Emilie CauÃ«t

List of Publications by Year
in descending order

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20 papers	724 citations	567281 15 h-index	752698 20 g-index
21 all docs	21 docs citations	21 times ranked	997 citing authors

#	Article	IF	Citations
1	Red Absorbing Cyclometalated Ir(III) Diimine Photosensitizers Competent for Hydrogen Photocatalysis. Inorganic Chemistry, 2022, 61, 5245-5254.	4.0	5
2	Accessing Photoredox Transformations with an Iron(III) Photosensitizer and Green Light. Journal of the American Chemical Society, 2021, 143, 15661-15673.	13.7	62
3	Excited-state behavior and photoinduced electron transfer of pH-sensitive Ir(III) complexes with cyclometallation (C/Nâ€“) ratios between 0/6 and 3/3. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 405, 112957.	3.9	8
4	Conceptual and Computational DFTâ€based In Silico Fragmentation Method for the Identification of Metabolite Mass Spectra. Chemistry Methods, 2021, 1, 101-115.	3.8	2
5	Mechanistic investigation of a visible light mediated dehalogenation/cyclisation reaction using iron(<scp>iii</scp>), iridium(<scp>iii</scp>) and ruthenium(<scp>ii</scp>) photosensitizers. Catalysis Science and Technology, 2021, 11, 8037-8051.	4.1	18
6	On the coupling of solvent characteristics to the electronic structure of solute molecules. Physical Chemistry Chemical Physics, 2014, 16, 3807.	2.8	2
7	Sequence dependence of electron-induced DNA strand breakage revealed by DNA nanoarrays. Scientific Reports, 2014, 4, 7391.	3.3	45
8	Electron-Attachment-Induced DNA Damage: Instantaneous Strand Breaks. Journal of Physical Chemistry B, 2013, 117, 9669-9676.	2.6	20
9	Near-Quantitative Agreement of Model-Free DFT-MD Predictions with XAFS Observations of the Hydration Structure of Highly Charged Transition-Metal Ions. Journal of Physical Chemistry Letters, 2012, 3, 2588-2593.	4.6	40
10	Ion Association in AlCl3 Aqueous Solutions from Constrained First-Principles Molecular Dynamics. Inorganic Chemistry, 2012, 51, 10856-10869.	4.0	15
11	Probing Electron-Induced Bond Cleavage at the Single-Molecule Level Using DNA Origami Templates. ACS Nano, 2012, 6, 4392-4399.	14.6	66
12	Conformations Consistent with Charge Migration Observed in DNA and RNA X-ray Structures. Journal of Biomolecular Structure and Dynamics, 2011, 28, 949-954.	3.5	13
13	Unique Hole-Trapping Property of the Human Telomere Sequence. Journal of Biomolecular Structure and Dynamics, 2011, 29, 557-561.	3.5	19
14	Influence of F^{â^'} Coordination on Al³⁺ Hydrolysis Reactions from Density Functional Theory Calculations. Journal of Physical Chemistry C, 2011, 115, 6910-6921.	3.1	18
15	Vertical Ionization Potentials of Nucleobases in a Fully Solvated DNA Environment. Journal of Physical Chemistry B, 2010, 114, 5886-5894.	2.6	69
16	Structure and dynamics of the hydration shells of the Zn2+ ion from ab initio molecular dynamics and combined ab initio and classical molecular dynamics simulations. Journal of Chemical Physics, 2010, 132, 194502.	3.0	95
17	Ab Initio Study of the Electron Transfer in an Ionized Stacked Complex of Guanines. Journal of Physical Chemistry A, 2009, 113, 9881-9890.	2.5	18
18	Radical Cations of the Nucleic Bases and Radiation Damage to DNA: Ab Initio Study. Advances in Quantum Chemistry, 2007, , 121-147.	0.8	26

#	Article	IF	Citations
19	Ab Initio Study of the Ionization of the DNA Bases:â€‰ Ionization Potentials and Excited States of the Cations. Journal of Physical Chemistry A, 2006, 110, 9200-9211.	2.5	73
20	Histidineâˆ’Aromatic Interactions in Proteins and Proteinâˆ’Ligand Complexes:â€‰ Quantum Chemical Study of X-ray and Model Structures. Journal of Chemical Theory and Computation, 2005, 1, 472-483.	5.3	110