

M Merced Montero-Campillo

List of Publications by Year in descending order

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66
papers

715
citations

567281

15
h-index

713466

21
g-index

67
all docs

67
docs citations

67
times ranked

538
citing authors

#	ARTICLE	IF	CITATIONS
1	Trapping CO ₂ by Adduct Formation with Nitrogen Heterocyclic Carbenes (NHCs): A Theoretical Study. <i>Chemistry - A European Journal</i> , 2017, 23, 10604-10609.	3.3	45
2	The beryllium bond. <i>Advances in Inorganic Chemistry</i> , 2019, 73, 73-121.	1.0	36
3	Alkaline-earth (Be, Mg and Ca) bonds at the origin of huge acidity enhancements. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2413-2420.	2.8	32
4	Modulating weak intramolecular interactions through the formation of beryllium bonds: complexes between squaric acid and BeH ₂ . <i>Journal of Molecular Modeling</i> , 2013, 19, 2759-2766.	1.8	24
5	Weak Interactions Get Strong: Synergy between Tetrel and Alkaline-Earth Bonds. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7124-7132.	2.5	24
6	Thermodynamic stability of PFOS: M06-2X and B3LYP comparison. <i>Computational and Theoretical Chemistry</i> , 2014, 1046, 81-92.	2.5	22
7	Characterizing magnesium bonds: main features of a non-covalent interaction. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	21
8	Binding indirect greenhouse gases OCS and CS ₂ by nitrogen heterocyclic carbenes (NHCs). <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19552-19559.	2.8	20
9	Ternary Complexes Stabilized by Chalcogen and Alkaline-Earth Bonds: Crucial Role of Cooperativity and Secondary Noncovalent Interactions. <i>Chemistry - A European Journal</i> , 2019, 25, 11688-11695.	3.3	20
10	On the mechanism of rhodium-catalyzed [6+2] cycloaddition of 2-vinylcyclobutanones and alkenes. <i>Tetrahedron</i> , 2008, 64, 6215-6220.	1.9	19
11	Thermodynamic Stability of Neutral and Anionic PFOS: A Gas-Phase, <i>n</i> -Octanol, and Water Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10148-10155.	2.5	19
12	Alkyl mercury compounds: an assessment of DFT methods. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	1.4	19
13	Spontaneous H ₂ Loss through the Interaction of Squaric Acid Derivatives and BeH ₂ . <i>Chemistry - A European Journal</i> , 2014, 20, 5309-5316.	3.3	19
14	Study of the ferrocene-lithium cation interaction by DFT calculations: an in-depth analysis of the existence of a planetary system. <i>Tetrahedron</i> , 2009, 65, 2368-2371.	1.9	17
15	Ab initio and DFT study of the aromaticity of some Fulvalenes derived from Methylidenecyclopropabenzene. <i>Journal of Molecular Modeling</i> , 2007, 13, 919-926.	1.8	16
16	Modulating the Proton Affinity of Silanol and Siloxane Derivatives by Tetrel Bonds. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7424-7431.	2.5	16
17	Theoretical Study of the [2+2+2+1] Cycloaddition Mechanism of Eneidyne and Carbon Monoxide Catalyzed by Rhodium. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2423-2427.	2.5	15
18	Hydrogen-Bonding Acceptor Character of Be ₃ , the Beryllium Three-Membered Ring. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1472-1478.	2.5	15

