

Mercedes Alonso

List of Publications by Year in descending order

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76
papers

2,052
citations

236925
25
h-index

265206
42
g-index

82
all docs

82
docs citations

82
times ranked

1935
citing authors

#	ARTICLE	IF	CITATIONS
1	Imine hydrogenation with simple alkaline earth metal catalysts. <i>Nature Catalysis</i> , 2018, 1, 40-47.	34.4	151
2	A benchmark for the non-covalent interaction (NCI) index or π is it really all in the geometry?. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	124
3	Understanding the Fundamental Role of π , π , and π Dispersion Interactions in Shaping Carbon-Based Materials. <i>Chemistry - A European Journal</i> , 2014, 20, 4931-4941.	3.3	109
4	Simple Alkaline-Earth Metal Catalysts for Effective Alkene Hydrogenation. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15177-15182.	13.8	87
5	New electron delocalization tools to describe the aromaticity in porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2787-2796.	2.8	86
6	From Dibismuthenes to Three- and Two-Coordinated Bismuthinidenes by Fine Ligand Tuning: Evidence for Aromatic BiC_3N Rings through a Combined Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2015, 21, 16917-16928.	3.3	76
7	Alkene Transfer Hydrogenation with Alkaline-Earth Metal Catalysts. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 4248-4253.	13.8	65
8	Conductance Switching in Expanded Porphyrins through Aromaticity and Topology Changes. <i>Journal of the American Chemical Society</i> , 2018, 140, 1313-1326.	13.7	56
9	Revisiting sulfur H-bonds in proteins: The example of peroxiredoxin AhpE. <i>Scientific Reports</i> , 2016, 6, 30369.	3.3	52
10	Stibinidene and Bismuthinidene as Two-Electron Donors for Transition Metals (Co and Mn). <i>Chemistry - A European Journal</i> , 2016, 22, 7376-7380.	3.3	51
11	Topology Switching in [32]Heptaphyrins Controlled by Solvent, Protonation, and meso -Substituents. <i>Chemistry - A European Journal</i> , 2013, 19, 1617-1628.	3.3	49
12	Viability of M^{II} Topologies in [26]- and [28]Hexaphyrins. <i>Chemistry - A European Journal</i> , 2012, 18, 10916-10928.	3.3	48
13	A comparative study of the structure and bonding in heavier pnictinidene complexes $[(\text{ArE})\text{M}(\text{CO})_n]$ (E = As, Sb and Bi; M = Cr, Mo, W and Fe). <i>Dalton Transactions</i> , 2017, 46, 3556-3568.	3.3	44
14	Performance of Localized Coupled Cluster Methods in a Moderately Strong Correlation Regime: H_4chel - M^{II} Interconversions in Expanded Porphyrins. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3641-3653.	5.3	44
15	Exploring the structure-aromaticity relationship in H_4chel and M^{II} N-fused pentaphyrins using DFT. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14396-14407.	2.8	41
16	Global and local aromaticity of acenes from the information-theoretic approach in density functional reactivity theory. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18195-18210.	2.8	41
17	Different Products of the Reduction of (N),C,N-Chelated Antimony(III) Compounds: Competitive Formation of Monomeric Stibinidenes versus $1\text{-H-}2,1\text{-Benzazastiboles}$. <i>Chemistry - A European Journal</i> , 2017, 23, 2340-2349.	3.3	39
18	A universal scale of aromaticity for π -organic compounds. <i>Journal of Computational Chemistry</i> , 2010, 31, 917-928.	3.3	38

