

Mercedes Alonso

List of Publications by Year in descending order

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2,052
citations

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docs citations

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times ranked

2120
citing authors

#	ARTICLE	IF	CITATIONS
1	Uncovering the Activity of Alkaline Earth Metal Hydrogenation Catalysis Through Molecular Volcano Plots. <i>Topics in Catalysis</i> , 2022, 65, 289-295.	1.3	3
2	SuFEx-enabled, chemoselective synthesis of triflates, triflamides and triflimidates. <i>Chemical Science</i> , 2022, 13, 2270-2279.	3.7	7
3	Mechanochemically Triggered Topology Changes in Expanded Porphyrins. <i>Chemistry - A European Journal</i> , 2021, 27, 3397-3406.	1.7	14
4	Single-molecule conductance in a unique cross-conjugated tetra(aminoaryl)ethene. <i>Chemical Communications</i> , 2021, 57, 591-594.	2.2	9
5	Towards the understanding of halogenation in peptide hydrogels: a quantum chemical approach. <i>Materials Advances</i> , 2021, 2, 4792-4803.	2.6	3
6	Quantifying aromaticity according to the energetic criterion. , 2021, , 195-235.		1
7	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.	1.7	11
8	Designing Force Probes Based on Reversible 6 π -Electrocyclizations in Polyenes Using Quantum Chemical Calculations. <i>Journal of Organic Chemistry</i> , 2021, 86, 7477-7489.	1.7	5
9	Computational Tools to Rationalize and Predict the Self-Assembly Behavior of Supramolecular Gels. <i>Gels</i> , 2021, 7, 87.	2.1	13
10	Fine-Tuning of Nonlinear Optical Contrasts of Hexaphyrin-Based Molecular Switches Using Inverse Design. <i>Frontiers in Chemistry</i> , 2021, 9, 786036.	1.8	5
11	Rationalising Supramolecular Hydrogelation of Bis-Urea-Based Gelators through a Multiscale Approach. <i>ChemPlusChem</i> , 2020, 85, 267-276.	1.3	9
12	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.	3.7	21
13	Rationalising Supramolecular Hydrogelation of Bis-Urea-Based Gelators through a Multiscale Approach. <i>ChemPlusChem</i> , 2020, 85, 266-266.	1.3	1
14	Synthesis and Reactivity of Spirocarbocycles as Scaffolds for Nucleoside Analogues. <i>Journal of Organic Chemistry</i> , 2020, 85, 14989-15005.	1.7	1
15	Molecular dynamics based descriptors for predicting supramolecular gelation. <i>Chemical Science</i> , 2020, 11, 4226-4238.	3.7	29
16	Switching between H π -stacking and M π -aromaticity: a density functional theory and information-theoretic approach study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4715-4730.	1.3	25
17	Performance of Electronic Structure Methods for the Description of H π -stacking \leftrightarrow M π -Interconversions in Extended π -Systems. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2380-2397.	1.1	22
18	Ambident Nucleophilic Substitution: Understanding Non-HSAB Behavior through Activation Strain and Conceptual DFT Analyses. <i>Chemistry - A European Journal</i> , 2020, 26, 3884-3893.	1.7	23

