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	Histidineâ^'Aromatic Interactions in Proteins and Proteinâ^'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
2	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
3	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
4	Vertical Ionization Potentials of Nucleobases in a Fully Solvated DNA Environment. Journal of Physical Chemistry B, 2010, 114, 5886-5894.	2.6	69
5	Probing Electron-Induced Bond Cleavage at the Single-Molecule Level Using DNA Origami Templates. ACS Nano, 2012, 6, 4392-4399.	14.6	66
6	Accessing Photoredox Transformations with an Iron(III) Photosensitizer and Green Light. Journal of the American Chemical Society, 2021, 143, 15661-15673.	13.7	62
7	Sequence dependence of electron-induced DNA strand breakage revealed by DNA nanoarrays. Scientific Reports, 2014, 4, 7391.	3.3	45
8	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
9	Radical Cations of the Nucleic Bases and Radiation Damage to DNA: Ab Initio Study. Advances in Quantum Chemistry, 2007, , 121-147.	0.8	26
10	Electron-Attachment-Induced DNA Damage: Instantaneous Strand Breaks. Journal of Physical Chemistry B, 2013, 117, 9669-9676.	2.6	20
11	Unique Hole-Trapping Property of the Human Telomere Sequence. Journal of Biomolecular Structure and Dynamics, 2011, 29, 557-561.	3.5	19
12	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
13	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
14	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
15	Ion Association in AlCl3 Aqueous Solutions from Constrained First-Principles Molecular Dynamics. Inorganic Chemistry, 2012, 51, 10856-10869.	4.0	15
16	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
17	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
18	Red Absorbing Cyclometalated Ir(III) Diimine Photosensitizers Competent for Hydrogen Photocatalysis. Inorganic Chemistry, 2022, 61, 5245-5254.	4.0	5

#	Article	IF	Citations
19	On the coupling of solvent characteristics to the electronic structure of solute molecules. Physical Chemistry Chemical Physics, 2014, 16, 3807.	2.8	2
20	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