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	Does the composition in PtGe clusters play any role in fighting CO poisoning?. Journal of Chemical Physics, 2022, 156, 174301.	3.0	3
2	Building machine learning assisted phase diagrams: Three chemically relevant examples. AIP Advances, 2022, 12, 075206.	1.3	0
3	Electronic Structure and Electron Delocalization in Bare and Dressed Boron Pentamer Clusters. Journal of Physical Chemistry A, 2021, 125, 5246-5255.	2.5	0
4	Doping Platinum with Germanium: An Effective Way to Mitigate the CO Poisoning. ChemPhysChem, 2021, 22, 1603-1610.	2.1	5
5	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
6	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
7	The aromaticity of dicupra[10]annulenes. Physical Chemistry Chemical Physics, 2017, 19, 9669-9675.	2.8	33
8	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
9	Structural and optical properties of the naked and passivated Al5Au5 bimetallic nanoclusters. Journal of Chemical Physics, 2016, 144, 114302.	3.0	6
10	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
11	Frontispiece: The Electronic Structure of the Al3â^'Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, n/a-n/a.	3.3	0
12	The Electronic Structure of the Al₃^{â^'} Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, 9610-9614.	3.3	23
13	Recent developments and future prospects of all-metal aromatic compounds. Chemical Society Reviews, 2015, 44, 6519-6534.	38.1	128
14	Planar pentacoordinate carbons in CBe₅^{4â^'} derivatives. Physical Chemistry Chemical Physics, 2015, 17, 4620-4624.	2.8	66
15	Doped Aluminum Cluster Anions: Size Matters. Journal of Physical Chemistry A, 2014, 118, 4309-4314.	2.5	14
16	ALUMINIUM IN BIOLOGICAL ENVIRONMENTS: A COMPUTATIONAL APPROACH. Computational and Structural Biotechnology Journal, 2014, 9, e201403002.	4.1	41
17	Reâ€examination of the C₆Li₆ Structure: To Be, or not To Be Symmetric. Chemistry - A European Journal, 2013, 19, 12668-12672.	3.3	20
18	Vibrational spectroscopy of selfâ€assembling aromatic peptide derivates. Journal of Raman Spectroscopy, 2012, 43, 1397-1406.	2.5	18

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19	CBe5Eâˆ’ (E = Al, Ga, In, Tl): planar pentacoordinate carbon in heptaatomic clusters. Physical Chemistry Chemical Physics, 2012, 14, 14764.	2.8	55
20	Planar tetracoordinate carbon in CE42âˆ’ (E=Alâ€“Tl) clusters. Chemical Physics Letters, 2012, 519-520, 29-33.	2.6	56
21	sp3 Hybrid orbitals and ionization energies of methane from PNOF5. Chemical Physics Letters, 2012, 531, 272-274.	2.6	14
22	Sandwich Complexes of the Metalloaromatic Î·³-Al₃R₃ Ligand. Journal of the American Chemical Society, 2009, 131, 6949-6951.	13.7	16
23	Magnetic Endohedral Transitionâ€Metalâ€Doped Semiconductingâ€Nanoclusters. Chemistry - A European Journal, 2008, 14, 8547-8554.	3.3	10
24	New Solids Based on B₁₂N₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.	3.1	72
25	Complexation of Al^{III} by Aromatic Amino Acids in the Gas Phase. Inorganic Chemistry, 2007, 46, 6413-6419.	4.0	11
26	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
27	Protein Side Chains Facilitate Mg/Al Exchange in Model Protein Binding Sites. ChemPhysChem, 2007, 8, 2119-2124.	2.1	22
28	Endohedral Stannaspherenes Mn@Sn₁₂ and its Dimer: Ferromagnetic or Antiferromagnetic?. ChemPhysChem, 2007, 8, 2096-2099.	2.1	24
29	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
30	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
31	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
32	Comparison of Ti, Zr, and Hf as Cations for Metallocene-Catalyzed Olefin Polymerization. Organometallics, 2006, 25, 4483-4490.	2.3	26
33	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
34	Sandwich Complexes Based on the â€œAll-Metalâ€•Al42âˆ’ Aromatic Ring. Chemistry - A European Journal, 2006, 12, 4495-4502.	3.3	40
35	Electronic excitation energies of ZniSinanoparticles. Nanotechnology, 2006, 17, 4100-4105.	2.6	16
36	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