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19	Large Proton Affinity Enhancements Triggered by Noncovalent Interactions. <i>Chemistry - A European Journal</i> , 2018, 24, 1971-1977.	3.3	15
20	Some Interesting Features of Non-Covalent Interactions. <i>Croatica Chemica Acta</i> , 2014, 87, 291-306.	0.4	14
21	Ferrocene and Silicon-Containing Oxathiacrown Macrocycles and Linear Oligo-Oxathioethers Obtained via Thiol-Ene Chemistry of a Redox-Active Bifunctional Vinyldisiloxane. <i>Macromolecules</i> , 2015, 48, 6955-6969.	4.8	14
22	Boron-Boron One-Electron Sigma Bonds versus Boron-Bridged Structures. <i>Chemistry - A European Journal</i> , 2016, 22, 13697-13704.	3.3	13
23	Modulating the intrinsic reactivity of molecules through non-covalent interactions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2222-2233.	2.8	13
24	Mutual Influence of Pnictogen Bonds and Beryllium Bonds: Energies and Structures in the Spotlight. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5871-5878.	2.5	13
25	Multi-Ferrocene-Containing Silanols as Redox-Active Anion Receptors. <i>Organometallics</i> , 2016, 35, 3507-3519.	2.3	12
26	Photochemical Behavior of Beryllium Complexes with Subporphyrzines and Subphthalocyanines. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4845-4852.	2.5	12
27	One-Electron Bonds in Frustrated Lewis Pair TPB Ligands: Boron Behaving as a Lewis Base. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 6788-6792.	13.8	11
28	UV/Vis Spectra of Subporphyrzines and Subphthalocyanines with Aluminum and Gallium: A Time-Dependent DFT Study. <i>ChemPhysChem</i> , 2013, 14, 915-922.	2.1	10
29	Activation of Dinitrogen as A Dipolarophile in 1,3-Dipolar Cycloadditions: A Theoretical Study Using Nitrile Imines as Octet-1,3-Dipoles. <i>Scientific Reports</i> , 2017, 7, 6115.	3.3	10
30	Beryllium-based fluorenes as efficient anion sponges. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23052-23059.	2.8	10
31	Weak interactions and cooperativity effects on disiloxane: a look at the building block of silicones. <i>Molecular Physics</i> , 2018, 116, 1539-1550.	1.7	10
32	Using protonation to change a Cl-N halogen bond in N-Base:ClOH complexes to a Cl-O halogen bond. <i>Chemical Physics Letters</i> , 2018, 710, 123-128.	2.6	10
33	Behavior of Carboxylic Acids upon Complexation with Beryllium Compounds. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5720-5726.	2.5	9
34	Protonation of methyluracils in the gas phase: The particular case of 3-methyluracil. <i>International Journal of Mass Spectrometry</i> , 2018, 429, 47-55.	1.5	9
35	One-Electron Bonds in Frustrated Lewis Pair TPB Ligands: Boron Behaving as a Lewis Base. <i>Angewandte Chemie</i> , 2017, 129, 6892-6896.	2.0	8
36	Be- and Mg-Based Electron and Anion Sponges. <i>ChemPhysChem</i> , 2018, 19, 1701-1706.	2.1	8