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19	Performance of Localized Coupled Cluster Methods in a Moderately Strong Correlation Regime: H ₄ chelâ€“MÃ¶bius Interconversions in Expanded Porphyrins. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3641-3653.	2.3	44
20	Stereoselective Reductions of 3-Substituted Cyclobutanones: A Comparison between Experiment and Theory. <i>Journal of Organic Chemistry</i> , 2020, 85, 7803-7816.	1.7	5
21	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.	1.3	41
22	A Benchmark of Density Functional Approximations For Thermochemistry and Kinetics of Hydride Reductions of Cyclohexanones. <i>ChemistryOpen</i> , 2019, 8, 788-806.	0.9	7
23	Alkene Transfer Hydrogenation with Alkalineâ€“Earth Metal Catalysts. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 4248-4253.	7.2	65
24	Alkene Transfer Hydrogenation with Alkalineâ€“Earth Metal Catalysts. <i>Angewandte Chemie</i> , 2019, 131, 4292-4297.	1.6	24
25	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.	1.3	25
26	Fingerprint of Aromaticity and Molecular Topology on the Photophysical Properties of Octaphyrins. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7318-7335.	1.5	32
27	Towards the Design of Optically Active Thiophene Sâ€“Oxides using Quantum Chemistry. <i>Chemistry - A European Journal</i> , 2019, 25, 2840-2851.	1.7	2
28	Conductance Switching in Expanded Porphyrins through Aromaticity and Topology Changes. <i>Journal of the American Chemical Society</i> , 2018, 140, 1313-1326.	6.6	56
29	New electron delocalization tools to describe the aromaticity in porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2787-2796.	1.3	86
30	Imine hydrogenation with simple alkaline earth metal catalysts. <i>Nature Catalysis</i> , 2018, 1, 40-47.	16.1	151
31	Qualitative Insights into the Transport Properties of H ₄ chel/MÃ¶bius (Anti)Aromatic Compounds: Application to Expanded Porphyrins. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19842-19856.	1.5	17
32	Toward the Design of Bithermoelectric Switches. <i>Journal of Physical Chemistry C</i> , 2018, 122, 24436-24444.	1.5	10
33	Simple Alkalineâ€“Earth Metal Catalysts for Effective Alkene Hydrogenation. <i>Angewandte Chemie</i> , 2018, 130, 15397-15402.	1.6	33
34	Simple Alkalineâ€“Earth Metal Catalysts for Effective Alkene Hydrogenation. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15177-15182.	7.2	87
35	Aromaticity as a Guiding Concept for Spectroscopic Features and Nonlinear Optical Properties of Porphyrinoids. <i>Molecules</i> , 2018, 23, 1333.	1.7	38
36	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.	0.8	22

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37	A comparative study of the structure and bonding in heavier pnictinidene complexes [(ArE)M(CO) _n] (E = As, Sb and Bi; M = Cr, Mo, W and Fe). Dalton Transactions, 2017, 46, 3556-3568.	1.6	44
38	Different Products of the Reduction of (N),C,N-Chelated Antimony(III) Compounds: Competitive Formation of Monomeric Stibinidenes versus 1,2-Benzazastiboles. Chemistry - A European Journal, 2017, 23, 2340-2349.	1.7	39
39	Spontaneous Double Hydrometallation Induced by N ⁺ M Coordination in Organometallic Hydrides of Group 14 Elements. Chemistry - A European Journal, 2016, 22, 5620-5628.	1.7	16
40	Synthesis and reactivity of a germylene stabilized by a boraguanidinate ligand. RSC Advances, 2016, 6, 19377-19388.	1.7	18
41	A benchmark for the non-covalent interaction (NCI) index or δ is it really all in the geometry?. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	124
42	Revisiting sulfur H-bonds in proteins: The example of peroxiredoxin AhpE. Scientific Reports, 2016, 6, 30369.	1.6	52
43	The active site architecture in peroxiredoxins: a case study on Mycobacterium tuberculosis AhpE. Chemical Communications, 2016, 52, 10293-10296.	2.2	16
44	Stibinidene and Bismuthinidene as Two σ -Electron Donors for Transition Metals (Co and Mn). Chemistry - A European Journal, 2016, 22, 7376-7380.	1.7	51
45	Understanding conductivity in molecular switches: a real space approach in octaphyrins. Physical Chemistry Chemical Physics, 2016, 18, 11829-11838.	1.3	10
46	Understanding the molecular switching properties of octaphyrins. Physical Chemistry Chemical Physics, 2016, 18, 11885-11900.	1.3	29
47	Metalated Hexaphyrins: From Understanding to Rational Design. Chemistry - A European Journal, 2015, 21, 17631-17638.	1.7	14
48	From Dibismuthenes to Three- and Two- Coordinated Bismuthinidenes by Fine Ligand Tuning: Evidence for Aromatic BiC ₃ N Rings through a Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2015, 21, 16917-16928.	1.7	76
49	Oxidative Additions of Homoleptic Tin(II) Amidinate. Organometallics, 2015, 34, 606-615.	1.1	13
50	Reactivity of bis(organoamino)phosphanes with magnesium(σ) compounds. Dalton Transactions, 2015, 44, 4533-4545.	1.6	5
51	Reactivity of Tin(II) Guanidinate with 1,2- and 1,3-Diones: Oxidative Cycloaddition or Ligand Substitution?. Organometallics, 2015, 34, 2202-2211.	1.1	8
52	Scrutinizing ion- π and ion- π^* interactions using the noncovalent index and energy decomposition analysis. Computational and Theoretical Chemistry, 2015, 1053, 150-164.	1.1	9
53	Comparison of reactivity of σ -C, σ -N-chelated and Lappert's stannylenes with trimethylsilylazide. Canadian Journal of Chemistry, 2014, 92, 434-440.	0.6	12
54	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, 4931-4941.	1.7	109

