JosÃ© Maria Mercero

List of Publications by Year
in descending order

66	1,996	236925 25	254184 43
papers	citations	h-index	g-index

72	72	72	1909
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Water-Promoted Hydrolysis of a Highly Twisted Amide:Â Rate Acceleration Caused by the Twist of the Amide Bond. Journal of the American Chemical Society, 2005, 127, 4445-4453.	13.7	136
2	Recent developments and future prospects of all-metal aromatic compounds. Chemical Society Reviews, 2015, 44, 6519-6534.	38.1	128
3	Theoretical methods that help understanding the structure and reactivity of gas phase ions. International Journal of Mass Spectrometry, 2005, 240, 37-99.	1.5	104
4	Sandwich-Like Complexes Based on â€œAll-Metalâ€•(Al42-) Aromatic Compounds. Journal of the American Chemical Society, 2004, 126, 3380-3381.	13.7	102
5	Electronic Excitation Energies of ZniOiClusters. Journal of the American Chemical Society, 2003, 125, 9494-9499.	13.7	98
6	A Joint Experimental and Theoretical Study of Cationâˆ’Ï€ Interactions:Â Multiple-Decker Sandwich Complexes of Ferrocene with Alkali Metal Ions (Li+, Na+, K+, Rb+, Cs+). Journal of the American Chemical Society, 2005, 127, 10656-10666.	13.7	81
7	New Solids Based on B₁₂N₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.	3.1	72
8	Planar pentacoordinate carbons in CBe₅^{4âˆ’} derivatives. Physical Chemistry Chemical Physics, 2015, 17, 4620-4624.	2.8	66
9	Clusters of IIâˆ’VI Materials:Â CdiXi, X = S, Se, Te,iâ‰¤ 16. Journal of Physical Chemistry A, 2004, 108, 10502-10508.	2.5	56
10	Planar tetracoordinate carbon in CE42âˆ’ (E=Alâ€“Tl) clusters. Chemical Physics Letters, 2012, 519-520, 29-33.	2.6	56
11	CBe5Eâˆ’ (E = Al, Ga, In, Tl): planar pentacoordinate carbon in heptaatomic clusters. Physical Chemistry Chemical Physics, 2012, 14, 14764.	2.8	55
12	The Ferroceneâˆ’Lithium Cation Complex in the Gas Phase. Journal of the American Chemical Society, 2001, 123, 5040-5043.	13.7	51
13	A Theoretical Evaluation of the pKa for Twisted Amides Using Density Functional Theory and Dielectric Continuum Methods. Journal of Physical Chemistry A, 2003, 107, 6099-6107.	2.5	49
14	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring. Angewandte Chemie - International Edition, 2004, 43, 5485-5488.	13.8	42
15	Hydrogen-Bonding Interactions between Formic Acid and Pyridine. Journal of Physical Chemistry A, 2002, 106, 4187-4191.	2.5	41
16	ALUMINIUM IN BIOLOGICAL ENVIRONMENTS: A COMPUTATIONAL APPROACH. Computational and Structural Biotechnology Journal, 2014, 9, e201403002.	4.1	41
17	A study of the coordination shell of aluminum(III) and magnesium(II) in model protein environments: Thermodynamics of the complex formation and metal exchange reactions. Journal of Inorganic Biochemistry, 2006, 100, 374-384.	3.5	40
18	Sandwich Complexes Based on the â€œAll-Metalâ€•Al42âˆ’ Aromatic Ring. Chemistry - A European Journal, 2006, 12, 4495-4502.	3.3	40

