Bogdan FrecuÈ

List of Publications by Year
in descending order

15 papers	176 citations	1040056 9 h-index	1058476 14 g-index
15 all docs	15 docs citations	15 times ranked	345 citing authors

#	Article	IF	Citations
1	Intra- and Inter-Molecular Spin Coupling in Phenalenyl Dimeric Systems. Journal of Physical Chemistry A, 2021, 125, 6893-6901.	2.5	7
2	Molecular and Supramolecular Interactions in Systems with Nitroxide-Based Radicals. International Journal of Molecular Sciences, 2019, 20, 4733.	4.1	6
3	Valence Bond Account of Triangular Polyaromatic Hydrocarbons with Spin: Combining Ab Initio and Phenomenological Approaches. Journal of Physical Chemistry C, 2019, 123, 6869-6880.	3.1	18
4	On The Density Functional Theory Treatment of Lanthanide Coordination Compounds: A Comparative Study in a Series of Cuâ€“Ln (Ln = Gd, Tb, Lu) Binuclear Complexes. Inorganic Chemistry, 2017, 56, 9474-9485.	4.0	22
5	Noble gas endohedral fullerenes, Ng@C60 (Ng=Ar, Kr): a particular benchmark for assessing the account of non-covalent interactions by density functional theory calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	11
6	On exchange coupling and bonding in the Gd₂@C₈₀ and Gd₂@C₇₉N endohedral dimetallo-fullerenes. Molecular Physics, 2015, 113, 1712-1727.	1.7	17
7	Ab initio study of exchange coupling for the consistent understanding of the magnetic ordering at room temperature in V[TCNE] x. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	9
8	Disorder, exchange and magnetic anisotropy in the room-temperature molecular magnet V[TCNE]x â€“ A theoretical study. Computational Materials Science, 2014, 91, 320-328.	3.0	11
9	EPR spin Hamiltonian parameters of encapsulated spin-labels: impact of the hydrogen bonding topology. Physical Chemistry Chemical Physics, 2013, 15, 2427.	2.8	4
10	Ï€-Stacking effects on the EPR parameters of a prototypical DNA spin label. Physical Chemistry Chemical Physics, 2013, 15, 10466.	2.8	2
11	Encapsulation Influence on EPR Parameters of Spin-Labels: 2,2,6,6-Tetramethyl-4-methoxypiperidine-1-oxyl in Cucurbit[8]uril. Journal of Chemical Theory and Computation, 2012, 8, 257-263.	5.3	19
12	Density Functional Restrictedâ€“Unrestricted/Molecular Mechanics Theory for Hyperfine Coupling Constants of Molecules in Solution. Journal of Chemical Theory and Computation, 2011, 7, 3261-3271.	5.3	18
13	DFT study of structureâ€“properties correlations in [MnTPP][TCNE] quasi-one-dimensional molecular magnets. Theoretical Chemistry Accounts, 2011, 129, 847-857.	1.4	8
14	DFT study of electronic structure and optical properties of some Ru- and Rh-based complexes for dye-sensitized solar cells. Molecular Physics, 2011, 109, 2511-2523.	1.7	14
15	The DFT rationalization of exchange and anisotropy in one-dimensional d-p magnets: The [MnIII(porphyrin)][TCNE] case study. Polyhedron, 2009, 28, 2039-2043.	2.2	10