

Olivier Holtomo

List of Publications by Year in descending order

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Version: 2024-02-01

12
papers

52
citations

1937685

4
h-index

1588992

8
g-index

12
all docs

12
docs citations

12
times ranked

41
citing authors

#	ARTICLE	IF	CITATIONS
1	DFT study of the effect of solvent on the H-atom transfer involved in the scavenging of the free radicals $\dot{\text{O}}_2$ and $\dot{\text{O}}_2^-$ by caffeic acid phenethyl ester and some of its derivatives. <i>Journal of Molecular Modeling</i> , 2014, 20, 2509.	1.8	21
2	DFT Study of Photochemical Properties and Radiative Forcing Efficiency Features of the Stereoisomers <i>cis</i> - and <i>trans</i> - $\text{CHCl}-\text{CH}=\text{CF}_3$. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10437-10445.	2.5	11
3	Structure, antioxidative potency and potential scavenging of OH and OOH of phenylethyl-3,4-dihydroxyhydrocinnamate in protic and aprotic media: DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 78, 221-233.	2.4	7
4	Thermodynamic of solvation, solute \rightarrow Solvent electron transfer and ionization potential of BSCAPE molecule and its UV-vis spectra in aqueous solution. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 92, 100-111.	2.4	5
5	Infrared spectra of PEHA molecule and its resistance to oxidation in water and methanol media at 298.15 K: solvent cluster size dependency. <i>Journal of Molecular Modeling</i> , 2020, 26, 323.	1.8	3
6	Basis set dependence of $1\text{H}-X$ spin-spin coupling constants in non-empirical pure DFT framework, $X = 1\text{H}, 13\text{C}, 19\text{F}, 35\text{Cl}$: Case of $\text{CHCl}=\text{CH}=\text{CF}_3$ stereoisomers. <i>AIP Advances</i> , 2021, 11, .	1.3	2
7	Insight and performance of LC-DFT vs DFT in the NMR shielding and chemical shift calculations: Case of $\text{CHCl}=\text{CH}=\text{CF}_3$. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26408.	2.0	1
8	Insight of UV-vis spectra and atmospheric implication for the reaction of $\dot{\text{E}}^{\text{TM}}\text{OH}$ radical towards glyphosate herbicide and its hydrates. <i>RSC Advances</i> , 2021, 11, 16404-16418.	3.6	1
9	Infrared absorption cross section and radiative forcing efficiency features of four hydrofluoropolyethers: Performance of some DFT functionals. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113798.	2.5	1
10	Temperature-dependent oxidation of BSCAPE molecule in methanol medium. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107850.	2.4	0
11	Theoretical investigation of the atmospheric implication for the reaction of $\dot{\text{C}}\text{OH}$ radical with $\text{CF}_2\text{C}(\text{CH}_3)-\text{CX}_3$, $\text{X} = \text{H}, \text{F}$. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 106, 107905.	2.4	0
12	Reaction of $\dot{\text{C}}\text{OH}$ with $\text{CHCl}=\text{CH}-\text{CHF}_2$ and its atmospheric implication for future environmental-friendly refrigerant. <i>Pure and Applied Chemistry</i> , 2021, .	1.9	0