ValÃ©rie Vallet

List of Publications by Year
in descending order

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107	3,389	185998	161609
papers	citations	28 h-index	54 g-index

118	118	118	2363
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Time-dependent quantum wave-packet description of the Ï€1Ïƒ* photochemistry of phenol. Journal of Chemical Physics, 2005, 122, 224315.	1.2	177
2	Solution coordination chemistry of actinides: Thermodynamics, structure and reaction mechanisms. Coordination Chemistry Reviews, 2006, 250, 784-815.	9.5	177
3	Structure of Uranium(VI) in Strong Alkaline Solutions. A Combined Theoretical and Experimental Investigation. Journal of Physical Chemistry A, 1999, 103, 8257-8264.	1.1	169
4	A two-step uncontracted determinantal effective Hamiltonian-based SOâ€“CI method. Journal of Chemical Physics, 2000, 113, 1391-1402.	1.2	140
5	Solvent Effects on Uranium(VI) Fluoride and Hydroxide Complexes Studied by EXAFS and Quantum Chemistry. Inorganic Chemistry, 2001, 40, 3516-3525.	1.9	138
6	The Mechanism for Water Exchange in [UO2(H2O)5]2+and [UO2(oxalate)2(H2O)]2-, as Studied by Quantum Chemical Methods. Journal of the American Chemical Society, 2001, 123, 11999-12008.	6.6	123
7	Photochemistry of pyrrole: Time-dependent quantum wave-packet description of the dynamics at the Ï€1Ïƒ*-S0 conical intersections. Journal of Chemical Physics, 2005, 123, 144307.	1.2	120
8	Actinide Chemistry in Solution, Quantum Chemical Methods and Models. Theoretical Chemistry Accounts, 2006, 115, 145-160.	0.5	114
9	Probing the Nature of Chemical Bonding in Uranyl(VI) Complexes with Quantum Chemical Methods. Journal of Physical Chemistry A, 2012, 116, 12373-12380.	1.1	113
10	Reduction of uranyl by hydrogen: an ab initio study. Chemical Physics, 1999, 244, 185-193.	0.9	81
11	Can density functional methods be used for open-shell actinide molecules? Comparison with multiconfigurational spin-orbit studies. Journal of Chemical Physics, 2004, 121, 5312-5321.	1.2	81
12	Chelate Effect and Thermodynamics of Metal Complex Formation in Solution:Â A Quantum Chemical Study. Journal of the American Chemical Society, 2003, 125, 14941-14950.	6.6	78
13	Time-dependent quantum wave-packet description of the1Ï€Ïƒ* photochemistry of pyrrole. Faraday Discussions, 2004, 127, 283-293.	1.6	78
14	Theoretical investigation of the energies and geometries of photoexcited uranyl(VI) ion: A comparison between wave-function theory and density functional theory. Journal of Chemical Physics, 2007, 127, 214302.	1.2	75
15	Structure and Bonding in Solution of Dioxouranium(VI) Oxalate Complexes:Â Isomers and Intramolecular Ligand Exchange. Inorganic Chemistry, 2003, 42, 1982-1993.	1.9	68
16	An Investigation of the Accuracy of Different DFT Functionals on the Water Exchange Reaction in Hydrated Uranyl(VI) in the Ground State and the First Excited State. Journal of Chemical Theory and Computation, 2008, 4, 569-577.	2.3	64
17	The Mechanism of Water Exchange in AmO2(H2O)52+ and in the Isoelectronic UO2(H2O)5+ and NpO2(H2O)52+ Complexes as Studied by Quantum Chemical Methods. Journal of the American Chemical Society, 2004, 126, 7766-7767.	6.6	63
18	Benchmarking Electronic Structure Calculations on the Bare UO₂²⁺ Ion: How Different are Single and Multireference Electron Correlation Methods?. Journal of Physical Chemistry A, 2009, 113, 12504-12511.	1.1	62

