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	Trapping CO₂ by Adduct Formation with Nitrogen Heterocyclic Carbenes (NHCs): A Theoretical Study. Chemistry - A European Journal, 2017, 23, 10604-10609.	3.3	45
2	The beryllium bond. Advances in Inorganic Chemistry, 2019, 73, 73-121.	1.0	36
3	Cations brought together by hydrogen bonds: the protonated pyridineâ€“boronic acid dimer explained. Physical Chemistry Chemical Physics, 2019, 21, 5796-5802.	2.8	33
4	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
5	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
6	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
7	Weak Interactions Get Strong: Synergy between Tetrel and Alkaline-Earth Bonds. Journal of Physical Chemistry A, 2019, 123, 7124-7132.	2.5	24
8	First-principles modelling of lithium iron oxides as battery cathode materials. Journal of Power Sources, 2011, 196, 3955-3961.	7.8	23
9	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
10	Thermodynamic stability of PFOS: M06-2X and B3LYP comparison. Computational and Theoretical Chemistry, 2014, 1046, 81-92.	2.5	22
11	Characterizing magnesium bonds: main features of a non-covalent interaction. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	21
12	Binding indirect greenhouse gases OCS and CS2by nitrogen heterocyclic carbenes (NHCs). Physical Chemistry Chemical Physics, 2018, 20, 19552-19559.	2.8	20
13	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
14	On the mechanism of rhodium-catalyzed [6+2] cycloaddition of 2-vinylcyclobutanones and alkenes. Tetrahedron, 2008, 64, 6215-6220.	1.9	19
15	Thermodynamic Stability of Neutral and Anionic PFOS: A Gas-Phase, <i>n</i>-Octanol, and Water Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 10148-10155.	2.5	19
16	Alkyl mercury compounds: an assessment of DFT methods. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	19
17	Spontaneous H₂ Loss through the Interaction of Squaric Acid Derivatives and BeH₂. Chemistry - A European Journal, 2014, 20, 5309-5316.	3.3	19
18	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

#	Article	IF	Citations
19	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
20	Modulating the Proton Affinity of Silanol and Siloxane Derivatives by Tetrel Bonds. Journal of Physical Chemistry A, 2017, 121, 7424-7431.	2.5	16
21	Steric clash in real space: biphenyl revisited. Physical Chemistry Chemical Physics, 2020, 22, 21251-21256.	2.8	16
22	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
23	Mechanochemical and silica gel-mediated formation of highly electron-poor 1-cyanocarbonylferrocene. Chemical Communications, 2013, 49, 9785.	4.1	15
24	Hydrogen-Bonding Acceptor Character of Be₃, the Beryllium Three-Membered Ring. Journal of Physical Chemistry A, 2018, 122, 1472-1478.	2.5	15
25	Large Protonâ€Affinity Enhancements Triggered by Noncovalent Interactions. Chemistry - A European Journal, 2018, 24, 1971-1977.	3.3	15
26	Some Interesting Features of Non-Covalent Interactions. Croatica Chemica Acta, 2014, 87, 291-306.	0.4	14
27	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
28	Boronâ€Boron Oneâ€Electron Sigma Bonds versus Bâ€Xâ€B Bridged Structures. Chemistry - A European Journal, 2016, 22, 13697-13704.	3.3	13
29	Modulating the intrinsic reactivity of molecules through non-covalent interactions. Physical Chemistry Chemical Physics, 2019, 21, 2222-2233.	2.8	13
30	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
31	Multi-Ferrocene-Containing Silanols as Redox-Active Anion Receptors. Organometallics, 2016, 35, 3507-3519.	2.3	12
32	Photochemical Behavior of Beryllium Complexes with Subporphyrazines and Subphthalocyanines. Journal of Physical Chemistry A, 2016, 120, 4845-4852.	2.5	12
33	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
34	Relativistic Effects on NMR Parameters of Halogen-Bonded Complexes. Molecules, 2019, 24, 4399.	3.8	11
35	UV/Vis Spectra of Subporphyrazines and Subphthalocyanines with Aluminum and Gallium: A Timeâ€Dependent DFT Study. ChemPhysChem, 2013, 14, 915-922.	2.1	10
36	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