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19	On the Affinity Regulation of the Metal-Ion-Dependent Adhesion Sites in Integrins. Journal of the American Chemical Society, 2006, 128, 3554-3563.	13.7	39
20	Quantum mechanical calculations on phosphate hydrolysis reactions. Journal of Computational Chemistry, 2000, 21, 43-51.	3.3	37
21	Small clusters of group-(IIâ€“VI) materials:ZniXi,X=Se,Te,i=1â€“9. Physical Review A, 2001, 64, .	2.5	36
22	The aromaticity of dicupra[10]annulenes. Physical Chemistry Chemical Physics, 2017, 19, 9669-9675.	2.8	33
23	A theoretical study of the principles regulating the specificity for Al(III) against Mg(II) in protein cavities. Journal of Inorganic Biochemistry, 2007, 101, 1192-1200.	3.5	31
24	Reaction Mechanism of the Acidic Hydrolysis of Highly Twisted Amides:Â Rate Acceleration Caused by the Twist of the Amide Bond. Journal of Physical Chemistry B, 2006, 110, 15000-15011.	2.6	28
25	Comparison of Ti, Zr, and Hf as Cations for Metallocene-Catalyzed Olefin Polymerization. Organometallics, 2006, 25, 4483-4490.	2.3	26
26	Aluminum(III) Interactions with the Acidic Amino Acid Chains. Journal of Physical Chemistry A, 1998, 102, 7006-7012.	2.5	25
27	Endohedral Stannaspherenes Mn@Sn₁₂ and its Dimer: Ferromagnetic or Antiferromagnetic?. ChemPhysChem, 2007, 8, 2096-2099.	2.1	24
28	The Electronic Structure of the Al₃^{â^’} Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, 9610-9614.	3.3	23
29	Atomic configuration-interaction electron-electron counterbalance densities. Physical Review A, 1999, 59, 4255-4258.	2.5	22
30	Aluminum(III) Interactions with the Acid Derivative Amino Acid Chains. Journal of Physical Chemistry A, 2000, 104, 7053-7060.	2.5	22
31	Clusters of Group IIâ^’VI Materials:â€‰ CdiOi (i â‰ 15). Journal of Physical Chemistry A, 2003, 107, 9918-9923.	2.5	22
32	Protein Side Chains Facilitate Mg/Al Exchange in Model Protein Binding Sites. ChemPhysChem, 2007, 8, 2119-2124.	2.1	22
33	Reâ€examination of the C₆Li₆ Structure: To Be, or not To Be Symmetric. Chemistry - A European Journal, 2013, 19, 12668-12672.	3.3	20
34	The electronic states of Fe2+. Chemical Physics Letters, 2003, 376, 310-317.	2.6	19
35	The first solvation shell of aluminum (III) and magnesium (II) cations in a protein model environment. International Journal of Quantum Chemistry, 2004, 98, 409-424.	2.0	19
36	Ab-InitioStudies of Alternant X2Y2Rings (X = N, P, As, and Sb and Y = O, S, Se, and Te). PlanarversusButterfly Structures. Journal of Physical Chemistry A, 1997, 101, 5574-5579.	2.5	18

