

# Douglas Henrique Pereira

## List of Publications by Year in descending order

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45  
papers

601  
citations

623188

14  
h-index

642321

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.	5.3	76
2	DFT study of the application of polymers cellulose and cellulose acetate for adsorption of metal ions (Cd <sup>2+</sup> , Cu <sup>2+</sup> and Cr <sup>3+</sup> ) potentially toxic. <i>Polymer Bulletin</i> , 2020, 77, 3443-3456.	1.7	54
3	A DFT-based analysis of adsorption of Cd <sup>2+</sup> , Cr <sup>3+</sup> , Cu <sup>2+</sup> , Hg <sup>2+</sup> , Pb <sup>2+</sup> , and Zn <sup>2+</sup> , on vanillin monomer: a study of the removal of metal ions from effluents. <i>Journal of Molecular Modeling</i> , 2019, 25, 267.	0.8	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.	0.1	34
5	Fenton-type process using peracetic acid: Efficiency, reaction elucidations and ecotoxicity. <i>Journal of Hazardous Materials</i> , 2021, 403, 123949.	6.5	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.	1.2	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.	1.2	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.	1.0	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.	2.3	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.	1.2	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.	0.8	17
12	Theoretical insights about the possibility of removing Pb <sup>2+</sup> and Hg <sup>2+</sup> metal ions using adsorptive processes and matrices of carboxymethyl diethylaminoethyl cellulose and cellulose nitrate biopolymers. <i>Journal of Molecular Liquids</i> , 2021, 331, 115730.	2.3	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.	4.2	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.	1.1	16
15	Carboxymethylcellulose and cellulose xanthate matrices as potential adsorbent material for potentially toxic Cr <sup>3+</sup> , Cu <sup>2+</sup> and Cd <sup>2+</sup> -metal ions: a theoretical study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	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.	3.3	14
17	Understanding the substituent effect on the acidity of alcohols and <i>i</i> -substituted phenols. <i>Molecular Simulation</i> , 2009, 35, 1269-1278.	0.9	13
18	W1CEP theory for computational thermochemistry. <i>Computational and Theoretical Chemistry</i> , 2015, 1067, 84-92.	1.1	13

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19	Theoretical-experimental study of the advanced oxidative process using peracetic acid and solar radiation: Removal efficiency and thermodynamic elucidation of radical formation processes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 423, 113615.	2.0	13
20	Energy potential of biomass from two types of genetically improved rice husks in Brazil: A theoretical-experimental study. <i>Biomass and Bioenergy</i> , 2020, 142, 105816.	2.9	12
21	Synthesis, crystallographic studies, molecular modeling and in vitro biological studies of silver(I) complexes with aminoadamantane ligands. <i>Polyhedron</i> , 2019, 173, 114116.	1.0	11
22	Synthesis, crystal structures, DFT studies, antibacterial assays and interaction assessments with biomolecules of new platinum(II) complexes with adamantane derivatives. <i>New Journal of Chemistry</i> , 2020, 44, 11546-11556.	1.4	11
23	Synthesis, spectroscopic characterization and in vitro antibacterial and antiviral activities of novel silver(I) complexes with mafenide and ethyl-mafenide. <i>Journal of Molecular Structure</i> , 2021, 1246, 131261.	1.8	9
24	G3(MP2)-CEP theory and applications for compounds containing atoms from representative first, second and third row elements of the periodic table. <i>Journal of Molecular Modeling</i> , 2015, 21, 204.	0.8	8
25	Phe-Phe Di-Peptide Nanostructure Self-Assembling Modulated by Luminescent Additives. <i>ACS Omega</i> , 2019, 4, 606-619.	1.6	8
26	Carbonate anion photolyzed by solar radiation or combined with peracetic acid to form reactive species for dye degradation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 420, 113511.	2.0	8
27	An energetic analysis of the Diels-Alder endo:exo selectivity reaction by using composite methods. <i>Computational and Theoretical Chemistry</i> , 2018, 1123, 161-168.	1.1	7
28	Computational study of the interaction of heavy metal ions, Cd(II), Hg(II), and Pb(II) on lignin matrices. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 111, 108080.	1.3	7
29	Chemical, spectroscopic characterization, molecular modeling and antibacterial activity assays of a silver (I) complex with succinic acid. <i>Eletica Quimica</i> , 2021, 46, 26-35.	0.2	6
30	Plant and Bacterial Cellulose: Production, Chemical Structure, Derivatives and Applications. <i>Orbital</i> , 2019, 11, .	0.1	6
31	Theoretical study of the internal rotational barriers of fluorine, chlorine, bromine, and iodine-substituted ethanes. <i>Computational and Theoretical Chemistry</i> , 2019, 1166, 112589.	1.1	4
32	Adsorptive capacity of a g-C <sub>3</sub> N <sub>4</sub> matrix for thiamethoxam removal: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113816.	1.1	4
33	Theoretical study of internal rotational barriers of electrons donating and electrons withdrawing groups in aromatic compounds. <i>Heliyon</i> , 2020, 6, e04957.	1.4	3
34	Interaction of glyphosate in matrices of cellulose and diethylaminoethyl cellulose biopolymers: theoretical viewpoint of the adsorption process. <i>Journal of Molecular Modeling</i> , 2021, 27, 272.	0.8	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. <i>Journal of Molecular Structure</i> , 2021, 1236, 130316.	1.8	2
36	Interaction of Fe <sup>2+</sup> , Co <sup>2+</sup> , Ni <sup>2+</sup> , Cu <sup>2+</sup> , Zn <sup>2+</sup> , Pb <sup>2+</sup> , and Cr <sup>3+</sup> metal ions on B <sub>12</sub> N <sub>12</sub> fullerene-like cages: a theoretical study. <i>Monatshefte für Chemie</i> , 2021, 152, 915-922.	0.9	2

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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.	1.7	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.	0.4	1
40	Theoretical insights into the possibility of removing CH <sub>3</sub> Hg <sup>+</sup> using different adsorptive matrices: g-C <sub>3</sub> N <sub>4</sub> , cellulose xanthate, and vanillin-derived modified monomer. Journal of Molecular Liquids, 2022, 361, 119691.	2.3	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.	0.1	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.	0.0	0
45	Análise sensorial de bebida láctea de cupuaçu. Research, Society and Development, 2020, 9, e9749109441.	0.0	0