials of Actinide(VI)/Actinide(V) Couple in Water. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4500-4505.	2.5	38
16	Photoreactivity of Cr(CO) <sub>4</sub> (2,2'-Bipyridine): Quantum Chemistry and Photodissociation Dynamics. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1107-1114.	2.5	37
17	Combining theoretical chemistry and XANES multi-edge experiments to probe actinide valence states. <i>Comptes Rendus Chimie</i> , 2007, 10, 859-871.	0.5	37
18	Structure of early actinides(V) in acidic solutions. <i>Radiochimica Acta</i> , 2009, 97, 347-353.	1.2	37

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19	Synergism in a HDEHP/TOPO Liquid-Liquid Extraction System: An Intrinsic Ligands Property?. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2814-2823.	2.6	37
20	Photodissociation and Electronic Spectroscopy of Mn(H)(CO) <sub>3</sub> (H-DAB) (DAB = 1,4-Diaza-1,3-butadiene): Quantum Wave Packet Dynamics Based on ab Initio Potentials. <i>Journal of the American Chemical Society</i> , 1999, 121, 11733-11743.	13.7	36
21	Liquid-Liquid Extraction of Acids and Water by a Malonamide: I-Anion Specific Effects on the Polar Core Microstructure of the Aggregated Malonamide. <i>Solvent Extraction and Ion Exchange</i> , 2014, 32, 601-619.	2.0	35
22	Spin-Orbit Coupling Effects on the Metal-Hydrogen Bond Homolysis of M(H)(CO) <sub>3</sub> (H-DAB) (M = Mn, Re;). <i>J. Electroanal. Chem.</i> 2010, 620, 100-107.	2.5	34
23	Investigating the electronic structure and bonding in uranyl compounds by combining NEXAFS spectroscopy and quantum chemistry. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14253.	2.8	34
24	Electronic Structure of the Lowest Excited States of Cr(CO) <sub>4</sub> (2,2'-bipyridine): A CASSCF/CASPT2 Analysis. <i>Inorganic Chemistry</i> , 1997, 36, 1684-1688.	4.0	32
25	New Insights into Formation of Trivalent Actinides Complexes with DTPA. <i>Inorganic Chemistry</i> , 2012, 51, 12638-12649.	4.0	32
26	Americium(III) coordination chemistry: An unexplored diversity of structure and bonding. <i>Comptes Rendus Chimie</i> , 2010, 13, 839-848.	0.5	29
27	Modeling and Speciation Study of Uranium(VI) and Technetium(VII) Coextraction with DEHiBA. <i>Inorganic Chemistry</i> , 2016, 55, 6511-6519.	4.0	29
28	Thermodynamics and Structure of Actinide(IV) Complexes with Nitrilotriacetic Acid. <i>Inorganic Chemistry</i> , 2009, 48, 3943-3953.	4.0	28
29	A quantum chemical investigation of the metal-to-ligand-charge-transfer photochemistry. <i>Coordination Chemistry Reviews</i> , 1998, 177, 181-199.	18.8	27
30	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.	2.8	27
31	Crystal and Electronic Structure of a Mixed-Valent Np(IV)-Np(V) Compound: [BuMeIm] <sub>5</sub> [Np(NpO <sub>2</sub> ) <sub>3</sub> (H <sub>2</sub> O) <sub>6</sub> Cl <sub>12</sub> ]. <i>Inorganic Chemistry</i> , 2010, 49, 2077-2082.	4.0	26
32	First Evidence of a Water-Soluble Plutonium(IV) Hexanuclear Cluster. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 3536-3540.	2.0	26
33	Inner to outer-sphere coordination of plutonium(IV) with N,N-dialkyl amide: influence of nitric acid. <i>Dalton Transactions</i> , 2017, 46, 3812-3815.	3.3	26
34	Understanding the synergistic effect on lanthanides(III) solvent extraction by systems combining a malonamide and a dialkyl phosphoric acid. <i>Hydrometallurgy</i> , 2017, 169, 542-551.	4.3	25
35	Structural Versatility of Uranyl(VI) Nitrate Complexes That Involve the Diamide Ligand Et <sub>2</sub> N(C=O)(CH <sub>2</sub> ) <sub>n</sub> (C=O)NEt <sub>2</sub> (0 ≤ n ≤ 6). <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 3747-3763.	2.0	24
