Florent Louis

List of Publications by Year
in descending order

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74	898	471371	580701
papers	citations	17	25
		h-index	g-index

81	81	81	782
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Reactivity of Ru oxides with air radiolysis products investigated by theoretical calculations. Journal of Nuclear Materials, 2022, 558, 153395.	1.3	3
2	A study of single and quaternary adsorption of Cu2+, Co2+, Ni2+ and Ag+ on sludge modified by alkaline fusion. Chemical Engineering Journal, 2022, 433, 133674.	6.6	7
3	Application of a multilayer physical model for the critical analysis of the adsorption of nicotinamide and propranolol on magnetic-activated carbon. Environmental Science and Pollution Research, 2022, 29, 30184-30192.	2.7	8
4	New insights into the competition between antioxidant activities and pro-oxidant risks of rosmarinic acid. RSC Advances, 2022, 12, 1499-1514.	1.7	11
5	Thermochemical and kinetic studies of H-abstraction reaction of benzofurans and benzodioxins by H-atoms. Computational and Theoretical Chemistry, 2022, 1209, 113589.	1.1	0
6	Understanding the Cu2+ adsorption mechanism on activated carbon using advanced statistical physics modelling. Environmental Science and Pollution Research, 2022, , 1.	2.7	1
7	Detailed kinetic study of hydrogen abstraction reactions of triphenylene, benzo[e]pyrene, dibenzo[fg,op]naphtacene, and coronene by H atoms. International Journal of Chemical Kinetics, 2022, 54, 266-276.	1.0	0
8	Enhanced adsorption of ketoprofen and 2,4-dichlorophenoxyactic acid on Physalis peruviana fruit residue functionalized with H2SO4: Adsorption properties and statistical physics modeling. Chemical Engineering Journal, 2022, 445, 136773.	6.6	22
9	A theoretical study of the potential energy surface for the isomerization reaction of fluoranthene to aceanthrylene: Implications for combustion chemistry. Computational and Theoretical Chemistry, 2021, 1196, 113118.	1.1	1
10	Theoretical Study of the Monohydration of Mercury Compounds of Atmospheric Interest. Journal of Physical Chemistry A, 2021, 125, 5819-5828.	1.1	1
11	Thermochemical and kinetic studies of hydrogen abstraction reaction from C16H10 isomers by H atoms. Computational and Theoretical Chemistry, 2021, 1201, 113257.	1.1	4
12	Infrared matrix-isolation and theoretical studies of interactions between CH3I and water. Journal of Molecular Structure, 2021, 1236, 130342.	1.8	0
13	Physicochemical assessment of anionic dye adsorption on bone char using a multilayer statistical physics model. Environmental Science and Pollution Research, 2021, 28, 67248-67255.	2.7	20
14	Adsorption of 3-aminophenol and resorcinol on avocado seed activated carbon: Mathematical modelling, thermodynamic study and description of adsorbent performance. Journal of Molecular Liquids, 2021, 342, 116952.	2.3	21
15	Preparation of an avocado seed hydrochar and its application as heavy metal adsorbent: Properties and advanced statistical physics modeling. Chemical Engineering Journal, 2021, 419, 129472.	6.6	44
16	A statistical physics analysis of the adsorption of Fe3+, Al3+ and Cu2+ heavy metals on chitosan films via homogeneous and heterogeneous monolayer models. Journal of Molecular Liquids, 2021, 343, 117617.	2.3	12
17	Antioxidant and UV-radiation absorption activity of aaptamine derivatives â€“ potential application for natural organic sunscreens. RSC Advances, 2021, 11, 21433-21446.	1.7	6
18	Unraveling the Tropospheric Microhydration Processes of Iodous Acid HOIO. ACS Earth and Space Chemistry, 2020, 4, 92-100.	1.2	6

