MarÃ-a de la Merced Montero Campillo

List of Publications by Year
in descending order

79 papers	895 citations	516710 16 h-index	642732 23 g-index
80 all docs	80 docs citations	80 times ranked	792 citing authors

#	Article	IF	Citations
1	A Theoretical Survey of the UVâ€“Visible Spectra of Axially and Peripherally Substituted Boron Subphthalocyanines. Computation, 2022, 10, 14.	2.0	3
2	Malonaldehyde-like Systems: BeF2 Clustersâ€”A Subtle Balance between Hydrogen Bonds, Beryllium Bonds, and Resonance. Sci, 2022, 4, 7.	3.0	0
3	Stand up for Electrostatics: The Disiloxane Case. ChemPhysChem, 2022, 23, .	2.1	3
4	Spontaneous bond dissociation cascades induced by Be_n clusters (n = 2,4). Physical Chemistry Chemical Physics, 2021, 23, 6448-6454.	2.8	3
5	Large Stabilization Effects by Intramolecular Beryllium Bonds in Ortho-Benzene Derivatives. Molecules, 2021, 26, 3401.	3.8	1
6	Clustering of Electron Deficient Bâ€•and Beâ€Containing Analogues: In the Fight for Tetracoordination, Beryllium Takes the Lead. European Journal of Inorganic Chemistry, 2021, 2021, 4393-4401.	2.0	2
7	Significant bonding rearrangements triggered by Mg4 clusters. Journal of Chemical Physics, 2021, 154, 044302.	3.0	2
8	Looking for the Azeotrope: A Computational Study of (Ethanol)6â€“Water, (Methanol)6â€“Water, (Ethanol)7, and (Methanol)7 Heptamers. Journal of Physical Chemistry A, 2020, 124, 7080-7087.	2.5	4
9	Steric clash in real space: biphenyl revisited. Physical Chemistry Chemical Physics, 2020, 22, 21251-21256.	2.8	16
10	The Importance of Strain (Preorganization) in Beryllium Bonds. Molecules, 2020, 25, 5876.	3.8	2
11	Bonding between electron-deficient atoms: strong Lewis-acid character preserved in Xâ€“Yâ€“X (X = B, Al;) Tj ETQq1 1 0.784314 rgBT	2.8	2
12	Mutual Influence of Pnicogen Bonds and Beryllium Bonds: Energies and Structures in the Spotlight. Journal of Physical Chemistry A, 2020, 124, 5871-5878.	2.5	13
13	From Very Strong to Inexistent Beâ‹¯Be Bonds in the Interactions of Be₂ with Ïâ€Systems. ChemPhysChem, 2020, 21, 2701-2708.	2.1	5
14	Are Anions of Cyclobutane Beryllium Derivatives Stabilized through Four-Center One-Electron Bonds?. Journal of Physical Chemistry A, 2020, 124, 1515-1521.	2.5	3
15	Weak Interactions Get Strong: Synergy between Tetrel and Alkaline-Earth Bonds. Journal of Physical Chemistry A, 2019, 123, 7124-7132.	2.5	24
16	The beryllium bond. Advances in Inorganic Chemistry, 2019, 73, 73-121.	1.0	36
17	Modulating the intrinsic reactivity of molecules through non-covalent interactions. Physical Chemistry Chemical Physics, 2019, 21, 2222-2233.	2.8	13
18	Ternary Complexes Stabilized by Chalcogen and Alkalineâ€Earth Bonds: Crucial Role of Cooperativity and Secondary Noncovalent Interactions. Chemistry - A European Journal, 2019, 25, 11688-11695.	3.3	20

