Florent RÃ©al

List of Publications by Year
in descending order

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50 papers	1,004 citations	361413 20 h-index	454955 30 g-index
52 all docs	52 docs citations	52 times ranked	1007 citing authors

#	Article	IF	Citations
1	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.	3.0	75
2	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.	5.3	64
3	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.	2.5	62
4	On the universality of the long-/short-range separation in multiconfigurational density-functional theory. II. Investigating f actinide species. Journal of Chemical Physics, 2009, 131, 054107.	3.0	49
5	Quantum Chemical and Molecular Dynamics Study of the Coordination of Th(IV) in Aqueous Solvent. Journal of Physical Chemistry B, 2010, 114, 15913-15924.	2.6	48
6	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.	2.8	44
7	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.	2.5	42
8	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.	3.0	36
9	Aqueous chemistry of Ce(<scp>iv</scp>): estimations using actinide analogues. Dalton Transactions, 2017, 46, 13553-13561.	3.3	34
10	Further insights in the ability of classical nonadditive potentials to model actinide ionâ€“water interactions. Journal of Computational Chemistry, 2013, 34, 707-719.	3.3	29
11	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.	3.0	29
12	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.	13.7	28
13	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.	3.3	28
14	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.	3.0	27
15	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.	3.0	27
16	On the multi-reference nature of plutonium oxides: PuO22+, PuO2, PuO3 and PuO2(OH)2. Physical Chemistry Chemical Physics, 2017, 19, 4317-4329.	2.8	27
17	Electronic structure investigation of the evanescent AtO⁺ion. Physical Chemistry Chemical Physics, 2014, 16, 9238-9248.	2.8	25
18	Standard free energy of the equilibrium between the trans-monomer and the cyclic-dimer of acetic acid in the gas phase from infrared spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 7477-7488.	2.8	25

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19	Ab initio simulation of photoluminescence: Bi3+ in Y2O3 (S6 site). Optical Materials, 2003, 24, 221-230.	3.6	22
20	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.	3.0	20
21	How Does the Solvation Unveil AtO⁺ Reactivity?. Journal of Physical Chemistry B, 2013, 117, 5206-5211.	2.6	20
22	Predictive Simulations of Ionization Energies of Solvated Halide Ions with Relativistic Embedded Equation of Motion Coupled Cluster Theory. Physical Review Letters, 2018, 121, 266001.	7.8	19
23	Influence of the geometry of a hydrogen bond on conformational stability: a theoretical and experimental study of ethyl carbamate. Physical Chemistry Chemical Physics, 2009, 11, 1719.	2.8	18
24	Ab initio embedded cluster study of the excitation spectrum and Stokes shifts of Bi3+-doped Y2O3. Journal of Chemical Physics, 2007, 127, 104705.	3.0	17
25	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, .	2.5	16
26	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.	4.0	16
27	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.	4.0	15
28	Synthesis and photoluminescence of three bismuth(<scp>iii</scp>)-organic compounds bearing heterocyclic N-donor ligands. Dalton Transactions, 2020, 49, 11756-11771.	3.3	13
29	Structureâ€“Property Relationships in Photoluminescent Bismuth Halide Organic Hybrid Materials. Inorganic Chemistry, 2021, 60, 9727-9744.	4.0	12
30	Unraveling the Ground State and Excited State Structures and Dynamics of Hydrated Ce³⁺ Ions by Experiment and Theory. Inorganic Chemistry, 2018, 57, 10111-10121.	4.0	11
31	Accurate Predictions of Volatile Plutonium Thermodynamic Properties. Inorganic Chemistry, 2019, 58, 14507-14521.	4.0	11
32	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.	3.0	10
33	Rationalization of the Solvation Effects on the AtO⁺ Ground-State Change. Journal of Physical Chemistry B, 2013, 117, 10589-10595.	2.6	9
34	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.	3.0	9
35	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.	3.0	9
36	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.	4.0	9

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37	Unraveling the hydration-induced ground-state change of AtO⁺ by relativistic and multiconfigurational wave-function-based methods. Physical Chemistry Chemical Physics, 2016, 18, 32703-32712.	2.8	8
38	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.	3.3	7
39	Properties of the tetravalent actinide series in aqueous phase from a microscopic simulation self-consistent engine. Physical Chemistry Chemical Physics, 2020, 22, 2343-2350.	2.8	6
40	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.	0.3	5
41	Conformational Landscape of Oxygen-Containing Naphthalene Derivatives. Journal of Physical Chemistry A, 2020, 124, 4484-4495.	2.5	5
42	Facing the challenge of predicting the standard formation enthalpies ofn-butyl-phosphate species withab initiomethods. Journal of Chemical Physics, 2017, 146, 244312.	3.0	4
43	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.	4.0	3
44	X-ray diffraction and ab initio determinations of the structure of Rb4CdCl6. Solid State Communications, 2004, 131, 543-548.	1.9	2
45	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.	2.8	2
46	NaCl Salts in Finite Aqueous Environments at the Fine Particle Marine Aerosol Scale. ACS Earth and Space Chemistry, 2022, 6, 1612-1626.	2.7	2
47	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.	3.3	1
48	How to build accurate macroscopic models of actinide ions in aqueous solvents?. , 2014, , .		0
49	A Molecular Scale Investigation of Organic/Inorganic Ion Selectivity at the Airâ€“Liquid Interface. ACS Earth and Space Chemistry, 2022, 6, 1698-1716.	2.7	0
50	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.	4.9	0