

Douglas Henrique Pereira

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/6080658/publications.pdf>

Version: 2024-02-01

45
papers

601
citations

623734

14
h-index

642732

23
g-index

46
all docs

46
docs citations

46
times ranked

437
citing authors

#	ARTICLE	IF	CITATIONS
1	Peracetic acid: Structural elucidation for applications in wastewater treatment. <i>Water Research</i> , 2020, 168, 115143.	11.3	76
2	DFT study of the application of polymers cellulose and cellulose acetate for adsorption of metal ions (Cd ²⁺ , Cu ²⁺ and Cr ³⁺) potentially toxic. <i>Polymer Bulletin</i> , 2020, 77, 3443-3456.	3.3	54
3	A DFT-based analysis of adsorption of Cd ²⁺ , Cr ³⁺ , Cu ²⁺ , Hg ²⁺ , Pb ²⁺ , and Zn ²⁺ , on vanillin monomer: a study of the removal of metal ions from effluents. <i>Journal of Molecular Modeling</i> , 2019, 25, 267.	1.8	38
4	New Perspectives on the Role of Frontier Molecular Orbitals in the Study of Chemical Reactivity: A Review. <i>Revista Virtual De Quimica</i> , 2016, 8, 425-453.	0.4	34
5	Fenton-type process using peracetic acid: Efficiency, reaction elucidations and ecotoxicity. <i>Journal of Hazardous Materials</i> , 2021, 403, 123949.	12.4	32
6	Implementation of pseudopotential in the G3 theory for molecules containing first-, second-, and non-transition third-row atoms. <i>Journal of Chemical Physics</i> , 2011, 135, 034106.	3.0	24
7	G4CEP: A G4 theory modification by including pseudopotential for molecules containing first-, second- and third-row representative elements. <i>Journal of Chemical Physics</i> , 2016, 144, 204118.	3.0	21
8	Formation of Ag nanoparticles under electron beam irradiation: Atomistic origins from first-principles calculations. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25551.	2.0	21
9	Removal of fatty acid by natural and modified bentonites: Elucidation of adsorption mechanism. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 605, 125340.	4.7	19
10	Assessment of G3(MP2)//B3 theory including a pseudopotential for molecules containing first-, second-, and third-row representative elements. <i>Journal of Chemical Physics</i> , 2013, 139, 184108.	3.0	17
11	A study of the rotational barriers for some organic compounds using the G3 and G3CEP theories. <i>Journal of Molecular Modeling</i> , 2014, 20, 2199.	1.8	17
12	Theoretical insights about the possibility of removing Pb ²⁺ and Hg ²⁺ metal ions using adsorptive processes and matrices of carboxymethyl diethylaminoethyl cellulose and cellulose nitrate biopolymers. <i>Journal of Molecular Liquids</i> , 2021, 331, 115730.	4.9	17
13	When treatment increases the contaminant's ecotoxicity: A study of the Fenton process in the degradation of methylene blue. <i>Chemosphere</i> , 2021, 283, 131117.	8.2	17
14	Thermal and Solvent Effects On NMR Indirect Spin-Spin Coupling Constants of a Prototypical Chagas Disease Drug. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13504-13512.	2.5	16
15	Carboxymethylcellulose and cellulose xanthate matrices as potential adsorbent material for potentially toxic Cr ³⁺ , Cu ²⁺ and Cd ²⁺ -metal ions: a theoretical study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	16
16	Effect of dimethyl sulfoxide intercalation into kaolinite on etheramine adsorption: experimental and theoretical investigation. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 105503.	6.7	14
17	Understanding the substituent effect on the acidity of alcohols and <i>p</i> -substituted phenols. <i>Molecular Simulation</i> , 2009, 35, 1269-1278.	2.0	13
18	W1CEP theory for computational thermochemistry. <i>Computational and Theoretical Chemistry</i> , 2015, 1067, 84-92.	2.5	13