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19	Reduction Behavior of the Early Actinyl Ions in Aqueous Solution. Journal of Physical Chemistry A, 1999, 103, 9285-9289.	1.1	54
20	Quantum Chemical and Molecular Dynamics Study of the Coordination of Th(IV) in Aqueous Solvent. Journal of Physical Chemistry B, 2010, 114, 15913-15924.	1.2	48
21	Photoinduced multi-mode quantum dynamics of pyrrole at the â€“ conical intersections. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 177-189.	2.0	44
22	Towards systematically improvable models for actinides in condensed phase: the electronic spectrum of uranyl in Cs2UO2Cl4 as a test case. Physical Chemistry Chemical Physics, 2013, 15, 15153.	1.3	44
23	Investigation of the low-lying excited states of PuO22+. Chemical Physics, 1999, 244, 195-201.	0.9	42
24	An ab Initio Theoretical Study of the Electronic Structure of UO₂⁺ and [UO₂(CO₃)₃]^{5â^’}. Journal of Physical Chemistry A, 2009, 113, 1420-1428.	1.1	42
25	Multimode Jahnâ€“Teller and pseudo-Jahnâ€“Teller coupling effects in the photoelectron spectrum of CH3F. Chemical Physics, 2004, 304, 17-34.	0.9	41
26	Rates and Mechanism of Fluoride and Water Exchange in UO2F53-and [UO2F4(H2O)]2-Studied by NMR Spectroscopy and Wave Function Based Methods. Inorganic Chemistry, 2002, 41, 5626-5633.	1.9	37
27	Modeling the hydration of mono-atomic anions from the gas phase to the bulk phase: The case of the halide ions Fâ^’, Clâ^’, and Brâ^’. Journal of Chemical Physics, 2012, 136, 044509.	1.2	36
28	Aqueous chemistry of Ce(<scp>iv</scp>): estimations using actinide analogues. Dalton Transactions, 2017, 46, 13553-13561.	1.6	34
29	Further insights in the ability of classical nonadditive potentials to model actinide ionâ€“water interactions. Journal of Computational Chemistry, 2013, 34, 707-719.	1.5	29
30	Theoretical Study of Plutonium(IV) Complexes Formed within the PUREX Process: A Proposal of a Plutonium Surrogate in Fire Conditions. Journal of Physical Chemistry A, 2014, 118, 10073-10080.	1.1	29
31	Effective bond orders from two-step spinâ€“orbit coupling approaches: The I2, At2, IO+, and AtO+ case studies. Journal of Chemical Physics, 2015, 142, 094305.	1.2	29
32	On the structure and relative stability of uranyl(VI) sulfate complexes in solution. Comptes Rendus Chimie, 2007, 10, 905-915.	0.2	28
33	Ab Initio Study of the Mechanism for Photoinduced Yl-Oxygen Exchange in Uranyl(VI) in Acidic Aqueous Solution. Journal of the American Chemical Society, 2008, 130, 11742-11751.	6.6	28
34	First structural characterization of Pa(<scp>iv</scp>) in aqueous solution and quantum chemical investigations of the tetravalent actinides up to Bk(<scp>iv</scp>): the evidence of a curium break. Dalton Transactions, 2016, 45, 453-457.	1.6	28
35	Revisiting a many-body model for water based on a single polarizable site: From gas phase clusters to liquid and air/liquid water systems. Journal of Chemical Physics, 2013, 139, 114502.	1.2	27
36	Structural, dynamical, and transport properties of the hydrated halides: How do Atâ^’ bulk properties compare with those of the other halides, from Fâ^’ to Iâ^’?. Journal of Chemical Physics, 2016, 144, 124513.	1.2	27

