Julio C S Da Silva

List of Publications by Year
in descending order

23 papers	340 citations	933447 10 h-index	839539 18 g-index
23 all docs	23 docs citations	23 times ranked	559 citing authors

#	Article	IF	Citations
1	A combined experimental and computational study of novel nanocage-based metalâ€“organic frameworks for drug delivery. Dalton Transactions, 2015, 44, 19370-19382.	3.3	83
2	A radical rebound mechanism for the methane oxidation reaction promoted by the dicopper center of a pMMO enzyme: a computational perspective. Dalton Transactions, 2016, 45, 2492-2504.	3.3	40
3	Impact of the Molecular Environment on Thiolâ€“Ene Coupling For Biofunctionalization and Conjugation. Bioconjugate Chemistry, 2016, 27, 2111-2123.	3.6	39
4	Single-Amino Acid Modifications Reveal Additional Controls on the Proton Pathway of [FeFe]-Hydrogenase. Biochemistry, 2016, 55, 3165-3173.	2.5	29
5	Phosphorane lifetime and stereo-electronic effects along the alkaline hydrolysis of phosphate esters. Physical Chemistry Chemical Physics, 2016, 18, 18255-18267.	2.8	16
6	Molecular interaction of sulfonamides and ovalbumin, an allergenic egg protein, exploring biophysical, theoretical and biological studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117747.	3.9	14
7	DFT study of the full catalytic cycle for the propene hydroformylation catalyzed by a heterobimetallic HPt(SnCl₃)(PH₃)₂ model catalyst. Journal of Computational Chemistry, 2010, 31, 1986-2000.	3.3	13
8	Câ^'H Bond Activation of Methane Promoted by (Î·5-Phospholyl)Rh(CO)2:â€‰ A Theoretical Perspective. Organometallics, 2005, 24, 2262-2268.	2.3	12
9	Theoretical investigation of the structure and nature of the interaction in metalâ€“alkane Ïƒ-complexes of the type [M(CO)5(C2H6)] (M = Cr, Mo, and W). Chemical Physics, 2009, 365, 85-93.	1.9	12
10	QUANTUM CHEMICAL STUDY OF CISPLATIN-WATER COMPLEXES: AN INVESTIGATION OF ELECTRON CORRELATION EFFECTS. Journal of Theoretical and Computational Chemistry, 2011, 10, 371-391.	1.8	12
11	A rainbow multielectrochromic copolymer based on 2,5-di(thienyl)pyrrole derivative bearing a dansyl substituent and 3,4-ethylenedioxythiophene. Synthetic Metals, 2020, 269, 116545.	3.9	10
12	Multielectrochromic amide-based poly(2,5-dithienylpyrrole) bearing a fluorene derivative: Synthesis, characterization, and optoelectronic properties. Electrochimica Acta, 2021, 379, 138173.	5.2	10
13	Cï£¿H bond activation of methane in aqueous solution: A hybrid quantum mechanical/effective fragment potential study. Journal of Computational Chemistry, 2011, 32, 3383-3392.	3.3	9
14	Propene Hydroformylation Reaction Catalyzed by HRh(CO)(BISBI): A Thermodynamic and Kinetic Analysis of the Full Catalytic Cycle. European Journal of Inorganic Chemistry, 2020, 2020, 3907-3916.	2.0	9
15	Theoretical investigation of the neutral hydrolysis of diethyl 4-nitrophenyl phosphate (paraoxon) in aqueous solution. Journal of Molecular Modeling, 2018, 24, 259.	1.8	8
16	Ab initio thermodynamic study of the reaction of CF2Cl2 and CHF2Cl CFCs species with OH radical. Chemical Physics Letters, 2007, 448, 164-172.	2.6	7
17	Base Mechanism to the Hydrolysis of Phosphate Triester Promoted by the Cd²⁺/Cd²⁺ Active site of Phosphotriesterase: A Computational Study. Inorganic Chemistry, 2018, 57, 5888-5902.	4.0	6
18	AN EVALUATION OF QUANTUM CHEMICAL CALCULATIONS OF REACTION ENERGIES FOR CATALYTIC ACTIVATION PROCESSES: THE ACTIVATION OF PROPANE BY A RHODIUM CATALYST REVISITED. Journal of Theoretical and Computational Chemistry, 2012, 11, 297-312.	1.8	5

#	Article	IF	Citations
19	Insights into the coordination chemistry of alkanes to metal carbonyls from quantum chemical calculations. Journal of Organometallic Chemistry, 2015, 793, 241-247.	1.8	3
20	SISTEMAS DE INCENTIVOS GERENCIAIS E O DESEMPENHO ECONÃ”MICO-FINANCEIRO DAS EMPRESAS BRASILEIRAS. Advances in Scientific and Applied Accounting, 2019, 12, 082-100.	0.2	2
21	Medicinal Electrochemistry of Halogenated and Nitrated Pterocarpanquinones. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
22	Estudo de ProspecÃ§Ã£o em QuÃmica Computacional. Cadernos De ProspecÃ§Ã£o, 2019, 12, 538.	0.1	0
23	Refining details of the structural and electronic properties of the Cu_B site in pMMO enzyme through sequential molecular dynamics/CPKS-EPR calculations. Physical Chemistry Chemical Physics, 0, , .	2.8	0