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19	Aromaticity as a Guiding Concept for Spectroscopic Features and Nonlinear Optical Properties of Porphyrinoids. <i>Molecules</i> , 2018, 23, 1333.	3.8	38
20	Simple Alkaline-Earth Metal Catalysts for Effective Alkene Hydrogenation. <i>Angewandte Chemie</i> , 2018, 130, 15397-15402.	2.0	33
21	Fingerprint of Aromaticity and Molecular Topology on the Photophysical Properties of Octaphyrins. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7318-7335.	3.1	32
22	Neural Networks as a Tool To Classify Compounds According to Aromaticity Criteria. <i>Chemistry - A European Journal</i> , 2007, 13, 3913-3923.	3.3	29
23	Substituent effects on the aromaticity of carbocyclic five-membered rings. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1305-1317.	2.8	29
24	Understanding the molecular switching properties of octaphyrins. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11885-11900.	2.8	29
25	Molecular dynamics based descriptors for predicting supramolecular gelation. <i>Chemical Science</i> , 2020, 11, 4226-4238.	7.4	29
26	Conformational Control in [22]- and [24]Pentaphyrins(1.1.1.1.1) by Meso Substituents and their N-Fusion Reaction. <i>Journal of Organic Chemistry</i> , 2013, 78, 4419-4431.	3.2	25
27	Implementing the mechanical force into the conceptual DFT framework: understanding and predicting molecular mechanochemical properties. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7378-7388.	2.8	25
28	Switching between Hückel and Möbius aromaticity: a density functional theory and information-theoretic approach study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4715-4730.	2.8	25
29	Alkene Transfer Hydrogenation with Alkaline-Earth Metal Catalysts. <i>Angewandte Chemie</i> , 2019, 131, 4292-4297.	2.0	24
30	Chemical applications of neural networks: aromaticity of pyrimidine derivatives. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20564.	2.8	23
31	Hydrosilylation Induced by Na ⁺ /Si Intramolecular Coordination: Spontaneous Transformation of Organosilanes into 1-Aza-6-silole-Type Molecules in the Absence of a Catalyst. <i>Chemistry - A European Journal</i> , 2014, 20, 2542-2550.	3.3	23
32	Ambident Nucleophilic Substitution: Understanding Non-HSAB Behavior through Activation Strain and Conceptual DFT Analyses. <i>Chemistry - A European Journal</i> , 2020, 26, 3884-3893.	3.3	23
33	Synthesis and Structural Characterization of Heteroboroxines with MB ₂ O ₃ Core (M = Sb, Bi, Sn). <i>Inorganic Chemistry</i> , 2013, 52, 1424-1431.	4.0	22
34	A computational study on the role of noncovalent interactions in the stability of polymer/graphene nanocomposites. <i>Journal of Molecular Modeling</i> , 2017, 23, 43.	1.8	22
35	Performance of Electronic Structure Methods for the Description of Hückel-Möbius Interconversions in Extended π -Systems. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2380-2397.	2.5	22
36	Studies on aromatic compounds: inhibition of calpain I by biphenyl derivatives and peptide-biphenyl hybrids. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 2753-2757.	2.2	21

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37	The hunt for reactive alkynes in bio-orthogonal click reactions: insights from mechanochemical and conceptual DFT calculations. <i>Chemical Science</i> , 2020, 11, 1431-1439.	7.4	21
38	Decabromobiphenyl (PBB-209) Activates the Aryl Hydrocarbon Receptor While Decachlorobiphenyl (PCB-209) Is Inactive: Experimental Evidence and Computational Rationalization of the Different Behavior of Some Halogenated Biphenyls. <i>Chemical Research in Toxicology</i> , 2008, 21, 643-658.	3.3	19
39	Aromaticity changes along the reaction coordinate connecting the cyclobutadiene dimer to cubane and the benzene dimer to hexaprismane. <i>Structural Chemistry</i> , 2007, 18, 773-783.	2.0	18
40	Synthesis and reactivity of a germylene stabilized by a boraguanidinate ligand. <i>RSC Advances</i> , 2016, 6, 19377-19388.	3.6	18
41	Qualitative Insights into the Transport Properties of H ₂ and Methyl (Anti)Aromatic Compounds: Application to Expanded Porphyrins. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19842-19856.	3.1	17
42	ACTIVATION OF THE ARYL HYDROCARBON RECEPTOR BY CARBARYL: COMPUTATIONAL EVIDENCE OF THE ABILITY OF CARBARYL TO ASSUME A PLANAR CONFORMATION. <i>Environmental Toxicology and Chemistry</i> , 2006, 25, 3141.	4.3	16
43	Spontaneous Double Hydrometallation Induced by N ⁺ M Coordination in Organometallic Hydrides of Group 14 Elements. <i>Chemistry - A European Journal</i> , 2016, 22, 5620-5628.	3.3	16
44	The active site architecture in peroxiredoxins: a case study on Mycobacterium tuberculosis AhpE. <i>Chemical Communications</i> , 2016, 52, 10293-10296.	4.1	16
45	Biological and chemical studies on aryl hydrocarbon receptor induction by the p53 inhibitor pifithrin- α and its condensation product pifithrin- β . <i>Life Sciences</i> , 2011, 88, 774-783.	4.3	14
46	Metalated Hexaphyrins: From Understanding to Rational Design. <i>Chemistry - A European Journal</i> , 2015, 21, 17631-17638.	3.3	14
47	Mechanochemically Triggered Topology Changes in Expanded Porphyrins. <i>Chemistry - A European Journal</i> , 2021, 27, 3397-3406.	3.3	14
48	Oxidative Additions of Homoleptic Tin(II) Amidinate. <i>Organometallics</i> , 2015, 34, 606-615.	2.3	13
49	Computational Tools to Rationalize and Predict the Self-Assembly Behavior of Supramolecular Gels. <i>Gels</i> , 2021, 7, 87.	4.5	13
50	Comparison of reactivity of $\text{C}(\text{N})$ -chelated and Lappert's stannylenes with trimethylsilylazide. <i>Canadian Journal of Chemistry</i> , 2014, 92, 434-440.	1.1	12
51	8-Aryl substituted boron-dipyrromethene dyes: crystal structures and computational studies. <i>Journal of Molecular Structure</i> , 2004, 697, 29-40.	3.6	11
52	Reactivity of Single Transition Metal Atoms on a Hydroxylated Amorphous Silica Surface: A Periodic Conceptual DFT Investigation. <i>Chemistry - A European Journal</i> , 2021, 27, 6050-6063.	3.3	11
53	Studies on calpain inhibitors. Synthesis of partially reduced isoquinoline-1-thione derivatives and conversion to functionalized 1-chloroisoquinolines. <i>Tetrahedron Letters</i> , 2008, 49, 2275-2279.	1.4	10
54	Understanding conductivity in molecular switches: a real space approach in octaphyrins. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11829-11838.	2.8	10

