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	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
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	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
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	Computational study of the I2O5+ H2O = 2 HOIO2 gas-phase reaction. Chemical Physics Letters, 2016, 662, 114-119.	1.2	20
16	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
17	Kinetic study of the reactions of CF3O2 radicals with Cl and NO. Physical Chemistry Chemical Physics, 1999, 1, 5087-5096.	1.3	19
18	Detailed modeling of the atmospheric degradation mechanism of very-short lived brominated species. Atmospheric Environment, 2012, 59, 514-532.	1.9	17

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19	Thermodynamic Properties of Gaseous Ruthenium Species. Journal of Physical Chemistry A, 2015, 119, 4961-4971.	1.1	17
20	A theoretical study of the microhydration of iodic acid (HOIO2). Computational and Theoretical Chemistry, 2016, 1094, 98-107.	1.1	17
21	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
22	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
23	A Theoretical Study of the H-Abstraction Reactions from HOI by Moist Air Radiolytic Products (H, OH,) Tj ETQq1 1 0.784314 rgBT /Ove Chemistry A, 2011, 115, 6664-6674.	1.1	15
24	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
25	A Theoretical Study of the Kinetics of the Benzylperoxy Radical Isomerization. Journal of Physical Chemistry A, 2008, 112, 6045-6052.	1.1	14
26	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
27	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
28	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
29	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
30	Ab Initio Study of the Oxidation Reaction of CO by ClO Radicals. Journal of Physical Chemistry A, 2003, 107, 9931-9936.	1.1	11
31	New insights into the competition between antioxidant activities and pro-oxidant risks of rosmarinic acid. RSC Advances, 2022, 12, 1499-1514.	1.7	11
32	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
33	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
34	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
35	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
36	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

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37	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
38	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
39	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
40	Reactivity of Hydrogen Peroxide with Br and I Atoms. Journal of Physical Chemistry A, 2018, 122, 1053-1063.	1.1	8
41	Research Works on Iodine and Ruthenium Behavior in Severe Accident Conditions. Journal of Nuclear Engineering and Radiation Science, 2018, 4, .	0.2	8
42	Theoretical investigation of thermochemical properties of cesium borates species. Journal of Nuclear Materials, 2019, 517, 63-70.	1.3	8
43	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
44	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
45	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
46	Thermochemistry of small iodine species. Physica Scripta, 2013, 88, 058304.	1.2	7
47	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
48	Box modelling of gas-phase atmospheric iodine chemical reactivity in case of a nuclear accident. Atmospheric Environment, 2019, 214, 116838.	1.9	7
49	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
50	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
51	Gas-Phase Reactivity of Cesium-Containing Species by Quantum Chemistry. Journal of Physical Chemistry A, 2015, 119, 9373-9384.	1.1	6
52	A theoretical study of the microhydration processes of iodine nitrogen oxides. International Journal of Quantum Chemistry, 2019, 119, e25792.	1.0	6
53	Unraveling the Tropospheric Microhydration Processes of Iodous Acid HOIO. ACS Earth and Space Chemistry, 2020, 4, 92-100.	1.2	6
54	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

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55	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
56	The Kinetics of the Reaction C₂H₅ ^{â€¢}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	5
57	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
58	Caesium hydride: MS-CASPT2 potential energy curves and A1Î£+â†’X1Î£+ absorption/emission spectroscopy. Journal of Chemical Physics, 2017, 146, 104304.	1.2	4
59	Theoretical Study of the Reactions of H Atoms with CH₃I and CH₂I₂. Journal of Physical Chemistry A, 2018, 122, 6546-6557.	1.1	4
60	Theoretical Investigation of the Reaction of Pyrene Formation from Fluoranthene. Journal of Physical Chemistry A, 2019, 123, 7491-7498.	1.1	4
61	Thermochemical and kinetic studies of hydrogen abstraction reaction from C16H10 isomers by H atoms. Computational and Theoretical Chemistry, 2021, 1201, 113257.	1.1	4
62	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
63	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
64	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
65	Reactivity of Ru oxides with air radiolysis products investigated by theoretical calculations. Journal of Nuclear Materials, 2022, 558, 153395.	1.3	3
66	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
67	IRSN R&D Actions on FP Behaviour for RCS, Containment and FCVS in Severe Accident Conditions. , 2016, , .		1
68	MS-CASPT2 study of the ground and low lying states of CsH+. Journal of Molecular Modeling, 2017, 23, 339.	0.8	1
69	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
70	Theoretical Study of the Monohydration of Mercury Compounds of Atmospheric Interest. Journal of Physical Chemistry A, 2021, 125, 5819-5828.	1.1	1
71	Understanding the Cu2+ adsorption mechanism on activated carbon using advanced statistical physics modelling. Environmental Science and Pollution Research, 2022, , 1.	2.7	1
72	Infrared matrix-isolation and theoretical studies of interactions between CH3I and water. Journal of Molecular Structure, 2021, 1236, 130342.	1.8	0

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73	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
74	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