

Joaquã-n Barroso-Flores

List of Publications by Year in descending order

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44
papers

560
citations

759233

12
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677142

22
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48
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48
docs citations

48
times ranked

844
citing authors

#	ARTICLE	IF	CITATIONS
1	A water-stable luminescent Zn-MOF based on a conjugated π -electron ligand as an efficient sensor for atorvastatin and its application in pharmaceutical samples. <i>Journal of Materials Chemistry C</i> , 2022, 10, 5944-5955.	5.5	10
2	A boron, nitrogen-containing heterocyclic carbene (BNC) as a redox active ligand: synthesis and characterization of a lithium BNC-aurate complex. <i>Dalton Transactions</i> , 2022, 51, 7899-7906.	3.3	2
3	Impact of secondary salts, temperature, and pH on the colloidal stability of graphene oxide in water. <i>Nanoscale Advances</i> , 2022, 4, 2435-2443.	4.6	6
4	Synthesis, Optical Characterization in Solution and Solid-State, and DFT Calculations of 3-Acetyl and 3-(1- β -(2-Phenylhydrazono)ethyl)-coumarin-(7)-substituted Derivatives. <i>Molecules</i> , 2022, 27, 3677.	3.8	2
5	Electronic Structure Effects Related to the Origin of the Remarkable Near-Infrared Absorption of <i>Blastochloris viridis</i> Light Harvesting 1-Reaction Center Complex. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4555-4564.	5.3	2
6	Electrochemical reactivity of S-phenacyl-O-ethyl-xanthates in hydroalcoholic (MeOH/H ₂ O 4:1) and anhydrous acetonitrile media. <i>Electrochimica Acta</i> , 2021, 380, 138239.	5.2	2
7	Evaluation of Antiproliferative Palladium(II) Complexes of Synthetic Bisdemethoxycurcumin towards In Vitro Cytotoxicity and Molecular Docking on DNA Sequence. <i>Molecules</i> , 2021, 26, 4369.	3.8	7
8	Chemosensing of neurotransmitters with selectivity and naked eye detection of <i>l</i> -DOPA based on fluorescent Zn(II)-terpyridine bearing boronic acid complexes. <i>Dalton Transactions</i> , 2021, 50, 4255-4269.	3.3	9
9	Proton to hydride umpolung at a phosphonium center <i>via</i> electron relay: a new strategy for main-group based water reduction. <i>Chemical Science</i> , 2021, 12, 15603-15608.	7.4	4
10	Hydrophobic unnatural base pairs show a Watson-Crick pairing in micro-second molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 4098-4106.	3.5	5
11	Effect of the degree of oxidation of graphene oxide on As(III) adsorption. <i>Journal of Hazardous Materials</i> , 2020, 384, 121440.	12.4	53
12	Production of few-layer graphene by wet media milling using organic solvents and different types of graphite. <i>Ceramics International</i> , 2020, 46, 2413-2420.	4.8	7
13	A Digallane Gold Complex with a 12-Electron Auride Center: Synthesis and Computational Studies. <i>Organometallics</i> , 2020, 39, 4372-4379.	2.3	2
14	Accurate Estimation of pK_b Values for Amino Groups from Surface Electrostatic Potential ($V_{S,min}$) Calculations: The Isoelectric Points of Amino Acids as a Case Study. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1445-1452.	5.4	23
15	Effect of UV radiation on the structure of graphene oxide in water and its impact on cytotoxicity and As(III) adsorption. <i>Chemosphere</i> , 2020, 249, 126160.	8.2	29
16	Fluorescence decay rate of selected compounds from <i>Eysenhardtia polystachya</i> extracts and their viability as biosensors. <i>Materials Science and Engineering C</i> , 2019, 104, 109978.	7.3	2
17	Calculation of $V_{S,max}$ and Its Use as a Descriptor for the Theoretical Calculation of pK_a Values for Carboxylic Acids. <i>Molecules</i> , 2019, 24, 79.	3.8	13
18	Long range $^1H^{19}F$ coupling through multiple bond in thienopyridines, isoquinolines and 2-aza-carbazoles derivatives. <i>Journal of Molecular Structure</i> , 2019, 1176, 562-566.	3.6	1