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37	The separation of the dynamical and non-dynamical electron correlation effects. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 275-283.	1.5	18
38	Vibrational spectroscopy of selfâ€assembling aromatic peptide derivates. Journal of Raman Spectroscopy, 2012, 43, 1397-1406.	2.5	18
39	Aluminum (III) interactions with the side chains of aromatic aminoacids. International Journal of Quantum Chemistry, 2002, 90, 859-881.	2.0	17
40	Discordant results on the FeO+â€‰+â€‰H2reaction reconciled by quantum Monte Carlo theory. Molecular Physics, 2004, 102, 2635-2637.	1.7	17
41	Bound excited states ofHâ^'andHeâ^'in the statically screened Coulomb potential. Physical Review A, 1998, 57, 2550-2555.	2.5	16
42	Electronic excitation energies of ZniSinanoparticles. Nanotechnology, 2006, 17, 4100-4105.	2.6	16
43	Sandwich Complexes of the Metalloaromatic Î·³-Al₃R₃ Ligand. Journal of the American Chemical Society, 2009, 131, 6949-6951.	13.7	16
44	Asymmetric Synthesis of Adjacent Triâ€and Tetrasubstituted Carbon Stereocenters: Organocatalytic Aldol Reaction of an Hydantoin Surrogate with Azaarene 2â€Carbaldehydes. Chemistry - A European Journal, 2019, 25, 12431-12438.	3.3	15
45	sp3 Hybrid orbitals and ionization energies of methane from PNOF5. Chemical Physics Letters, 2012, 531, 272-274.	2.6	14
46	Doped Aluminum Cluster Anions: Size Matters. Journal of Physical Chemistry A, 2014, 118, 4309-4314.	2.5	14
47	Aluminum (III) Interactions with Sulfur-Containing Amino Acid Chains. Journal of Physical Chemistry A, 2001, 105, 7446-7453.	2.5	12
48	Incremental binding free energies of aluminum (III) vs. magnesium (II) complexes. Chemical Physics, 2003, 295, 175-184.	1.9	11
49	Complexation of Al^{III} by Aromatic Amino Acids in the Gas Phase. Inorganic Chemistry, 2007, 46, 6413-6419.	4.0	11
50	The stability of biradicaloid versus closed-shell [E(Î¼-XR)]₂ (E = P, As; X = N, P, As) rings. Does aromaticity play a role?. Physical Chemistry Chemical Physics, 2016, 18, 11879-11884.	2.8	11
51	Magnetic Endohedral Transitionâ€Metalâ€Doped Semiconductingâ€Nanoclusters. Chemistry - A European Journal, 2008, 14, 8547-8554.	3.3	10
52	Atomic charge states in a weakly coupled plasma environment. Physical Review E, 2002, 66, 026408.	2.1	9
53	Assessment of Approximate Density Functional Methods for the Study of the Interactions of Al(III) with Aromatic Amino Acids. Journal of Chemical Theory and Computation, 2007, 3, 1830-1836.	5.3	8
54	Electronic structures of the bound excited quartet states of the helium anion. Physical Review A, 1999, 60, 4375-4378.	2.5	7

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55	Structural and optical properties of the naked and passivated Al5Au5 bimetallic nanoclusters. Journal of Chemical Physics, 2016, 144, 114302.	3.0	6
56	The electron-pair density distribution of the^{1,3}Î_uexcited states of H₂. Canadian Journal of Chemistry, 2016, 94, 998-1001.	1.1	5
57	Doping Platinum with Germanium: An Effective Way to Mitigate the CO Poisoning. ChemPhysChem, 2021, 22, 1603-1610.	2.1	5
58	Molecular and Electronic Structures of TiXH6+(X = B, Al, Ga) Compounds. Journal of Physical Chemistry A, 1997, 101, 5953-5957.	2.5	4
59	Does the composition in PtGe clusters play any role in fighting CO poisoning?. Journal of Chemical Physics, 2022, 156, 174301.	3.0	3
60	Molecular and Electronic Structures of (TiXH6)0/-, X = B, Al, Ga, Compounds. Journal of Physical Chemistry A, 1998, 102, 2055-2064.	2.5	2
61	Experiment and Theory Clarify: Sc + Receives One Oxygen Atom from SO 2 to Form ScO + , which Proves to be a Catalyst for the Hidden Oxygenâ€Exchange with SO 2. ChemPhysChem, 2021, , .	2.1	2
62	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring.. ChemInform, 2004, 35, no.	0.0	0
63	Clusters of II?VI Materials: CdiXi, X: S, Se, Te, i ? 16.. ChemInform, 2005, 36, no.	0.0	0
64	Frontispiece: The Electronic Structure of the Al3â¯Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, n/a-n/a.	3.3	0
65	Electronic Structure and Electron Delocalization in Bare and Dressed Boron Pentamer Clusters. Journal of Physical Chemistry A, 2021, 125, 5246-5255.	2.5	0
66	Building machine learning assisted phase diagrams: Three chemically relevant examples. AIP Advances, 2022, 12, 075206.	1.3	0