36	Through-Space Exciton Coupling and Multimodal Na <sup>+</sup> /K <sup>+</sup> Sensing Properties of Calix[4]arene-crowns with the Thienylene Analogue of para-Terphenyl as Chromophore. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 2925-2928.	13.8	22

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37	Structural Characterization of Am(III)- and Pu(III)-DOTA Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 12248-12259.	4.0	22
38	Radiolytic stability of N,N-dialkyl amide: effect on Pu(IV) complexes in solution. <i>Dalton Transactions</i> , 2018, 47, 251-263.	3.3	22
39	Metal-to-ligand charge-transfer photochemistry: quantum chemistry and dynamics of the systems $M(CO)_3(DAB)$ ( $M \rightarrow Mn$ ; $R \rightarrow H$ , methyl, ethyl; $M \rightarrow Re$ , $R \rightarrow H$ , $DAB \rightarrow 1,4$ -diaz-1,3-butadiene). <i>Coordination Chemistry Reviews</i> , 1998, 171, 439-459.	1.8	21
40	Insight of the Metal-Ligand Interaction in f-Element Complexes by Paramagnetic NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2019, 25, 4435-4451.	3.3	21
41	Coordination Structures of Uranium(VI) and Plutonium(IV) in Organic Solutions with Amide Derivatives. <i>Inorganic Chemistry</i> , 2020, 59, 1823-1834.	4.0	21
42	The nature of chemical bonding in actinide and lanthanide ferrocyanides determined by X-ray absorption spectroscopy and density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2887-2895.	2.8	19
43	Perrhenate and pertechnetate complexation by an azacryptand in nitric acid medium. <i>Dalton Transactions</i> , 2020, 49, 1446-1455.	3.3	19
44	Investigation of actinide compounds by coupling X-ray absorption spectroscopy and quantum chemistry. <i>Journal of Alloys and Compounds</i> , 2007, 444-445, 443-446.	5.5	18
45	Extraction of Uranium(VI) and Plutonium(IV) with Tetra-Alkylcarbamides. <i>Solvent Extraction and Ion Exchange</i> , 2019, 37, 111-125.	2.0	17
46	Structural and magnetic susceptibility characterization of Pu(IV) aqua ion using sonochemistry as a facile synthesis method. <i>Inorganic Chemistry Frontiers</i> , 2018, 5, 100-111.	6.0	16
47	Effect of metal complexation on diglycolamide radiolysis: a comparison between <i>ex situ</i> gamma and <i>in situ</i> alpha irradiation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 9213-9228.	2.8	16
48	Thermodynamic Study of the Complexation of Protactinium(V) with Diethylenetriaminepentaacetic Acid. <i>Inorganic Chemistry</i> , 2013, 52, 7497-7507.	4.0	15
49	Variation in Charge-Transfer Photochemistry Clarified by a CASSCF/MR-CCI Comparative Study of the Low-Lying Excited States of $M(R)(CO)_3(H-DAB)$ ( $M = Mn$ , $R = H$ , Methyl, Ethyl; $M = Re$ , $R = H$ ; $DAB =$ )	1.7	14
50	Photodissociation and electronic spectroscopy of transition metal hydrides carbonyls: quantum chemistry and wave packet dynamics. <i>Journal of Organometallic Chemistry</i> , 2000, 609, 66-76.	1.8	14
51	Uranium Extraction by a Bifunctional Amido-Phosphonic Acid: Coordination Structure and Aggregation. <i>Solvent Extraction and Ion Exchange</i> , 2016, 34, 260-273.	2.0	13
52	An experimental and computational look at the radiolytic degradation of TODGA and the effect on metal complexation. <i>New Journal of Chemistry</i> , 2021, 45, 12479-12493.	2.8	13
53	Mass spectrometry and theoretical investigation of di-alkylphosphoric acid-lanthanide complexes. <i>Radiochimica Acta</i> , 2008, 96, .	1.2	11
54	Paramagnetism of Aqueous Actinide Cations. Part II: Theoretical Aspects and New Measurements on An(IV). <i>Inorganic Chemistry</i> , 2016, 55, 12149-12157.	4.0	11

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55	Influence of the local atomic structure in the X-ray absorption near edge spectroscopy of neptunium oxo ions. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10396.	2.8	10
56	Aggregation of Bifunctional Extractants Used for Uranium(VI) Separation. <i>Journal of Physical Chemistry B</i> , 2021, 125, 10759-10771.	2.6	9