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37	On the multi-reference nature of plutonium oxides: PuO22+, PuO2, PuO3 and PuO2(OH)2. Physical Chemistry Chemical Physics, 2017, 19, 4317-4329.	1.3	27
38	Protactinium and the intersection of actinide and transition metal chemistry. Nature Communications, 2018, 9, 622.	5.8	27
39	Experimental and quantum chemical studies of structure and reaction mechanisms of dioxouranium(vi) complexes in solution. Dalton Transactions, 2004, , 3799-3807.	1.6	26
40	Effects of the first hydration sphere and the bulk solvent on the spectra of the f2isoelectronic actinide compounds: U4+, NpO2+, and PuO22+. Physical Chemistry Chemical Physics, 2010, 12, 1116-1130.	1.3	26
41	Electronic structure investigation of the evanescent AtO⁺ion. Physical Chemistry Chemical Physics, 2014, 16, 9238-9248.	1.3	25
42	Activation of Gas-Phase Uranyl: From an Oxo to a Nitrido Complex. Journal of Physical Chemistry A, 2014, 118, 325-330.	1.1	25
43	Spinâ€“orbit effects on the electronic spectroscopy of transition metal dihydrides H2M(CO)4 (M=Fe,) Tj ETQq1 1 0.784314 rgBT /Ove	0.9	23
44	On the combined use of discrete solvent models and continuum descriptions of solvent effects in ligand exchange reactions: a case study of the uranyl(VI) aquo ion. Theoretical Chemistry Accounts, 2009, 124, 377-384.	0.5	22
45	Ab initio study of the ground-state potential of XHâ¯ anions (X=He,Ne,Ar). Chemical Physics, 2001, 263, 33-40.	0.9	21
46	The structure and bonding of Y, Eu, U, Am and Cm complexes as studied by quantum chemical methods and X-ray crystallography. Dalton Transactions, 2010, 39, 7666.	1.6	21
47	Remarkable impact of intermode couplings on multimode vibronic dynamics: the photoelectron spectrum of CH3F. Journal of Chemical Physics, 2005, 123, 231103.	1.2	20
48	Spectroscopic effects of first-order relativistic vibronic coupling in linear triatomic molecules. Journal of Chemical Physics, 2005, 123, 124104.	1.2	20
49	Multiconfiguration Diracâ¯Hartreeâ¯Fock Adjusted Energy-Consistent Pseudopotential for Uranium: Spinâ¯Orbit Configuration Interaction and Fock-Space Coupled-Cluster Study of U⁴⁺ and U⁵⁺. Journal of Physical Chemistry A, 2009, 113, 11509-11516.	1.1	20
50	Improvement of the ab initio embedded cluster method for luminescence properties of doped materials by taking into account impurity induced distortions: The example of Y[sub 2]O[sub 3]:Bi[sup 3+]. Journal of Chemical Physics, 2009, 131, 194501.	1.2	20
51	Accurate ab initio study on the spectroscopy of Ag and Ag+ including spin-orbit couplings aimed at molecular calculations. Journal of Chemical Physics, 2001, 115, 3201-3207.	1.2	19
52	Predictive Simulations of Ionization Energies of Solvated Halide Ions with Relativistic Embedded Equation of Motion Coupled Cluster Theory. Physical Review Letters, 2018, 121, 266001.	2.9	19
53	Calculation of the vibronic structure of the XÌƒÎ2 photoelectron spectra of XCN,X=F, Cl, and Br. Journal of Chemical Physics, 2006, 124, 044317.	1.2	18
54	The luminescence spectrum of in 2GeF6 crystalsâ€”A quantum chemical study. Journal of Luminescence, 2007, 126, 779-783.	1.5	18

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55	Ab initio embedded cluster study of the excitation spectrum and Stokes shifts of Bi3+-doped Y2O3. Journal of Chemical Physics, 2007, 127, 104705.	1.2	17
56	Thermodynamic Properties of Gaseous Ruthenium Species. Journal of Physical Chemistry A, 2015, 119, 4961-4971.	1.1	17
