Stepan Stepanovic

List of Publications by Year in descending order

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20 papers	300 citations	933447 10 h-index	888059 17 g-index
22 all docs	22 docs citations	22 times ranked	596 citing authors

#	Article	IF	Citations
1	Unique mononuclear Mn^{II}complexes of an end-off compartmental Schiff base ligand: experimental and theoretical studies on their bio-relevant catalytic promiscuity. Dalton Transactions, 2016, 45, 12409-12422.	3.3	55
2	Benchmarking density functional tight binding models for barrier heights and reaction energetics of organic molecules. Journal of Computational Chemistry, 2017, 38, 2171-2185.	3.3	39
3	A Nonâ€Heme Iron Photocatalyst for Lightâ€Driven Aerobic Oxidation of Methanol. Angewandte Chemie - International Edition, 2018, 57, 3207-3211.	13.8	34
4	A density functional study of the spin state energetics of polypyrazolylborato complexes of first-row transition metals. Physical Chemistry Chemical Physics, 2014, 16, 14514.	2.8	20
5	Lewis versus BrÃ¸nsted Acid Activation of a Mn(IV) Catalyst for Alkene Oxidation. Inorganic Chemistry, 2019, 58, 14924-14930.	4.0	20
6	Role of Spin State and Ligand Charge in Coordination Patterns in Complexes of 2,6-Diacetylpyridinebis(semioxamazide) with 3d-Block Metal Ions: A Density Functional Theory Study. Inorganic Chemistry, 2013, 52, 13415-13423.	4.0	19
7	Spin state relaxation of iron complexes: The case for OPBE and S12g. Journal of the Serbian Chemical Society, 2015, 80, 1399-1410.	0.8	15
8	Experimental and theoretical investigation of octahedral and square-planar isothiocyanato complexes of Ni(II) with acylhydrazones of 2-(diphenylphosphino)benzaldehyde. Polyhedron, 2015, 89, 271-279.	2.2	13
9	Magnetic Anisotropy in â€œScorpionateâ€•Firstâ€Row Transitionâ€Metal Complexes: A Theoretical Investigation. Chemistry - A European Journal, 2015, 21, 3716-3726.	3.3	12
10	Challenges in assignment of orbital populations in a high spin manganese(<scp>iii</scp>) complex. Dalton Transactions, 2016, 45, 6702-6708.	3.3	11
11	Resolving the origin of the multimode Jahnâ€“Teller effect in metallophthalocyanines. Physical Chemistry Chemical Physics, 2016, 18, 29122-29130.	2.8	10
12	Structural diversity of isothiocyanato Cd(II) and Zn(II) Girardâ€™s T hydrazone complexes in solution and solid state: effect of H-bonding on coordination number and supramolecular assembly of Cd(II) complex in solid state. Structural Chemistry, 2018, 29, 1797-1806.	2.0	10
13	Density functional approximations for consistent spin and oxidation states of oxoiron complexes. International Journal of Quantum Chemistry, 2020, 120, e26121.	2.0	10
14	The role of spin states in the catalytic mechanism of the intra- and extradiol cleavage of catechols by O₂. Organic and Biomolecular Chemistry, 2017, 15, 7860-7868.	2.8	9
15	A Nonâ€Heme Iron Photocatalyst for Lightâ€Driven Aerobic Oxidation of Methanol. Angewandte Chemie, 2018, 130, 3261-3265.	2.0	5
16	Selective Photo-Induced Oxidation with O₂ of a Non-Heme Iron(III) Complex to a Bis(imine-pyridyl)iron(II) Complex. Inorganic Chemistry, 2018, 57, 4510-4515.	4.0	5
17	The Irony of Manganocene: An Interplay between the Jahnâ€“Teller Effect and Close-Lying Electronic and Spin States. Journal of Chemical Information and Modeling, 2019, 59, 1806-1810.	5.4	4
18	Decarbonylative Dibromination of 5-Phenylthiophene-2-carbaldehyde with Bromine. Synthesis, 2016, 48, 4423-4430.	2.3	3

#	Article	IF	Citations
19	High-yielding method for preparation of carbocyclic or N-containing heterocyclic Î²-keto esters using in situ activated sodium hydride in dimethyl sulphoxide. Green Chemistry Letters and Reviews, 2016, 9, 61-68.	4.7	3
20	Improvement of dâ€“d interactions in density functional tight binding for transition metal ions with a ligand field model: assessment of a DFTB3+U model on nickel coordination compounds. Physical Chemistry Chemical Physics, 2020, 22, 27084-27095.	2.8	3