

# Bogdan FrecuÈ

## List of Publications by Year in descending order

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15  
papers

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docs citations

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#	ARTICLE	IF	CITATIONS
1	On The Density Functional Theory Treatment of Lanthanide Coordination Compounds: A Comparative Study in a Series of Cu <sup>II</sup> -Ln (Ln = Gd, Tb, Lu) Binuclear Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 9474-9485.	4.0	22
2	Encapsulation Influence on EPR Parameters of Spin-Labels: 2,2,6,6-Tetramethyl-4-methoxypiperidine-1-oxyl in Cucurbit[8]uril. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 257-263.	5.3	19
3	Density Functional Restricted/Unrestricted/Molecular Mechanics Theory for Hyperfine Coupling Constants of Molecules in Solution. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3261-3271.	5.3	18
4	Valence Bond Account of Triangular Polyaromatic Hydrocarbons with Spin: Combining Ab Initio and Phenomenological Approaches. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6869-6880.	3.1	18
5	On exchange coupling and bonding in the Gd <sub>2</sub> @C <sub>80</sub> and Gd <sub>2</sub> @C <sub>79</sub> N endohedral dimetallo-fullerenes. <i>Molecular Physics</i> , 2015, 113, 1712-1727.	1.7	17
6	DFT study of electronic structure and optical properties of some Ru- and Rh-based complexes for dye-sensitized solar cells. <i>Molecular Physics</i> , 2011, 109, 2511-2523.	1.7	14
7	Disorder, exchange and magnetic anisotropy in the room-temperature molecular magnet V[TCNE] <sub>x</sub> – A theoretical study. <i>Computational Materials Science</i> , 2014, 91, 320-328.	3.0	11
8	Noble gas endohedral fullerenes, Ng@C <sub>60</sub> (Ng=Ar, Kr): a particular benchmark for assessing the account of non-covalent interactions by density functional theory calculations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	11
9	The DFT rationalization of exchange and anisotropy in one-dimensional d-p magnets: The [MnIII(porphyrin)][TCNE] case study. <i>Polyhedron</i> , 2009, 28, 2039-2043.	2.2	10
10	Ab initio study of exchange coupling for the consistent understanding of the magnetic ordering at room temperature in V[TCNE] <sub>x</sub> . <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	9
11	DFT study of structure-properties correlations in [MnTPP][TCNE] quasi-one-dimensional molecular magnets. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 847-857.	1.4	8
12	Intra- and Inter-Molecular Spin Coupling in Phenalenyl Dimeric Systems. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6893-6901.	2.5	7
13	Molecular and Supramolecular Interactions in Systems with Nitroxide-Based Radicals. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4733.	4.1	6
14	EPR spin Hamiltonian parameters of encapsulated spin-labels: impact of the hydrogen bonding topology. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 2427.	2.8	4
15	π-Stacking effects on the EPR parameters of a prototypical DNA spin label. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10466.	2.8	2