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19	Efficient fluorescent chemosensing of iodide based on a cationic meso-tetraarylporphyrin in pure water. <i>Sensors and Actuators B: Chemical</i> , 2019, 281, 462-470.	7.8	16
20	An Allosterically Regulated, Four-State Macrocyclic. <i>Inorganic Chemistry</i> , 2018, 57, 3568-3578.	4.0	14
21	Real-Time Visualization of Cell Membrane Damage Using Gadolinium–Schiff Base Complex-Doped Quantum Dots. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 35859-35868.	8.0	19
22	A Redox-Switchable, Allosteric Coordination Complex. <i>Journal of the American Chemical Society</i> , 2018, 140, 14590-14594.	13.7	18
23	Spectroscopic UV–Vis implications of an intramolecular I^{2+} –Mg coordination in bacteriochlorophyll <i>a</i> from the Fenna–Matthews–Olson complex. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25663.	2.0	3
24	Structural and dynamical instability of DNA caused by high occurrence of d5SICS and dNaM unnatural nucleotides. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10571-10580.	2.8	11
25	Evolution of the Fenna–Matthews–Olson Complex and Its Quantum Coherence Features. Which Led the Way?. <i>ACS Central Science</i> , 2017, 3, 1061-1062.	11.3	5
26	Molecular Group 13 Metallaborates Derived from $\text{M}^{\text{O}}\text{M}$ Cleavage Promoted by BH_3 . <i>Inorganic Chemistry</i> , 2017, 56, 7890-7899.	4.0	5
27	Aromatization of pyridinylidenes into pyridines is inhibited by exocyclic delocalization. A theoretical mechanistic assessment. <i>Tetrahedron</i> , 2016, 72, 4194-4200.	1.9	2
28	Synthesis and Crystal Structures of Stable 4-Aryl-2-(trichloromethyl)-1,3-diaza-1,3-butadienes. <i>Synthesis</i> , 2016, 48, 2205-2212.	2.3	5
29	In silico design of calixarene-based arsenic acid removal agents. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2016, 85, 169-174.	1.6	2
30	Reactivity of electrophilic chlorine atoms due to σ^* -holes: a mechanistic assessment of the chemical reduction of a trichloromethyl group by sulfur nucleophiles. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27300-27307.	2.8	9
31	A mixed DFT^{MD} methodology for the <i>in silico</i> development of drug releasing macrocycles. Calix and thia-calix[n]arenes as carriers for Bosutinib and Sorafenib. <i>Journal of Computational Chemistry</i> , 2016, 37, 940-946.	3.3	9
32	Synthesis and Crystal Structure of the First Selenonyl Bis(carboxylate) $\text{SeO}_2(\text{O}_2\text{CCH}_3)_2$. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 2923-2927.	2.0	2
33	Sensitive water-soluble fluorescent chemosensor for chloride based on a bisquinolinium pyridine-dicarboxamide compound. <i>Sensors and Actuators B: Chemical</i> , 2015, 221, 1348-1355.	7.8	33
34	Theoretical Assessment of the Selective Fluorescence Quenching of 1-Amino-8-naphthol-3,6-disulfonic Acid (H-Acid) Complexes with Zn^{2+} , Cd^{2+} , and Hg^{2+} : A DFT and TD-DFT Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 12178-12183.	2.5	12
35	Calix[n]arene-based drug carriers: A DFT study of their electronic interactions with a chemotherapeutic agent used against leukemia. <i>Computational and Theoretical Chemistry</i> , 2014, 1035, 84-91.	2.5	24
36	A Multi-State, Allosterically-Regulated Molecular Receptor With Switchable Selectivity. <i>Journal of the American Chemical Society</i> , 2014, 136, 10340-10348.	13.7	78

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37	In Silico Design of Monomolecular Drug Carriers for the Tyrosine Kinase Inhibitor Drug Imatinib Based on Calix- and Thiacalix[n]arene Host Molecules: A DFT and Molecular Dynamics Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 825-834.	5.3	26
38	Ab initio calculations of electronic interactions in inclusion complexes of calix- and thiacalix[n]arenes and block s cations. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2013, 75, 39-46.	1.6	3
39	Selective Optical Sensing of Hg(II) in Aqueous Media by H-Acid/SBA-15: A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 9281-9289.	3.1	41
40	Molecular Heterobimetallic Aluminoxanes and Aluminoxane Sulfides Containing Group 4 Metals. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 2849-2857.	2.0	12
41	Synthesis of new β -lactones from preactivated monosubstituted pyrazines and TMS- α -ketene acetals. <i>Canadian Journal of Chemistry</i> , 2012, 90, 469-482.	1.1	10
42	Influence of intramolecular Sn \cdots chalcogen interactions on the conformational preferences for three diorganotin(IV) xanthates. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4937-4944.	1.8	2
43	Phosphane-free C \cdots C Heck couplings catalyzed by Pd(II) fluorinated aniline complexes of the type trans-[PdCl ₂ (NH ₂ ArF) ₂]. <i>Journal of Molecular Catalysis A</i> , 2006, 247, 65-72.	4.8	9
44	Synthesis of the anisobidentate compound bis(2-amino-cyclopent-1-ene-carbodithioate)diethyltin (IV). Experimental and theoretical study. <i>Journal of Organometallic Chemistry</i> , 2004, 689, 2096-2102.	1.8	9