57	In silico prediction of atomic static electric-dipole polarizabilities of the early tetravalent actinide ions:Th4+(5f0),Pa4+(5f1), andU4+(5f2). Physical Review A, 2008, 78, .	1.0	16
58	Influence of Alkaline Earth Metal Ions on Structures and Luminescent Properties of Na_mM_nUO₂(CO₃)₃<sup>(4â€“mâ€“2n)â (M = Mg, Ca; m, n = 0â€“2): Time-Resolved Fluorescence Spectroscopy and Ab Initio Studies. Inorganic Chemistry, 2020, 59, 15036-15049.	1.9	16
59	The electronic spectroscopy of transition metal di-hydrides H2M(CO)4(Mâ€‰=â€‰Fe,Os): a theoretical study based on CASSCF/MS-CASPT2 and TD-DFT. Physical Chemistry Chemical Physics, 2003, 5, 2948-2953.	1.3	15
60	Importance of Spin-Orbit Coupling for the Assignment of the Photodetachment Spectra of AuX2â^' (X=Cl, Br, and I). ChemPhysChem, 2006, 7, 723-727.	1.0	15
61	Investigation of the Luminescence of [UO₂X₄]^{2â€“} (X = Cl, Br) Complexes in the Organic Phase Using Time-Resolved Laser-Induced Fluorescence Spectroscopy and Quantum Chemical Simulations. Inorganic Chemistry, 2020, 59, 5896-5906.	1.9	15
62	Spinâ^'Orbit Effects in Electron Transfer in Neptunyl(VI)â^'Neptunyl(V) Complexes in Solution. Journal of Physical Chemistry A, 2005, 109, 4957-4960.	1.1	14
63	Water Exchange Mechanism in the First Excited State of Hydrated Uranyl(VI). Inorganic Chemistry, 2009, 48, 11310-11313.	1.9	14
64	Alkali-metal ion coordination in uranyl(<scp>vi</scp>) poly-peroxide complexes in solution. Part 1: the Li⁺, Na⁺ and K⁺ â€“ peroxideâ€“hydroxide systems. Dalton Transactions, 2015, 44, 1549-1556.	1.6	13
65	Synthesis and photoluminescence of three bismuth(<scp>iii</scp>)-organic compounds bearing heterocyclic N-donor ligands. Dalton Transactions, 2020, 49, 11756-11771.	1.6	13
66	Spin-orbit configuration interaction study of the electronic structure of the 5f2 manifold of U4+ and the 5f manifold of U5+. Journal of Chemical Physics, 2008, 128, 154310.	1.2	12
67	Structureâ€“Property Relationships in Photoluminescent Bismuth Halide Organic Hybrid Materials. Inorganic Chemistry, 2021, 60, 9727-9744.	1.9	12
68	Comment on â€œThe Waterâ€Exchange Mechanism of the [UO₂(OH₂)₅]²⁺ Ion Revisited: The Importance of a Proper Treatment of Electron Correlationâ€•[F. P. Rotzinger Chem. Eur. J., 2007, 13, 800]. Chemistry - A European Journal, 2007, 13, 10294-10297.	1.7	11
69	Unraveling the Ground State and Excited State Structures and Dynamics of Hydrated Ce³⁺ Ions by Experiment and Theory. Inorganic Chemistry, 2018, 57, 10111-10121.	1.9	11
70	Accurate Predictions of Volatile Plutonium Thermodynamic Properties. Inorganic Chemistry, 2019, 58, 14507-14521.	1.9	11
71	Ab initio study of a Bi3+ impurity in Cs2NaYCl6 and Y2O3: Comparison of perturbative and variational electron correlation methods. Journal of Chemical Physics, 2006, 125, 174709.	1.2	10
72	Ground- and Excited-State Properties of the Mixed-Valence Complex [(NH₃)₅Ru^{III}NCRu^{II}(CN)₅]^{â^'}. Journal of Physical Chemistry A, 2008, 112, 5467-5477.	1.1	10

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73	Theoretical spectroscopy of molecular iodine. 1. Ab initio study on the B0⁺ _u â^' X0⁺ _g, A1_u â^' X0⁺ _g and Bâ€²1_u â^' X0⁺ _g radiative transition intensities. Molecular Physics, 2000, 98, 1973-1979.	0.8	9
