Mercedes Alonso

List of Publications by Year
in descending order

76 papers	2,052 citations	236612 25 h-index	264894 42 g-index
82 all docs	82 docs citations	82 times ranked	1935 citing authors

#	Article	IF	Citations
1	Uncovering the Activity of Alkaline Earth Metal Hydrogenation Catalysis Through Molecular Volcano Plots. Topics in Catalysis, 2022, 65, 289-295.	1.3	3
2	SuFEx-enabled, chemoselective synthesis of triflates, triflamides and triflimidates. Chemical Science, 2022, 13, 2270-2279.	3.7	7
3	Mechanochemically Triggered Topology Changes in Expanded Porphyrins. Chemistry - A European Journal, 2021, 27, 3397-3406.	1.7	14
4	Single-molecule conductance in a unique cross-conjugated tetra(aminoaryl)ethene. Chemical Communications, 2021, 57, 591-594.	2.2	9
5	Towards the understanding of halogenation in peptide hydrogels: a quantum chemical approach. Materials Advances, 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. Chemistry - A European Journal, 2021, 27, 6050-6063.	1.7	11
8	Designing Force Probes Based on Reversible 6Ї€-Electrocyclizations in Polyenes Using Quantum Chemical Calculations. Journal of Organic Chemistry, 2021, 86, 7477-7489.	1.7	5
9	Computational Tools to Rationalize and Predict the Self-Assembly Behavior of Supramolecular Gels. Gels, 2021, 7, 87.	2.1	13
10	Fine-Tuning of Nonlinear Optical Contrasts of Hexaphyrin-Based Molecular Switches Using Inverse Design. Frontiers in Chemistry, 2021, 9, 786036.	1.8	5
11	Rationalising Supramolecular Hydrogelation of Bisâ€Ureaâ€Based Gelators through a Multiscale Approach. ChemPlusChem, 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. Chemical Science, 2020, 11, 1431-1439.	3.7	21
13	Rationalising Supramolecular Hydrogelation of Bisâ€Ureaâ€Based Gelators through a Multiscale Approach. ChemPlusChem, 2020, 85, 266-266.	1.3	1
14	Synthesis and Reactivity of Spirocarbocycles as Scaffolds for Nucleoside Analogues. Journal of Organic Chemistry, 2020, 85, 14989-15005.	1.7	1
15	Molecular dynamics based descriptors for predicting supramolecular gelation. Chemical Science, 2020, 11, 4226-4238.	3.7	29
16	Switching between HÃ¼ckel and MÃ¶bius aromaticity: a density functional theory and information-theoretic approach study. Physical Chemistry Chemical Physics, 2020, 22, 4715-4730.	1.3	25
17	Performance of Electronic Structure Methods for the Description of HÃ¼ckelâ€“MÃ¶bius Interconversions in Extended Ї€-Systems. Journal of Physical Chemistry A, 2020, 124, 2380-2397.	1.1	22
18	Ambident Nucleophilic Substitution: Understanding Nonâ€HSAB Behavior through Activation Strain and Conceptual DFT Analyses. Chemistry - A European Journal, 2020, 26, 3884-3893.	1.7	23

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19	Performance of Localized Coupled Cluster Methods in a Moderately Strong Correlation Regime: HÃ¼ckelâ€“MÃ¶bius Interconversions in Expanded Porphyrins. Journal of Chemical Theory and Computation, 2020, 16, 3641-3653.	2.3	44
20	Stereoselective Reductions of 3-Substituted Cyclobutanones: A Comparison between Experiment and Theory. Journal of Organic Chemistry, 2020, 85, 7803-7816.	1.7	5
21	Global and local aromaticity of acenes from the information-theoretic approach in density functional reactivity theory. Physical Chemistry Chemical Physics, 2019, 21, 18195-18210.	1.3	41
22	A Benchmark of Density Functional Approximations For Thermochemistry and Kinetics of Hydride Reductions of Cyclohexanones. ChemistryOpen, 2019, 8, 788-806.	0.9	7
23	Alkene Transfer Hydrogenation with Alkalineâ€Earth Metal Catalysts. Angewandte Chemie - International Edition, 2019, 58, 4248-4253.	7.2	65
24	Alkene Transfer Hydrogenation with Alkalineâ€Earth Metal Catalysts. Angewandte Chemie, 2019, 131, 4292-4297.	1.6	24
25	Implementing the mechanical force into the conceptual DFT framework: understanding and predicting molecular mechanochemical properties. Physical Chemistry Chemical Physics, 2019, 21, 7378-7388.	1.3	25
26	Fingerprint of Aromaticity and Molecular Topology on the Photophysical Properties of Octaphyrins. Journal of Physical Chemistry C, 2019, 123, 7318-7335.	1.5	32
27	Towards the Design of Optically Active Thiophene Sâ€Oxides using Quantum Chemistry. Chemistry - A European Journal, 2019, 25, 2840-2851.	1.7	2
28	Conductance Switching in Expanded Porphyrins through Aromaticity and Topology Changes. Journal of the American Chemical Society, 2018, 140, 1313-1326.	6.6	56
29	New electron delocalization tools to describe the aromaticity in porphyrinoids. Physical Chemistry Chemical Physics, 2018, 20, 2787-2796.	1.3	86
30	Imine hydrogenation with simple alkaline earth metal catalysts. Nature Catalysis, 2018, 1, 40-47.	16.1	151
31	Qualitative Insights into the Transport Properties of HÃ¼ckel/MÃ¶bius (Anti)Aromatic Compounds: Application to Expanded Porphyrins. Journal of Physical Chemistry C, 2018, 122, 19842-19856.	1.5	17
32	Toward the Design of Bithermoelectric Switches. Journal of Physical Chemistry C, 2018, 122, 24436-24444.	1.5	10
33	Simple Alkalineâ€Earth Metal Catalysts for Effective Alkene Hydrogenation. Angewandte Chemie, 2018, 130, 15397-15402.	1.6	33
34	Simple Alkalineâ€Earth Metal Catalysts for Effective Alkene Hydrogenation. Angewandte Chemie - International Edition, 2018, 57, 15177-15182.	7.2	87
35	Aromaticity as a Guiding Concept for Spectroscopic Features and Nonlinear Optical Properties of Porphyrinoids. Molecules, 2018, 23, 1333.	1.7	38
36	A computational study on the role of noncovalent interactions in the stability of polymer/graphene nanocomposites. Journal of Molecular Modeling, 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,Nâ€Chelated Antimony(III) Compounds: Competitive Formation of Monomeric Stibinidenes versus 1Hâ€2,1â€Benzazastiboles. Chemistry - A European Journal, 2017, 23, 2340-2349.	1.7	39
39	Spontaneous Double Hydrometallation Induced by Nâ†'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 orâ€¦ 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 Twoâ€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 Threeâ€•and Twoâ€Coordinated Bismuthinidenes by Fine Ligand Tuning: Evidence for Aromatic BiC₃N 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(<scp>II</scp>) 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-Ï€ and ion-Ïƒ 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 C,N-chelated and Lappertâ€™s stannylenes with trimethylsilylazide. Canadian Journal of Chemistry, 2014, 92, 434-440.	0.6	12
54	Understanding the Fundamental Role of Ï€Ï€, ÏƒÏƒ, and ÏƒÏ€ Dispersion Interactions in Shaping Carbonâ€Based Materials. Chemistry - A European Journal, 2014, 20, 4931-4941.	1.7	109