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19	BrHgO^{â€¢} + CO: Analogue of OH + CO and Reduction Path for Hg(II) in the Atmosphere. ACS Earth and Space Chemistry, 2020, 4, 1777-1784.	1.2	16
20	On the applicability of the MP2.5 approximation for open-shell systems. Case study of atmospheric reactivity. Computational and Theoretical Chemistry, 2020, 1186, 112901.	1.1	2
21	Theoretical Investigation of the Reaction of Pyrene Formation from Fluoranthene. Journal of Physical Chemistry A, 2019, 123, 7491-7498.	1.1	4
22	Microhydration of caesium metaborate: structural and thermochemical properties of CsBO2â€‰+â€‰n H2O (nâ€‰=â€‰1â€“4) aggregates. Journal of Molecular Modeling, 2019, 25, 207.	0.8	3
23	Box modelling of gas-phase atmospheric iodine chemical reactivity in case of a nuclear accident. Atmospheric Environment, 2019, 214, 116838.	1.9	7
24	Theoretical investigation of thermochemical properties of cesium borates species. Journal of Nuclear Materials, 2019, 517, 63-70.	1.3	8
25	A theoretical study of the microhydration processes of iodine nitrogen oxides. International Journal of Quantum Chemistry, 2019, 119, e25792.	1.0	6
26	Reactivity of Hydrogen Peroxide with Br and I Atoms. Journal of Physical Chemistry A, 2018, 122, 1053-1063.	1.1	8
27	Research Works on Iodine and Ruthenium Behavior in Severe Accident Conditions. Journal of Nuclear Engineering and Radiation Science, 2018, 4, .	0.2	8
28	Theoretical Study of the Reactions of H Atoms with CH₃I and CH₂I₂. Journal of Physical Chemistry A, 2018, 122, 6546-6557.	1.1	4
29	Thermochemistry of HIO₂ Species and Reactivity of Iodous Acid with OH Radical: A Computational Study. ACS Earth and Space Chemistry, 2017, 1, 39-49.	1.2	12
30	Investigation of the Reaction Mechanism and Kinetics of Iodic Acid with OH Radical Using Quantum Chemistry. ACS Earth and Space Chemistry, 2017, 1, 227-235.	1.2	10
31	Caesium hydride: MS-CASPT2 potential energy curves and A1Î£+â†'X1Î£+ absorption/emission spectroscopy. Journal of Chemical Physics, 2017, 146, 104304.	1.2	4
32	MS-CASPT2 study of the ground and low lying states of CsH+. Journal of Molecular Modeling, 2017, 23, 339.	0.8	1
33	IRSN R&D Actions on FP Behaviour for RCS, Containment and FCVS in Severe Accident Conditions. , 2016, , .		1
34	A theoretical study of the microhydration of iodic acid (HOIO2). Computational and Theoretical Chemistry, 2016, 1094, 98-107.	1.1	17
35	Computational study of the I2O5+ H2O = 2 HOIO2 gas-phase reaction. Chemical Physics Letters, 2016, 662, 114-119.	1.2	20
36	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

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37	A Density Functional Theory and ab Initio Investigation of the Oxidation Reaction of CO by IO Radicals. Journal of Physical Chemistry A, 2016, 120, 1737-1749.	1.1	13
38	A Theoretical Study of the Kinetics of the Hydrogen Atom Abstraction Reactions from Cyclopropane by H, O (³P), and Cl (²P_{3/2}) Atoms and OH Radicals. International Journal of Chemical Kinetics, 2015, 47, 232-245.	1.0	3
39	Thermodynamic Properties of Gaseous Ruthenium Species. Journal of Physical Chemistry A, 2015, 119, 4961-4971.	1.1	17
40	The Kinetics of the Reaction C₂H₅ ^{â€¢}â€“HIâ€”â†’â€“C₂H₆â€“+â€¯I^{â€¢} over an Extended Temperature Range (213â€“623â€¯K): Experiment and Modeling. Zeitschrift Fur Physikalische Chemie, 2015, 229, 1475-1501.	1.4	3
41	Gas-Phase Reactivity of Cesium-Containing Species by Quantum Chemistry. Journal of Physical Chemistry A, 2015, 119, 9373-9384.	1.1	6
42	Reactivity of CHI3 with OH Radicals: X-Abstraction Reaction Pathways (X = H, I), Atmospheric Chemistry, and Nuclear Safety. Journal of Physical Chemistry A, 2014, 118, 9512-9520.	1.1	3
43	AÂTheoretical Study of the X-Abstraction Reactions (XÂ=ÂH, Br, or I) from CH2IBr by OH Radicals: Implications for Atmospheric Chemistry. Zeitschrift Fur Physikalische Chemie, 2013, , 130613021201008.	1.4	6
44	Advances in mechanistic understanding of iodine behaviour in PHEBUS-FP tests with the help of ab initio calculations. Annals of Nuclear Energy, 2013, 61, 170-178.	0.9	21
45	Atmospheric Reactivity of CH2ICl with OH Radicals: High-Level OVOS CCSD(T) Calculations for the X-Abstraction Pathways (X = H, Cl, or I). Journal of Physical Chemistry A, 2013, 117, 771-782.	1.1	15
46	Thermochemistry of small iodine species. Physica Scripta, 2013, 88, 058304.	1.2	7
47	Thermochemical Data and Additivity Group Values for Ten Species of o-Xylene Low-Temperature Oxidation Mechanism. Journal of Physical Chemistry A, 2012, 116, 592-610.	1.1	7
48	Ab initio calculations and iodine kinetic modeling in the reactor coolant system of a pressurized water reactor in case of severe nuclear accident. Computational and Theoretical Chemistry, 2012, 990, 194-208.	1.1	25
49	Theoretical Study of H-Abstraction Reactions from CH₃Cl and CH₃Br Molecules by ClO and BrO Radicals. Journal of Physical Chemistry A, 2012, 116, 4396-4408.	1.1	8
50	Detailed modeling of the atmospheric degradation mechanism of very-short lived brominated species. Atmospheric Environment, 2012, 59, 514-532.	1.9	17
51	Molecular structures and thermodynamic properties of 12 gaseous cesium-containing species of nuclear safety interest: Cs2, CsH, CsO, Cs2O, CsX, and Cs2X2 (X=OH, Cl, Br, and I). Journal of Nuclear Materials, 2012, 420, 452-462.	1.3	25
52	A Theoretical Study of the H-Abstraction Reactions from HOI by Moist Air Radiolytic Products (H, OH,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Chemistry A, 2011, 115, 6664-6674.	1.1	15
53	A theoretical study of the kinetics of the forward and reverse reactions HI+CH3=I+CH4. Chemical Physics Letters, 2011, 517, 149-154.	1.2	22
54	Atmospheric reactivity of CH3I and CH2I2 with OH radicals: A comparative study of the H- versus I-abstraction. Computational and Theoretical Chemistry, 2011, 965, 275-284.	1.1	22