74	Benchmark binding energies of ammonium and alkyl-ammonium ions interacting with water. Are ammoniumâ€“water hydrogen bonds strong?. Chemical Physics Letters, 2015, 618, 168-173.	1.2	9
75	Linking Solution Structures and Energetics: Thorium Nitrate Complexes. Journal of Physical Chemistry B, 2017, 121, 8577-8584.	1.2	9
76	Organic ion association in aqueous phase and ab initio-based force fields: The case of carboxylate/ammonium salts. Journal of Chemical Physics, 2017, 147, 161720.	1.2	9
77	Ion hydration free energies and water surface potential in water nano drops: The cluster pair approximation and the proton hydration Gibbs free energy in solution. Journal of Chemical Physics, 2019, 151, 174504.	1.2	9
78	Influence of the First Coordination of Uranyl on Its Luminescence Properties: A Study of Uranyl Binitrate with N,N-Dialkyl Amide DEHiBA and Water. Inorganic Chemistry, 2022, 61, 890-901.	1.9	9
79	Relativistic Pseudopotential Calculations for Electronic Excited States. Theoretical and Computational Chemistry, 2004, 14, 476-551.	0.2	8
80	Calculation of the vibronic structure of the photodetachment spectra of CCClâ^' and CCBrâ^'. Journal of Chemical Physics, 2006, 125, 164327.	1.2	8
81	Structure and dynamics of binary and ternary lanthanide(iii) and actinide(iii) tris[4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedione] (TTA) complexes. Part 2, the structure and dynamics of binary and ternary complexes in the Y(iii)/Eu(iii) â€“TTA â€“ tributylphosphate (TBP) system in chloroform as studied by NMR spectroscopy. Dalton Transactions, 2010, 39, 10944.	1.6	8
82	Alkaliâ€“metal ion coordination in uranyl(<scp>vi</scp>) poly-peroxo complexes in solution, inorganic analogues to crown-ethers. Part 2. Complex formation in the tetramethyl ammonium-, Li⁺-, Na⁺- and K⁺-uranyl(<scp>vi</scp>)â€“peroxideâ€“carbonate systems. Dalton Transactions, 2015, 44, 16565-16572.	1.6	8
83	Structural and Electronic Properties of Fluoride Complexes of Nb V , Ta V , and Pa V : The Influence of Relativistic Effects on Group V Elements. European Journal of Inorganic Chemistry, 2016, 2016, 5467-5476.	1.0	8
84	Structure and dynamics of binary and ternary lanthanide(iii) and actinide(iii) tris[4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedione] (TTA) â€“ tributylphosphate (TBP) complexes. Part 3, the structure, thermodynamics and reaction mechanisms of 8- and 9-coordinated binary and ternary Y-TTA-TBP complexes studied by quantum chemical methods. Dalton Transactions, 2011, 40, 3154.	1.6	7
85	Thermochemistry of Ruthenium Oxyhydroxide Species and Their Impact on Volatile Speciations in Severe Nuclear Accident Conditions. Journal of Physical Chemistry A, 2016, 120, 606-614.	1.1	7
86	Improving the description of solvent pairwise interactions using local solute/solvent threeâ€body functions. The case of halides and carboxylates in aqueous environment. Journal of Computational Chemistry, 2019, 40, 1209-1218.	1.5	7
87	Investigating solvent effects on the magnetic properties of molybdate ions () with relativistic embedding. International Journal of Quantum Chemistry, 2020, 120, e26207.	1.0	7
88	Investigation of the dynamics of two coupled oscillators with mixed quantum-classical methods. Journal of Chemical Physics, 2006, 124, 184105.	1.2	6
