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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	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
2	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.	2.0	13
3	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.	1.3	7
4	Fenton Processes in Dye Removal. Sustainable Textiles, 2022, , 21-36.	0.4	1
5	Theoretical insights into the possibility of removing CH3Hg+ using different adsorptive matrices: g-C3N4, cellulose xanthate, and vanillin-derived modified monomer. Journal of Molecular Liquids, 2022, 361, 119691.	2.3	1
6	Adsorptive capacity of a g-C3N4 matrix for thiamethoxam removal: A DFT study. Computational and Theoretical Chemistry, 2022, 1215, 113816.	1.1	4
7	Fenton-type process using peracetic acid: Efficiency, reaction elucidations and ecotoxicity. Journal of Hazardous Materials, 2021, 403, 123949.	6.5	32
8	CaracterizaÃ§Ã£o da biomassa de bagaÃ§o de cana-de-aÃ§Ãºcar com vistas energÃ©ticas. ForScience, 2021, 9, e00928.	0.1	1
9	Chemical, spectroscopic characterization, molecular modeling and antibacterial activity assays of a silver (I) complex with succinic acid. Ecletica Quimica, 2021, 46, 26-35.	0.2	6
10	Theoretical insights about the possibility of removing Pb2+ and Hg2+ metal ions using adsorptive processes and matrices of carboxymethyl diethylaminoethyl cellulose and cellulose nitrate biopolymers. Journal of Molecular Liquids, 2021, 331, 115730.	2.3	17
11	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.	1.8	2
12	Interaction of Fe2+, Co2+, Ni2+, Cu2+, Zn2+, Pb2+, and Cr3+ metal ions on B12N12 fullerene-like cages: a theoretical study. Monatshefte FÃ¼r Chemie, 2021, 152, 915-922.	0.9	2
13	Effect of dimethyl sulfoxide intercalation into kaolinite on etheramine adsorption: experimental and theoretical investigation. Journal of Environmental Chemical Engineering, 2021, 9, 105503.	3.3	14
14	Interaction of glyphosate in matrices of cellulose and diethylaminoethyl cellulose biopolymers: theoretical viewpoint of the adsorption process. Journal of Molecular Modeling, 2021, 27, 272.	0.8	3
15	When treatment increases the contaminant's ecotoxicity: A study of the Fenton process in the degradation of methylene blue. Chemosphere, 2021, 283, 131117.	4.2	17
16	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.	2.0	8
17	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.	1.8	9
18	Peracetic acid: Structural elucidation for applications in wastewater treatment. Water Research, 2020, 168, 115143.	5.3	76

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19	DFT study of the application of polymers cellulose and cellulose acetate for adsorption of metal ions (Cd2+, Cu2+ and Cr3+) potentially toxic. Polymer Bulletin, 2020, 77, 3443-3456.	1.7	54
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.	2.9	12
21	Theoretical study of internal rotational barriers of electrons donating and electrons withdrawing groups in aromatic compounds. Heliyon, 2020, 6, e04957.	1.4	3
22	Removal of fatty acid by natural and modified bentonites: Elucidation of adsorption mechanism. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2020, 605, 125340.	2.3	19
23	Carboxymethylcellulose and cellulose xanthate matrices as potential adsorbent material for potentially toxic Cr3+, Cu2+ and Cd2+metal ions: a theoretical study. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	16
24	Synthesis, crystal structures, DFT studies, antibacterial assays and interaction assessments with biomolecules of new platinum(<scp>ii</scp>) complexes with adamantane derivatives. New Journal of Chemistry, 2020, 44, 11546-11556.	1.4	11
25	CÃ¡lculos teÃ³ricos para elucidaÃ§Ã£o eletrÃ´nica de barreiras rotacionais: teoria e aplicaÃ§Ãµes. Journal of Biotechnology and Biodiversity, 2020, 8, 136-147.	0.1	0
26	Emprego de compostos naturais para a obtenÃ§Ã£o e projeÃ§Ã£o de um produto destinado ao tratamento de resÃduos de instalaÃ§Ãµes zootÃ©cnicas. Research, Society and Development, 2020, 9, e830974519.	0.0	0
27	AnÃ¡lise sensorial de bebida lÃ¡ctea de cupuaÃ§u. Research, Society and Development, 2020, 9, e9749109441.	0.0	0
28	A DFT-based analysis of adsorption of Cd2+, Cr3+, Cu2+, Hg2+, Pb2+, and Zn2+, on vanillin monomer: a study of the removal of metal ions from effluents. Journal of Molecular Modeling, 2019, 25, 267.	0.8	38
29	Synthesis, crystallographic studies, molecular modeling and in vitro biological studies of silver(I) complexes with aminoadamantane ligands. Polyhedron, 2019, 173, 114116.	1.0	11
30	Theoretical study of the internal rotational barriers of fluorine, chlorine, bromine, and iodine-substituted ethanes. Computational and Theoretical Chemistry, 2019, 1166, 112589.	1.1	4
31	Pheâ€“Phe Di-Peptide Nanostructure Self-Assembling Modulated by Luminescent Additives. ACS Omega, 2019, 4, 606-619.	1.6	8
32	Plant and Bacterial Cellulose: Production, Chemical Structure, Derivatives and Applications. Orbital, 2019, 11, .	0.1	6
33	An energetic analysis of the Diels-Alder endo:exo selectivity reaction by using composite methods. Computational and Theoretical Chemistry, 2018, 1123, 161-168.	1.1	7
34	Formation of Ag nanoparticles under electron beam irradiation: Atomistic origins from firstâ€principles calculations. International Journal of Quantum Chemistry, 2018, 118, e25551.	1.0	21
35	Photoluminescence of Solvent-Selected Fluorescent Moieties in MEH-PPV Solutions and Films. Journal of the Brazilian Chemical Society, 2017, , .	0.6	0
36	G4CEP: A G4 theory modification by including pseudopotential for molecules containing first-, second- and third-row representative elements. Journal of Chemical Physics, 2016, 144, 204118.	1.2	21

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37	New Perspectives on the Role of Frontier Molecular Orbitals in the Study of Chemical Reactivity: A Review. Revista Virtual De Quimica, 2016, 8, 425-453.	0.1	34
38	Quantum Theory: An Approach Quantized on its Evolution - Part I. Revista Virtual De Quimica, 2016, 8, 319-337.	0.1	0
39	W1CEP theory for computational thermochemistry. Computational and Theoretical Chemistry, 2015, 1067, 84-92.	1.1	13
40	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.	0.8	8
41	A study of the rotational barriers for some organic compounds using the G3 and G3CEP theories. Journal of Molecular Modeling, 2014, 20, 2199.	0.8	17
42	Assessment of G3(MP2)//B3 theory including a pseudopotential for molecules containing first-, second-, and third-row representative elements. Journal of Chemical Physics, 2013, 139, 184108.	1.2	17
43	Thermal and Solvent Effects On NMR Indirect Spinâ€“Spin Coupling Constants of a Prototypical Chagas Disease Drug. Journal of Physical Chemistry A, 2011, 115, 13504-13512.	1.1	16
44	Implementation of pseudopotential in the G3 theory for molecules containing first-, second-, and non-transition third-row atoms. Journal of Chemical Physics, 2011, 135, 034106.	1.2	24
45	Understanding the substituent effect on the acidity of alcohols andpara-substituted phenols. Molecular Simulation, 2009, 35, 1269-1278.	0.9	13