57	Influence of the First Coordination of Uranyl on Its Luminescence Properties: A Study of Uranyl Binitrate with <i>N,N</i> -Dialkyl Amide DEHIBA and Water. <i>Inorganic Chemistry</i> , 2022, 61, 890-901.	4.0	9
58	A CASSCF study of the relaxation effects in the lowest 3MLCT excited state of HMn(CO) 3(dab). <i>Chemical Physics Letters</i> , 1996, 257, 1-7.	2.6	7
59	X-ray absorption spectroscopy and actinide electrochemistry: a setup dedicated to radioactive samples applied to neptunium chemistry. <i>Journal of Synchrotron Radiation</i> , 2022, 29, 1-10.	2.4	7
60	Experimental and theoretical study of the degradation of malonamide extractant molecules under ionizing radiation. <i>RSC Advances</i> , 2012, 2, 3954.	3.6	6
61	Modeling and Speciation Study of Uranium(VI) and Technetium(VII) with TBP. <i>Solvent Extraction and Ion Exchange</i> , 2021, 39, 305-327.	2.0	5
62	Characterization of a Hexanuclear Plutonium(IV) Nanostructure in an Acetate Solution via Visible-Near Infrared Absorption Spectroscopy, Extended X-ray Absorption Fine Structure Spectroscopy, and Density Functional Theory. <i>Inorganic Chemistry</i> , 2022, 61, 4806-4817.	4.0	5
63	The electronic structure of f-element Prussian blue analogs determined by soft X-ray absorption spectroscopy. <i>Chemical Communications</i> , 2018, 54, 12206-12209.	4.1	4
64	Coupling Raman spectroscopy and DFT study for enhanced description of nitrosyl nitrate nitrite ruthenium(III) complexes in nitric acid. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2020, 326, 1213-1223.	1.5	4
65	Modeling Selectivity in Liquid/Liquid Extraction. <i>Nuclear Science and Engineering</i> , 2006, 153, 207-222.	1.1	3
66	Thermodynamics of plutonium(III) and curium(III) complexation with a N-donor ligand. <i>Dalton Transactions</i> , 2019, 48, 839-842.	3.3	3
67	Exploring the Coordination of Plutonium and Mixed Plutonyl-Uranyl Complexes of Imidodiphosphinates. <i>Inorganic Chemistry</i> , 2019, 58, 6904-6917.	4.0	3
68	Role of the Hydroxo Group in the Coordination of Citric Acid to Trivalent Americium. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1331-1344.	2.0	3
69	Force Field Parameterization of Actinyl Molecular Cations Using the 12-6-4 Model. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2432-2445.	5.4	3
70	A comparative study of actinide complexation in three ligand systems with increasing complexity. <i>Journal of Physics: Conference Series</i> , 2009, 190, 012185.	0.4	2
71	Molecular solids of actinide hexacyanoferrate: Structure and bonding. <i>IOP Conference Series: Materials Science and Engineering</i> , 2010, 9, 012026.	0.6	2
72	Insights from quantum chemical calculations into inner and outer-sphere complexation of plutonium(IV) by monoamide and carbamide extractants. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2229-2237.	2.8	2

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73	Extraction of Uranium(VI) and Plutonium(IV) by New Tri Alkylcarbamides. Solvent Extraction and Ion Exchange, 0, , 1-22.	2.0	2
74	Studies of Structural and Electronic Properties of Uranium Compounds, by XANES Spectroscopy. Materials Research Society Symposia Proceedings, 2005, 893, 1.	0.1	1
75	Molecular Characterization of Actinide Oxocations from Protactinium to Plutonium. AIP Conference Proceedings, 2007, , .	0.4	1
76	On the use of X-ray absorption spectroscopy to elucidate the structure of lutetium adenosine mono- and triphosphate complexes. Analytical and Bioanalytical Chemistry, 2014, 406, 1049-1061.	3.7	1
77	Electronic Structure of High Oxidation State Actinide Species: Theoretical and Experimental Approaches. Nuclear Science and Engineering, 2006, 153, 203-206.	1.1	0