89	Properties of the tetravalent actinide series in aqueous phase from a microscopic simulation self-consistent engine. Physical Chemistry Chemical Physics, 2020, 22, 2343-2350.	1.3	6
90	Can Quantum Chemical Methods be used to Predict Gibbs Energies for Reactions in Solution? A Case Study using Binary and Ternary Lanthanide(III) and Actinide(III) - Tris[4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedione] (TTA) â€“ Tributyl/Trimethyl phosphate (TBP/TMP) Complexes. Solvent Extraction and Ion Exchange, 2013, 31, 358-369.	0.8	5

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91	Structure and Bonding in Uranyl(VI) Peroxide and Crown Ether Complexes; Comparison of Quantum Chemical and Experimental Data. Inorganic Chemistry, 2017, 56, 15231-15240.	1.9	5
92	Measurement of double differential cross-section of light water at high temperature and pressure to generate S(Î±,Î²). EPJ Web of Conferences, 2017, 146, 13006.	0.1	5
93	Conformational Landscape of Oxygen-Containing Naphthalene Derivatives. Journal of Physical Chemistry A, 2020, 124, 4484-4495.	1.1	5
94	Facing the challenge of predicting the standard formation enthalpies ofn-butyl-phosphate species withab initiomethods. Journal of Chemical Physics, 2017, 146, 244312.	1.2	4
95	Global 15-Meter Mosaic Derived from Simulated True-Color ASTER Imagery. Remote Sensing, 2019, 11, 441.	1.8	3
96	Revisiting the Complexation of Cm(III) with Aqueous Phosphates: What Can We Learn from the Complex Structures Using Luminescence Spectroscopy and Ab Initio Simulations?. Inorganic Chemistry, 2021, 60, 10656-10673.	1.9	3
97	Reactivity of Ru oxides with air radiolysis products investigated by theoretical calculations. Journal of Nuclear Materials, 2022, 558, 153395.	1.3	3
98	Environment Effects on X-Ray Absorption Spectra With Quantum Embedded Real-Time Time-Dependent Density Functional Theory Approaches. Frontiers in Chemistry, 2022, 10, 823246.	1.8	3
99	Insights from quantum chemical calculations into inner and outer-sphere complexation of plutonium(iv) by monoamide and carbamide extractants. Physical Chemistry Chemical Physics, 2021, 23, 2229-2237.	1.3	2
100	NaCl Salts in Finite Aqueous Environments at the Fine Particle Marine Aerosol Scale. ACS Earth and Space Chemistry, 2022, 6, 1612-1626.	1.2	2
101	Carbonâ€“sulfur bond strength in methanesulfinate and benzenesulfinate ligands directs decomposition of Np(<scp>v</scp>) and Pu(<scp>v</scp>) coordination complexes. Dalton Transactions, 2020, 49, 3293-3303.	1.6	1
102	The Mechanism of Water Exchange in AmO2(H2O)52+ and in the Isoelectronic UO2(H2O)5+ and NpO2(H2O)52+ Complexes as Studied by Quantum Chemical Methods.. ChemInform, 2004, 35, no.	0.1	0
103	Experimental and Quantum Chemical Studies of Structure and Reaction Mechanisms of Dioxouranium(VI) Complexes in Solution. ChemInform, 2005, 36, no.	0.1	0
104	Cover Image, Volume 120, Issue 21. International Journal of Quantum Chemistry, 2020, 120, e26496.	1.0	0
105	The importance of electron correlation and intermediate coupling in the spectroscopy of actinides molecules. , 2006, , 1302-1305.		0
106	How to build accurate macroscopic models of actinide ions in aqueous solvents?. , 2014, , .		0
107	Structural and thermodynamics properties of pure phase alkanes, monoamides and alkane/monoamide mixtures with an ab initio based force-field model. Journal of Molecular Liquids, 2022, 363, 119797.	2.3	0