#	ARTICLE	IF	CITATIONS
19	Theoretical-experimental study of the advanced oxidative process using peracetic acid and solar radiation: Removal efficiency and thermodynamic elucidation of radical formation processes. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 423, 113615.	3.9	13
20	Energy potential of biomass from two types of genetically improved rice husks in Brazil: A theoretical-experimental study. Biomass and Bioenergy, 2020, 142, 105816.	5.7	12
21	Synthesis, crystallographic studies, molecular modeling and in vitro biological studies of silver(I) complexes with aminoadamantane ligands. Polyhedron, 2019, 173, 114116.	2.2	11
22	Synthesis, crystal structures, DFT studies, antibacterial assays and interaction assessments with biomolecules of new platinum(II) complexes with adamantane derivatives. New Journal of Chemistry, 2020, 44, 11546-11556.	2.8	11
23	Synthesis, spectroscopic characterization and in vitro antibacterial and antiviral activities of novel silver(I) complexes with mafenide and ethyl-mafenide. Journal of Molecular Structure, 2021, 1246, 131261.	3.6	9
24	G3(MP2)-CEP theory and applications for compounds containing atoms from representative first, second and third row elements of the periodic table. Journal of Molecular Modeling, 2015, 21, 204.	1.8	8
25	Phe-Phe Di-Peptide Nanostructure Self-Assembling Modulated by Luminescent Additives. ACS Omega, 2019, 4, 606-619.	3.5	8
26	Carbonate anion photolyzed by solar radiation or combined with peracetic acid to form reactive species for dye degradation. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 420, 113511.	3.9	8
27	An energetic analysis of the Diels-Alder endo:exo selectivity reaction by using composite methods. Computational and Theoretical Chemistry, 2018, 1123, 161-168.	2.5	7
28	Computational study of the interaction of heavy metal ions, Cd(II), Hg(II), and Pb(II) on lignin matrices. Journal of Molecular Graphics and Modelling, 2022, 111, 108080.	2.4	7
29	Chemical, spectroscopic characterization, molecular modeling and antibacterial activity assays of a silver (I) complex with succinic acid. Ecletica Quimica, 2021, 46, 26-35.	0.5	6
30	Plant and Bacterial Cellulose: Production, Chemical Structure, Derivatives and Applications. Orbital, 2019, 11, .	0.3	6
31	Theoretical study of the internal rotational barriers of fluorine, chlorine, bromine, and iodine-substituted ethanes. Computational and Theoretical Chemistry, 2019, 1166, 112589.	2.5	4
32	Adsorptive capacity of a g-C ₃ N ₄ matrix for thiamethoxam removal: A DFT study. Computational and Theoretical Chemistry, 2022, 1215, 113816.	2.5	4
33	Theoretical study of internal rotational barriers of electrons donating and electrons withdrawing groups in aromatic compounds. Heliyon, 2020, 6, e04957.	3.2	3
34	Interaction of glyphosate in matrices of cellulose and diethylaminoethyl cellulose biopolymers: theoretical viewpoint of the adsorption process. Journal of Molecular Modeling, 2021, 27, 272.	1.8	3
35	A novel water-soluble platinum(II) complex with the amino acid deoxyalliin: synthesis, crystal structure, theoretical studies and investigations about its antibacterial activity. Journal of Molecular Structure, 2021, 1236, 130316.	3.6	2
36	Interaction of Fe ²⁺ , Co ²⁺ , Ni ²⁺ , Cu ²⁺ , Zn ²⁺ , Pb ²⁺ , and Cr ³⁺ metal ions on B ₁₂ N ₁₂ fullerene-like cages: a theoretical study. Monatshefte für Chemie, 2021, 152, 915-922.	1.8	2

#	ARTICLE	IF	CITATIONS
37	Theoretical study of glyphosate adsorption potential on methylcellulose and cellulose xanthate matrices compared to activated carbon: role of biopolymers in the adsorption process. Polymer Bulletin, 2022, 79, 9331-9344.	3.3	2
38	Caracterização da biomassa de bagaço de cana-de-açúcar com vistas energéticas. ForScience, 2021, 9, e00928.	0.1	1
39	Fenton Processes in Dye Removal. Sustainable Textiles, 2022, , 21-36.	0.7	1
40	Theoretical insights into the possibility of removing CH ₃ Hg ⁺ using different adsorptive matrices: g-C ₃ N ₄ , cellulose xanthate, and vanillin-derived modified monomer. Journal of Molecular Liquids, 2022, 361, 119691.	4.9	1
41	Photoluminescence of Solvent-Selected Fluorescent Moieties in MEH-PPV Solutions and Films. Journal of the Brazilian Chemical Society, 2017, , .	0.6	0
42	Quantum Theory: An Approach Quantized on its Evolution - Part I. Revista Virtual De Química, 2016, 8, 319-337.	0.4	0
43	Cálculos teóricos para elucidar o efeito eletrônica de barreiras rotacionais: teoria e aplicações. Journal of Biotechnology and Biodiversity, 2020, 8, 136-147.	0.1	0
44	Emprego de compostos naturais para a obtenção e projeto de um produto destinado ao tratamento de resíduos de instalações zootécnicas. Research, Society and Development, 2020, 9, e830974519.	0.1	0
45	Análise sensorial de bebida láctea de cupuaçu. Research, Society and Development, 2020, 9, e9749109441.	0.1	0