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19	Gas-phase reactivity tuned through the interaction with alkaline-earth derivatives. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	5
20	Cations brought together by hydrogen bonds: the protonated pyridineâ€“boronic acid dimer explained. Physical Chemistry Chemical Physics, 2019, 21, 5796-5802.	2.8	33
21	Relativistic Effects on NMR Parameters of Halogen-Bonded Complexes. Molecules, 2019, 24, 4399.	3.8	11
22	Alkylation of uracil and thymine in the gas phase through interaction with alkylmercury compounds. International Journal of Mass Spectrometry, 2019, 436, 153-165.	1.5	5
23	Complexes between H₂ and neutral oxyacid beryllium derivatives. The role of angular strain. Molecular Physics, 2019, 117, 1142-1150.	1.7	5
24	Weak interactions and cooperativity effects on disiloxane: a look at the building block of silicones. Molecular Physics, 2018, 116, 1539-1550.	1.7	10
25	Beâ€•and Mgâ€Based Electron and Anion Sponges. ChemPhysChem, 2018, 19, 1701-1706.	2.1	8
26	Remote modulation of singletâ€“triplet gaps in carbenes. Chemical Physics Letters, 2018, 694, 48-52.	2.6	4
27	Trapping One Electron between Three Beryllium Atoms: Very Strong Oneâ€Electron Threeâ€Center Bonds. ChemPhysChem, 2018, 19, 1068-1074.	2.1	6
28	Hydrogen-Bonding Acceptor Character of Be₃, the Beryllium Three-Membered Ring. Journal of Physical Chemistry A, 2018, 122, 1472-1478.	2.5	15
29	Alkaline-earth (Be, Mg and Ca) bonds at the origin of huge acidity enhancements. Physical Chemistry Chemical Physics, 2018, 20, 2413-2420.	2.8	32
30	Are beryllium-containing biphenyl derivatives efficient anion sponges?. Journal of Molecular Modeling, 2018, 24, 16.	1.8	7
31	Fostering the Basic Instinct of Boron in Boronâ€“Beryllium Interactions. Journal of Physical Chemistry A, 2018, 122, 3313-3319.	2.5	8
32	Protonation of methyluracils in the gas phase: The particular case of 3-methyluracil. International Journal of Mass Spectrometry, 2018, 429, 47-55.	1.5	9
33	Large Protonâ€Affinity Enhancements Triggered by Noncovalent Interactions. Chemistry - A European Journal, 2018, 24, 1971-1977.	3.3	15
34	Using protonation to change a Clâ‹¯N halogen bond in N-Base:ClOH complexes to a Clâ‹¯O halogen bond. Chemical Physics Letters, 2018, 710, 123-128.	2.6	10
35	Complexes between neutral oxyacid beryllium salts and dihydrogen: a possible way for hydrogen storage?. Dalton Transactions, 2018, 47, 12516-12520.	3.3	7
36	Enhancement of Thermodynamic Gasâ€Phase Acidity and Basicity of Water by Means of Secondary Interactions. ChemPhysChem, 2018, 19, 2486-2491.	2.1	2

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37	Intramolecular magnesium bonds in malonaldehyde-like systems: a critical view of the resonance-assisted phenomena. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	8
38	Binding indirect greenhouse gases OCS and CS2by nitrogen heterocyclic carbenes (NHCs). Physical Chemistry Chemical Physics, 2018, 20, 19552-19559.	2.8	20
39	Characterizing magnesium bonds: main features of a non-covalent interaction. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	21
40	Oneâ€Electron Bonds in Frustrated Lewis Pair TPB Ligands: Boron Behaving as a Lewis Base. Angewandte Chemie, 2017, 129, 6892-6896.	2.0	8
41	Trapping CO₂ by Adduct Formation with Nitrogen Heterocyclic Carbenes (NHCs): A Theoretical Study. Chemistry - A European Journal, 2017, 23, 10604-10609.	3.3	45
42	Oneâ€Electron Bonds in Frustrated Lewis Pair TPB Ligands: Boron Behaving as a Lewis Base. Angewandte Chemie - International Edition, 2017, 56, 6788-6792.	13.8	11
43	Modulating the Proton Affinity of Silanol and Siloxane Derivatives by Tetrel Bonds. Journal of Physical Chemistry A, 2017, 121, 7424-7431.	2.5	16
44	Activation of Dinitrogen as A Dipolarophile in 1,3-Dipolar Cycloadditions: A Theoretical Study Using Nitrile Imines as â€œOctetâ€•1,3-Dipoles. Scientific Reports, 2017, 7, 6115.	3.3	10
45	Formation of unexpected silicon- and disiloxane-bridged multiferrocenyl derivatives bearing Siâ€“Oâ€“CHî€CH₂ and Siâ€“(CH₂)₂C(CH₃)₃ substituents via cleavage of tetrahydrofuran and trapping of its ring fragments. Dalton Transactions, 2017, 46, 11584-11597.	3.3	5
46	Beryllium-based fluorenes as efficient anion sponges. Physical Chemistry Chemical Physics, 2017, 19, 23052-23059.	2.8	10
47	Gasâ€Phase Infrared Spectroscopy of Substituted Cyanobutadiynes: Roles of the Bromine Atom and Methyl Group as Substituents. ChemPhysChem, 2016, 17, 1018-1024.	2.1	8
48	Charge Transfer in Beryllium Bonds and Cooperativity of Beryllium and Halogen Bonds. A New Perspective. Challenges and Advances in Computational Chemistry and Physics, 2016, , 461-489.	0.6	1
49	Multi-Ferrocene-Containing Silanols as Redox-Active Anion Receptors. Organometallics, 2016, 35, 3507-3519.	2.3	12
50	Boronâ€Boron Oneâ€Electron Sigma Bonds versus Bâ€“Xâ€“B Bridged Structures. Chemistry - A European Journal, 2016, 22, 13697-13704.	3.3	13
51	Beryllium subphthalocyanines self-assembling properties. Canadian Journal of Chemistry, 2016, 94, 1015-1021.	1.1	3
52	Photochemical Behavior of Beryllium Complexes with Subporphyrazines and Subphthalocyanines. Journal of Physical Chemistry A, 2016, 120, 4845-4852.	2.5	12
53	Ferrocene and Silicon-Containing Oxathiacrown Macrocycles and Linear Oligo-Oxathioethers Obtained via Thiolâ€“Ene Chemistry of a Redox-Active Bifunctional Vinyldisiloxane. Macromolecules, 2015, 48, 6955-6969.	4.8	14
54	Intervalence charge transfer across noncovalent interactions on vinyl silyl bridged biferrocenyl compounds. Computational and Theoretical Chemistry, 2015, 1053, 281-288.	2.5	5