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55	Understanding the Fundamental Role of Ï€/Ï€, Ïƒ/Ïƒ, and Ïƒ/Ï€ Dispersion Interactions in Shaping Carbon-Based Materials. Chemistry - A European Journal, 2014, 20, 4845-4845.	1.7	3
56	Exploring the structureâ€“aromaticity relationship in HÃ¼ckel and MÃ¶bius N-fused pentaphyrins using DFT. Physical Chemistry Chemical Physics, 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. European Journal of Inorganic Chemistry, 2014, 2014, 5193-5203.	1.0	8
58	Hydrosilylation Induced by Nâ†'Si Intramolecular Coordination: Spontaneous Transformation of Organosilanes into 1â€Azaâ€Siloleâ€Type Molecules in the Absence of a Catalyst. Chemistry - A European Journal, 2014, 20, 2542-2550.	1.7	23
59	Topology Switching in [32]Heptaphyrins Controlled by Solvent, Protonation, and mesoâ€...Substituents. Chemistry - A European Journal, 2013, 19, 1617-1628.	1.7	49
60	Synthesis and Structural Characterization of Heteroboroxines with MB₂O₃ Core (M = Sb, Bi, Sn). Inorganic Chemistry, 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. Journal of Organic Chemistry, 2013, 78, 4419-4431.	1.7	25
62	Viability of MÃ¶bius Topologies in [26]â€•and [28]Hexaphyrins. Chemistry - A European Journal, 2012, 18, 10916-10928.	1.7	48
63	Chemical applications of neural networks: aromaticity of pyrimidine derivatives. Physical Chemistry Chemical Physics, 2011, 13, 20564.	1.3	23
64	Biological and chemical studies on aryl hydrocarbon receptor induction by the p53 inhibitor pifithrin-Î± and its condensation product pifithrin-Î². Life Sciences, 2011, 88, 774-783.	2.0	14
65	A universal scale of aromaticity for Ï€â€organic compounds. Journal of Computational Chemistry, 2010, 31, 917-928.	1.5	38
66	Aryl hydrocarbon receptor induction by alpha- and ss-pifithrin. Toxicology Letters, 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. Journal of Organic Chemistry, 2010, 75, 342-352.	1.7	5
68	Substituent effects on the aromaticity of carbocyclic five-membered rings. Physical Chemistry Chemical Physics, 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. Tetrahedron Letters, 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. Chemical Research in Toxicology, 2008, 21, 643-658.	1.7	19
71	Neural Networks as a Tool To Classify Compounds According to Aromaticity Criteria. Chemistry - A European Journal, 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. Structural Chemistry, 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. Environmental Toxicology and Chemistry, 2006, 25, 3141.	2.2	16
74	Derivatives of 3-sec-Butyl-1-oxo-2,3-dihydroisoquinoline as Inhibitors of Î¼-Calpain. ChemMedChem, 2006, 1, 710-714.	1.6	7
75	Studies on aromatic compounds: inhibition of calpain I by biphenyl derivatives and peptide-biphenyl hybrids. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 2753-2757.	1.0	21
76	8-Aryl substituted boron-dipyrromethene dyes: crystal structures and computational studies. Journal of Molecular Structure, 2004, 697, 29-40.	1.8	11