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55	Understanding the Fundamental Role of π/π , π/f , and f/f Dispersion Interactions in Shaping Carbon-Based Materials. <i>Chemistry - A European Journal</i> , 2014, 20, 4845-4845.	1.7	3
56	Exploring the structure–aromaticity relationship in Hückel and Möbius N-fused pentaphyrins using DFT. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14396-14407.	1.3	41
57	Reactivity of Bis(organoamino)phosphanes with Aluminum(III) Compounds: Straightforward Access to Diiminophosphinates by Means of Hydrogen-Atom Migration - An Experimental and Theoretical Study. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 5193-5203.	1.0	8
58	Hydrosilylation Induced by Na ⁺ Si Intramolecular Coordination: Spontaneous Transformation of Organosilanes into σ -Alkylsilole-Type Molecules in the Absence of a Catalyst. <i>Chemistry - A European Journal</i> , 2014, 20, 2542-2550.	1.7	23
59	Topology Switching in [32]Heptaphyrins Controlled by Solvent, Protonation, and <i>meso</i> -Substituents. <i>Chemistry - A European Journal</i> , 2013, 19, 1617-1628.	1.7	49
60	Synthesis and Structural Characterization of Heteroboroxines with MB ₂ O ₃ Core (M = Sb, Bi, Sn). <i>Inorganic Chemistry</i> , 2013, 52, 1424-1431.	1.9	22
61	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.	1.7	25
62	Viability of Möbius Topologies in [26]- and [28]Hexaphyrins. <i>Chemistry - A European Journal</i> , 2012, 18, 10916-10928.	1.7	48
63	Chemical applications of neural networks: aromaticity of pyrimidine derivatives. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20564.	1.3	23
64	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.	2.0	14
65	A universal scale of aromaticity for π -organic compounds. <i>Journal of Computational Chemistry</i> , 2010, 31, 917-928.	1.5	38
66	Aryl hydrocarbon receptor induction by α - and β -pifithrin. <i>Toxicology Letters</i> , 2010, 196, S258.	0.4	0
67	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. <i>Journal of Organic Chemistry</i> , 2010, 75, 342-352.	1.7	5
68	Substituent effects on the aromaticity of carbocyclic five-membered rings. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1305-1317.	1.3	29
69	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.	0.7	10
70	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.	1.7	19
71	Neural Networks as a Tool To Classify Compounds According to Aromaticity Criteria. <i>Chemistry - A European Journal</i> , 2007, 13, 3913-3923.	1.7	29
72	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.	1.0	18

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73	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.	2.2	16
74	Derivatives of 3-sec-Butyl-1-oxo-2,3-dihydroisoquinoline as Inhibitors of $\hat{1}/4$ -Calpain. <i>ChemMedChem</i> , 2006, 1, 710-714.	1.6	7
75	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.	1.0	21
76	8-Aryl substituted boron-dipyrromethene dyes: crystal structures and computational studies. <i>Journal of Molecular Structure</i> , 2004, 697, 29-40.	1.8	11