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55	Some Interesting Features of Non-Covalent Interactions. Croatica Chemica Acta, 2014, 87, 291-306.	0.4	14
56	On the Structures, Lifetimes, and Infrared Spectra of Alkylmercury Hydrides. ChemPhysChem, 2014, 15, 530-541.	2.1	3
57	Spontaneous H₂ Loss through the Interaction of Squaric Acid Derivatives and BeH₂. Chemistry - A European Journal, 2014, 20, 5309-5316.	3.3	19
58	Thermodynamic stability of PFOS: M06-2X and B3LYP comparison. Computational and Theoretical Chemistry, 2014, 1046, 81-92.	2.5	22
59	Behavior of Carboxylic Acids upon Complexation with Beryllium Compounds. Journal of Physical Chemistry A, 2014, 118, 5720-5726.	2.5	9
60	On the stability of [Pb(Proline)]2+ complexes. Reconciling theory with experiment. Chemical Physics Letters, 2014, 598, 91-95.	2.6	6
61	Alkyl mercury compounds: an assessment of DFT methods. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	19
62	Mechanochemical and silica gel-mediated formation of highly electron-poor 1-cyanocarbonylferrocene. Chemical Communications, 2013, 49, 9785.	4.1	15
63	Modulating weak intramolecular interactions through the formation of beryllium bonds: complexes between squaric acid and BeH2. Journal of Molecular Modeling, 2013, 19, 2759-2766.	1.8	24
64	Mechanism of aziridination of styrene catalyzed by copper(I) bis(oxazoline). International Journal of Quantum Chemistry, 2013, 113, 2002-2011.	2.0	4
65	UV/Vis Spectra of Subporphyrazines and Subphthalocyanines with Aluminum and Gallium: A Timeâ€Dependent DFT Study. ChemPhysChem, 2013, 14, 915-922.	2.1	10
66	Lithium diffusion pathways and vacancy formation in the Pmmn-Li1â^'xFeO2 electrode material. Physical Chemistry Chemical Physics, 2011, 13, 11156.	2.8	7
67	First-principles modelling of lithium iron oxides as battery cathode materials. Journal of Power Sources, 2011, 196, 3955-3961.	7.8	23
68	Thermodynamic Stability of Neutral and Anionic PFOS: A Gas-Phase, n-Octanol, and Water Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 10148-10155.	2.5	19
69	Study of the ferroceneâ€“lithium cation interaction by DFT calculations: an in-depth analysis of the existence of a planetary system. Tetrahedron, 2009, 65, 2368-2371.	1.9	17
70	An Alternative Mechanism to Explain the Ruthenium(II)-Catalyzed [2 + 2 + 2] Cycloaddition of 1,6-Diynes and Tricarbonyl Compounds. Journal of Physical Chemistry A, 2009, 113, 9180-9184.	2.5	4
71	On the mechanism of rhodium-catalyzed [6+2] cycloaddition of 2-vinylcyclobutanones and alkenes. Tetrahedron, 2008, 64, 6215-6220.	1.9	19
72	A Theoretical Study of Pericyclic Rearrangements Catalyzed by Lithium. Journal of Physical Chemistry A, 2008, 112, 5218-5223.	2.5	2

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73	Theoretical Study of the [2+2+2+1] Cycloaddition Mechanism of Enediynes and Carbon Monoxide Catalyzed by Rhodium. Journal of Physical Chemistry A, 2008, 112, 2423-2427.	2.5	15
74	Density Functional Theory Study of Ruthenium (II)-Catalyzed [2+2+2] Cycloaddition of 1,6-Diynes with Tricarbonyl Compounds. Journal of Physical Chemistry A, 2008, 112, 8116-8120.	2.5	6
75	A Density Functional Theory Study of Rhodium-Catalyzed Hetero-[5+2]-cycloaddition of Cyclopropyl Imine Derivatives and Alkynes. Journal of Physical Chemistry A, 2008, 112, 9068-9074.	2.5	31
76	Ab initio and DFT study of the aromaticity of some Fulvalenes derived from Methylidenecyclopropabenzene. Journal of Molecular Modeling, 2007, 13, 919-926.	1.8	16
77	Ab Initio and DFT Study of the Reaction Mechanism of Diformylketene with Formamide. Journal of Physical Chemistry A, 2004, 108, 8373-8377.	2.5	22
78	Disrupting bonding in azoles through beryllium bonds: Unexpected coordination patterns and acidity enhancement. Journal of Chemical Physics, 0, , .	3.0	2
79	On predicting bonding patterns of small clusters of alkaline-earth (Be, Mg) and triel (B, Al) fluorides: a balance between atomic size and electron-deficient character. Molecular Physics, 0, , .	1.7	0