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55	Toward the Design of Bithermoelectric Switches. Journal of Physical Chemistry C, 2018, 122, 24436-24444.	3.1	10
56	Scrutinizing ion- π and ion- π interactions using the noncovalent index and energy decomposition analysis. Computational and Theoretical Chemistry, 2015, 1053, 150-164.	2.5	9
57	Rationalising Supramolecular Hydrogelation of Bis-urea-Based Gelators through a Multiscale Approach. ChemPlusChem, 2020, 85, 267-276.	2.8	9
58	Single-molecule conductance in a unique cross-conjugated tetra(aminoaryl)ethene. Chemical Communications, 2021, 57, 591-594.	4.1	9
59	Reactivity of Bis(organoamino)phosphanes with Aluminum(III) Compounds: Straightforward Access to Diiminophosphinates by Means of Hydrogen-Atom Migration - An Experimental and Theoretical Study. European Journal of Inorganic Chemistry, 2014, 2014, 5193-5203.	2.0	8
60	Reactivity of Tin(II) Guanidinate with 1,2- and 1,3-Diones: Oxidative Cycloaddition or Ligand Substitution ?. Organometallics, 2015, 34, 2202-2211.	2.3	8
61	Derivatives of 3-sec-Butyl-1-oxo-2,3-dihydroisoquinoline as Inhibitors of $\frac{1}{4}$ -Calpain. ChemMedChem, 2006, 1, 710-714.	3.2	7
62	A Benchmark of Density Functional Approximations For Thermochemistry and Kinetics of Hydride Reductions of Cyclohexanones. ChemistryOpen, 2019, 8, 788-806.	1.9	7
63	SuFEx-enabled, chemoselective synthesis of triflates, triflamides and triflimidates. Chemical Science, 2022, 13, 2270-2279.	7.4	7
64	X-ray Diffraction, Solution Structure, and Computational Studies on Derivatives of (3-sec-Butyl-2,3-dihydro-1H-isoquinolin-4-ylidene)acetic Acid: Compounds with Activity as Calpain Inhibitors. Journal of Organic Chemistry, 2010, 75, 342-352.	3.2	5
65	Reactivity of bis(organoamino)phosphanes with magnesium(σ -alkyl) compounds. Dalton Transactions, 2015, 44, 4533-4545.	3.3	5
66	Designing Force Probes Based on Reversible σ -Electrocyclizations in Polyenes Using Quantum Chemical Calculations. Journal of Organic Chemistry, 2021, 86, 7477-7489.	3.2	5
67	Stereoselective Reductions of 3-Substituted Cyclobutanones: A Comparison between Experiment and Theory. Journal of Organic Chemistry, 2020, 85, 7803-7816.	3.2	5
68	Fine-Tuning of Nonlinear Optical Contrasts of Hexaphyrin-Based Molecular Switches Using Inverse Design. Frontiers in Chemistry, 2021, 9, 786036.	3.6	5
69	Understanding the Fundamental Role of π - π , π - π , and π - π Dispersion Interactions in Shaping Carbon-Based Materials. Chemistry - A European Journal, 2014, 20, 4845-4845.	3.3	3
70	Towards the understanding of halogenation in peptide hydrogels: a quantum chemical approach. Materials Advances, 2021, 2, 4792-4803.	5.4	3
71	Uncovering the Activity of Alkaline Earth Metal Hydrogenation Catalysis Through Molecular Volcano Plots. Topics in Catalysis, 2022, 65, 289-295.	2.8	3
72	Towards the Design of Optically Active Thiophene σ -Oxides using Quantum Chemistry. Chemistry - A European Journal, 2019, 25, 2840-2851.	3.3	2

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73	Rationalising Supramolecular Hydrogelation of Bis-urea-Based Gelators through a Multiscale Approach. ChemPlusChem, 2020, 85, 266-266.	2.8	1
74	Synthesis and Reactivity of Spirocarbocycles as Scaffolds for Nucleoside Analogues. Journal of Organic Chemistry, 2020, 85, 14989-15005.	3.2	1
75	Quantifying aromaticity according to the energetic criterion. , 2021, , 195-235.		1
76	Aryl hydrocarbon receptor induction by alpha- and ss-pifithrin. Toxicology Letters, 2010, 196, S258.	0.8	0