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55	A theoretical study of the NCN (3Î£â^') biradical thermochemical properties: Implications for combustion chemistry. Computational and Theoretical Chemistry, 2011, 967, 67-74.	1.1	8
56	Theoretical Study of the Gas-Phase Reactions of Iodine Atoms (²P_{3/2}) with H₂, H₂O, HI, and OH. Journal of Physical Chemistry A, 2010, 114, 9270-9288.	1.1	32
57	Confocal Raman imaging and atomic force microscopy of the surface reaction of NO₂ and NaCl(100) under humidity. Journal of Raman Spectroscopy, 2009, 40, 157-163.	1.2	9
58	A CASPT2 Theoretical Study of the Kinetics of the 2-, 3-, and 4-Methylbenzylperoxy Radical Isomerization. Journal of Physical Chemistry A, 2009, 113, 2995-3003.	1.1	10
59	A Theoretical Study of the Kinetics of the Benzylperoxy Radical Isomerization. Journal of Physical Chemistry A, 2008, 112, 6045-6052.	1.1	14
60	Tropospheric multiphase chemistry of 2,5- and 2,6-dimethylphenols: determination of the mass accommodation coefficients and the Henryâ€™s law constants. Physical Chemistry Chemical Physics, 2006, 8, 1714.	1.3	4
61	Temperature Dependence of the Mass Accommodation Coefficients of 2-Nitrophenol, 2-Methylphenol, 3-Methylphenol, and 4-Methylphenol on Aqueous Surfaces. Journal of Physical Chemistry A, 2005, 109, 1864-1872.	1.1	10
62	Henry's law constant measurements for phenol, o-, m-, and p-cresol as a function of temperature. Atmospheric Environment, 2004, 38, 5577-5588.	1.9	43
63	Direct Combined ab Initio/Transition State Theory Study of the Kinetics of the Abstraction Reactions of Halogenated Methanes with Hydrogen Atoms. Journal of Physical Chemistry A, 2004, 108, 10586-10593.	1.1	26
64	Ab Initio Study of the Oxidation Reaction of CO by ClO Radicals. Journal of Physical Chemistry A, 2003, 107, 9931-9936.	1.1	11
65	Photochemistry of Bromine-Containing Fluorinated Alkenes:â€‰ Reactivity toward OH and UV Spectra. Journal of Physical Chemistry A, 2002, 106, 10195-10199.	1.1	38
66	An ab Initio Study of the Kinetics of the Reactions of Halomethanes with the Hydroxyl Radical. 3. Kinetic Parameters Predictions for the Potential Halon Replacements CH2FBr, CHFBr2, CHFClBr, CHCl2Br, and CHClBr2â€. Journal of Physical Chemistry A, 2001, 105, 1599-1604.	1.1	10
67	Computational Study of the Reactions of Methane with XO Radicals (X = F, Cl, or Br):â€‰ Implications in Combustion Chemistry. Journal of Physical Chemistry A, 2001, 105, 4284-4289.	1.1	5
68	General Expression for the Effective Mass in the One-Dimensional Treatment of Tunneling Corrections. Journal of Physical Chemistry A, 2001, 105, 11034-11040.	1.1	8
69	An ab Initio Study of the Kinetics of the Reactions of Halomethanes with the Hydroxyl Radical. 1. CH2Br2. Journal of Physical Chemistry A, 2000, 104, 2931-2938.	1.1	25
70	An ab Initio Study of the Kinetics of the Reactions of Halomethanes with the Hydroxyl Radical. 2. A Comparison between Theoretical and Experimental Values of the Kinetic Parameters for 12 Partially Halogenated Methanes. Journal of Physical Chemistry A, 2000, 104, 8773-8778.	1.1	50
71	Ab initio theoretical studies of the reactions between fluorine atoms and halomethanes of type CHCl3- xF x (x=0, 1, 2 or 3). Physical Chemistry Chemical Physics, 1999, 1, 383-389.	1.3	7
72	Kinetic study of the reactions of CF3O2 radicals with Cl and NO. Physical Chemistry Chemical Physics, 1999, 1, 5087-5096.	1.3	19

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73	Kinetics and products studies of reactions between fluorine atoms and CHF3, CHClF2, CHCl2F and CHCl3. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 1437-1445.	1.7	11
74	Rate Coefficients for the Gas Phase Reactions of CF3CH2F (HFC-134a) with Chlorine and Fluorine Atoms:â€‰ Experimental and ab Initio Theoretical Studies. Journal of Physical Chemistry A, 1997, 101, 8503-8507.	1.1	16