#	Article	IF	Citations
37	Beryllium-based fluorenes as efficient anion sponges. Physical Chemistry Chemical Physics, 2017, 19, 23052-23059.	2.8	10
38	Weak interactions and cooperativity effects on disiloxane: a look at the building block of silicones. Molecular Physics, 2018, 116, 1539-1550.	1.7	10
39	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
40	Behavior of Carboxylic Acids upon Complexation with Beryllium Compounds. Journal of Physical Chemistry A, 2014, 118, 5720-5726.	2.5	9
41	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
42	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
43	Oneâ€Electron Bonds in Frustrated Lewis Pair TPB Ligands: Boron Behaving as a Lewis Base. Angewandte Chemie, 2017, 129, 6892-6896.	2.0	8
44	Beâ€•and Mgâ€Based Electron and Anion Sponges. ChemPhysChem, 2018, 19, 1701-1706.	2.1	8
45	Fostering the Basic Instinct of Boron in Boronâ€“Beryllium Interactions. Journal of Physical Chemistry A, 2018, 122, 3313-3319.	2.5	8
46	Intramolecular magnesium bonds in malonaldehyde-like systems: a critical view of the resonance-assisted phenomena. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	8
47	Lithium diffusion pathways and vacancy formation in the Pmmn-Li1âˆ’xFeO2 electrode material. Physical Chemistry Chemical Physics, 2011, 13, 11156.	2.8	7
48	Are beryllium-containing biphenyl derivatives efficient anion sponges?. Journal of Molecular Modeling, 2018, 24, 16.	1.8	7
49	Complexes between neutral oxyacid beryllium salts and dihydrogen: a possible way for hydrogen storage?. Dalton Transactions, 2018, 47, 12516-12520.	3.3	7
50	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
51	On the stability of [Pb(Proline)]2+ complexes. Reconciling theory with experiment. Chemical Physics Letters, 2014, 598, 91-95.	2.6	6
52	Trapping One Electron between Three Beryllium Atoms: Very Strong Oneâ€Electron Threeâ€Center Bonds. ChemPhysChem, 2018, 19, 1068-1074.	2.1	6
53	Intervalence charge transfer across noncovalent interactions on vinyl silyl bridged biferrocenyl compounds. Computational and Theoretical Chemistry, 2015, 1053, 281-288.	2.5	5
54	Formation of unexpected silicon- and disiloxane-bridged multiferrocenyl derivatives bearing Siâ€“Oâ€“CHî€CH₂ and Siâ€“(CH₂)₂C(CH₃)₃ substituents <i>via</i> cleavage of tetrahydrofuran and trapping of its ring fragments. Dalton Transactions, 2017, 46, 11584-11597.	3.3	5

#	Article	IF	Citations
55	Gas-phase reactivity tuned through the interaction with alkaline-earth derivatives. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	5
56	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
57	Complexes between H₂ and neutral oxyacid beryllium derivatives. The role of angular strain. Molecular Physics, 2019, 117, 1142-1150.	1.7	5
58	From Very Strong to Inexistent Beâˆ’Be Bonds in the Interactions of Be₂ with Ï€â€Systems. ChemPhysChem, 2020, 21, 2701-2708.	2.1	5
59	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
60	Mechanism of aziridination of styrene catalyzed by copper(I) bis(oxazoline). International Journal of Quantum Chemistry, 2013, 113, 2002-2011.	2.0	4
61	Remote modulation of singletâ€“triplet gaps in carbenes. Chemical Physics Letters, 2018, 694, 48-52.	2.6	4
62	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
63	On the Structures, Lifetimes, and Infrared Spectra of Alkylmercury Hydrides. ChemPhysChem, 2014, 15, 530-541.	2.1	3
64	Beryllium subphthalocyanines self-assembling properties. Canadian Journal of Chemistry, 2016, 94, 1015-1021.	1.1	3
65	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
66	Spontaneous bond dissociation cascades induced by Be_n clusters (<i>n</i> = 2,4). Physical Chemistry Chemical Physics, 2021, 23, 6448-6454.	2.8	3
67	A Theoretical Survey of the UVâ€“Visible Spectra of Axially and Peripherally Substituted Boron Subphthalocyanines. Computation, 2022, 10, 14.	2.0	3
68	Stand up for Electrostatics: The Disiloxane Case. ChemPhysChem, 2022, 23, .	2.1	3
69	A Theoretical Study of Pericyclic Rearrangements Catalyzed by Lithium. Journal of Physical Chemistry A, 2008, 112, 5218-5223.	2.5	2
70	Enhancement of Thermodynamic Gasâ€Phase Acidity and Basicity of Water by Means of Secondary Interactions. ChemPhysChem, 2018, 19, 2486-2491.	2.1	2
71	The Importance of Strain (Preorganization) in Beryllium Bonds. Molecules, 2020, 25, 5876.	3.8	2
72	Bonding between electron-deficient atoms: strong Lewis-acid character preserved in Xâ€“Yâ€“X (X = B, Al;) Tj ETQq0 0 0 rgBT /Overlock	2.8	2

#	Article	IF	Citations
73	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
74	Significant bonding rearrangements triggered by Mg4 clusters. Journal of Chemical Physics, 2021, 154, 044302.	3.0	2
75	Disrupting bonding in azoles through beryllium bonds: Unexpected coordination patterns and acidity enhancement. Journal of Chemical Physics, 0, , .	3.0	2
76	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
77	Large Stabilization Effects by Intramolecular Beryllium Bonds in Ortho-Benzene Derivatives. Molecules, 2021, 26, 3401.	3.8	1
78	Malonaldehyde-like Systems: BeF2 Clustersâ€"A Subtle Balance between Hydrogen Bonds, Beryllium Bonds, and Resonance. Sci, 2022, 4, 7.	3.0	0
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