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37	Clusters of II?VI Materials: CdiXi, X: S, Se, Te, i ? 16.. ChemInform, 2005, 36, no.	0.0	0
38	A Joint Experimental and Theoretical Study of Cationâ^'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
39	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
40	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
41	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring. Angewandte Chemie - International Edition, 2004, 43, 5485-5488.	13.8	42
42	Mono- and Multidecker Sandwich-Like Complexes of the Tetraazacyclobutadiene Aromatic Ring.. ChemInform, 2004, 35, no.	0.0	0
43	Discordant results on the FeO+â€‰+â€‰H2reaction reconciled by quantum Monte Carlo theory. Molecular Physics, 2004, 102, 2635-2637.	1.7	17
44	Sandwich-Like Complexes Based on â€œAll-Metalâ€•(Al42-) Aromatic Compounds. Journal of the American Chemical Society, 2004, 126, 3380-3381.	13.7	102
45	Clusters of IIâ^'VI Materials:Â CdiXi, X = S, Se, Te,iâ‰ 16. Journal of Physical Chemistry A, 2004, 108, 10502-10508.	2.5	56
46	Incremental binding free energies of aluminum (III) vs. magnesium (II) complexes. Chemical Physics, 2003, 295, 175-184.	1.9	11
47	The electronic states of Fe2+. Chemical Physics Letters, 2003, 376, 310-317.	2.6	19
48	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
49	Electronic Excitation Energies of ZniOiClusters. Journal of the American Chemical Society, 2003, 125, 9494-9499.	13.7	98
50	Clusters of Group IIâ^'VI Materials:â€‰ CdiOi (i â‰ 15). Journal of Physical Chemistry A, 2003, 107, 9918-9923.	2.5	22
51	Atomic charge states in a weakly coupled plasma environment. Physical Review E, 2002, 66, 026408.	2.1	9
52	Hydrogen-Bonding Interactions between Formic Acid and Pyridine. Journal of Physical Chemistry A, 2002, 106, 4187-4191.	2.5	41
53	Aluminum (III) interactions with the side chains of aromatic aminoacids. International Journal of Quantum Chemistry, 2002, 90, 859-881.	2.0	17
54	The Ferroceneâ^'Lithium Cation Complex in the Gas Phase. Journal of the American Chemical Society, 2001, 123, 5040-5043.	13.7	51

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55	Aluminum (III) Interactions with Sulfur-Containing Amino Acid Chains. Journal of Physical Chemistry A, 2001, 105, 7446-7453.	2.5	12
56	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
57	Small clusters of group-(IIâ€“VI) materials:ZniXi,X=Se,Te,i=1â€“9. Physical Review A, 2001, 64, .	2.5	36
58	Quantum mechanical calculations on phosphate hydrolysis reactions. Journal of Computational Chemistry, 2000, 21, 43-51.	3.3	37
59	Aluminum(III) Interactions with the Acid Derivative Amino Acid Chains. Journal of Physical Chemistry A, 2000, 104, 7053-7060.	2.5	22
60	Atomic configuration-interaction electron-electron counterbalance densities. Physical Review A, 1999, 59, 4255-4258.	2.5	22
61	Electronic structures of the bound excited quartet states of the helium anion. Physical Review A, 1999, 60, 4375-4378.	2.5	7
62	Molecular and Electronic Structures of (TiXH6)0/-, X = B, Al, Ga, Compounds. Journal of Physical Chemistry A, 1998, 102, 2055-2064.	2.5	2
63	Aluminum(III) Interactions with the Acidic Amino Acid Chains. Journal of Physical Chemistry A, 1998, 102, 7006-7012.	2.5	25
64	Bound excited states ofHâ^'andHeâ^'in the statically screened Coulomb potential. Physical Review A, 1998, 57, 2550-2555.	2.5	16
65	Molecular and Electronic Structures of TiXH6+(X = B, Al, Ga) Compounds. Journal of Physical Chemistry A, 1997, 101, 5953-5957.	2.5	4
66	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