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37	Fostering the Basic Instinct of Boron in Boron-Beryllium Interactions. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3313-3319.	2.5	8
38	Intramolecular magnesium bonds in malonaldehyde-like systems: a critical view of the resonance-assisted phenomena. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	8
39	Are beryllium-containing biphenyl derivatives efficient anion sponges?. <i>Journal of Molecular Modeling</i> , 2018, 24, 16.	1.8	7
40	Complexes between neutral oxyacid beryllium salts and dihydrogen: a possible way for hydrogen storage?. <i>Dalton Transactions</i> , 2018, 47, 12516-12520.	3.3	7
41	Density Functional Theory Study of Ruthenium (II)-Catalyzed [2+2+2] Cycloaddition of 1,6-Diynes with Tricarbonyl Compounds. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8116-8120.	2.5	6
42	On the stability of [Pb(Proline)] ²⁺ complexes. Reconciling theory with experiment. <i>Chemical Physics Letters</i> , 2014, 598, 91-95.	2.6	6
43	Trapping One Electron between Three Beryllium Atoms: Very Strong One-Electron Three-Center Bonds. <i>ChemPhysChem</i> , 2018, 19, 1068-1074.	2.1	6
44	Intervale charge transfer across noncovalent interactions on vinyl silyl bridged biferrocenyl compounds. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 281-288.	2.5	5
45	Formation of unexpected silicon- and disiloxane-bridged multiferrocenyl derivatives bearing Si-O-C≡CH ₂ and Si-(CH ₂) ₂ C(CH ₃) ₃ substituents via cleavage of tetrahydrofuran and trapping of its ring fragments. <i>Dalton Transactions</i> , 2017, 46, 11584-11597.	3.3	5
46	Gas-phase reactivity tuned through the interaction with alkaline-earth derivatives. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	1.4	5
47	Alkylation of uracil and thymine in the gas phase through interaction with alkylmercury compounds. <i>International Journal of Mass Spectrometry</i> , 2019, 436, 153-165.	1.5	5
48	Complexes between H ₂ and neutral oxyacid beryllium derivatives. The role of angular strain. <i>Molecular Physics</i> , 2019, 117, 1142-1150.	1.7	5
49	From Very Strong to Inexistent Be-Be Bonds in the Interactions of Be ₂ with π -Systems. <i>ChemPhysChem</i> , 2020, 21, 2701-2708.	2.1	5
50	Remote modulation of singlet-triplet gaps in carbenes. <i>Chemical Physics Letters</i> , 2018, 694, 48-52.	2.6	4
51	On the Structures, Lifetimes, and Infrared Spectra of Alkylmercury Hydrides. <i>ChemPhysChem</i> , 2014, 15, 530-541.	2.1	3
52	Beryllium subphthalocyanines self-assembling properties. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1015-1021.	1.1	3
53	Are Anions of Cyclobutane Beryllium Derivatives Stabilized through Four-Center One-Electron Bonds?. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1515-1521.	2.5	3
54	Spontaneous bond dissociation cascades induced by Be _n clusters ($n = 2, 4$). <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6448-6454.	2.8	3

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55	A Theoretical Survey of the UV-Visible Spectra of Axially and Peripherally Substituted Boron Subphthalocyanines. <i>Computation</i> , 2022, 10, 14.	2.0	3
56	Stand up for Electrostatics: The Disiloxane Case. <i>ChemPhysChem</i> , 2022, 23, .	2.1	3
57	A Theoretical Study of Pericyclic Rearrangements Catalyzed by Lithium. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5218-5223.	2.5	2
58	Enhancement of Thermodynamic Gas-Phase Acidity and Basicity of Water by Means of Secondary Interactions. <i>ChemPhysChem</i> , 2018, 19, 2486-2491.	2.1	2
59	The Importance of Strain (Preorganization) in Beryllium Bonds. <i>Molecules</i> , 2020, 25, 5876.	3.8	2
60	Bonding between electron-deficient atoms: strong Lewis-acid character preserved in X_2Y_2 ($X = B, Al$); $Tj ETQq0.0 0 rgBT_2/Overlock$	2.8	2
61	Clustering of Electron Deficient B_2 - and Be_2 -Containing Analogues: In the Fight for Tetracoordination, Beryllium Takes the Lead. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 4393-4401.	2.0	2
62	Significant bonding rearrangements triggered by Mg_4 clusters. <i>Journal of Chemical Physics</i> , 2021, 154, 044302.	3.0	2
63	Charge Transfer in Beryllium Bonds and Cooperativity of Beryllium and Halogen Bonds. A New Perspective. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2016, , 461-489.	0.6	1
64	Large Stabilization Effects by Intramolecular Beryllium Bonds in Ortho-Benzene Derivatives. <i>Molecules</i> , 2021, 26, 3401.	3.8	1
65	Malonaldehyde-like Systems: BeF_2 Clusters – A Subtle Balance between Hydrogen Bonds, Beryllium Bonds, and Resonance. <i>Sci</i> , 2022, 4, 7.	3.0	0
66	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. <i>Molecular Physics</i> , 0, , .	1.7	0