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List of Publications by Year in descending order

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papers

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749
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#	ARTICLE	IF	CITATIONS
1	The Mechanism of Stereospecific C-H Oxidation by Fe(Pytacn) Complexes: Bioinspired Non-Heme Iron Catalysts Containing Labile Exchangeable Sites. <i>Chemistry - A European Journal</i> , 2013, 19, 6724-6738.	3.3	88
2	Oxidation States from Wave Function Analysis. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1501-1508.	5.3	78
3	Iron and Manganese Catalysts for the Selective Functionalization of Arene C(sp ²)-H Bonds by Carbene Insertion. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 6530-6534.	13.8	77
4	Reactivity Patterns of (Protonated) Compound II and Compound I of Cytochrome P450: Which is the Better Oxidant?. <i>Chemistry - A European Journal</i> , 2017, 23, 6406-6418.	3.3	71
5	On the existence and characterization of molecular electrides. <i>Chemical Communications</i> , 2015, 51, 4865-4868.	4.1	68
6	An Objective Alternative to IUPAC's Approach To Assign Oxidation States. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 10525-10529.	13.8	43
7	Mechanism of the Selective Fe-Catalyzed Arene Carbon-Hydrogen Bond Functionalization. <i>ACS Catalysis</i> , 2018, 8, 4313-4322.	11.2	32
8	Iron and Manganese Catalysts for the Selective Functionalization of Arene C(sp ²)-H Bonds by Carbene Insertion. <i>Angewandte Chemie</i> , 2016, 128, 6640-6644.	2.0	29
9	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. <i>Chemistry - A European Journal</i> , 2018, 24, 9853-9859.	3.3	28
10	Computational Insight into the Mechanism of Alkane Hydroxylation by Non-heme Fe(PyTACN) Iron Complexes. Effects of the Substrate and Solvent. <i>Inorganic Chemistry</i> , 2015, 54, 8223-8236.	4.0	24
11	An Objective Alternative to IUPAC's Approach To Assign Oxidation States. <i>Angewandte Chemie</i> , 2018, 130, 10685-10689.	2.0	23
12	Fluoreno[2,1-a]fluorene: an ortho-naphthoquinodimethane-based system with partial diradical character. <i>Chemical Communications</i> , 2019, 55, 14186-14189.	4.1	15
13	Quantum Mechanics/Molecular Mechanics Studies on the Relative Reactivities of Compound I and II in Cytochrome P450 Enzymes. <i>International Journal of Molecular Sciences</i> , 2018, 19, 1974.	4.1	14
14	Mild Open-Shell Character of BODIPY and Its Impact on Singlet and Triplet Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5825-5838.	5.3	12
15	Generation of multiple triplet states in an orthogonal bodipy dimer: a breakthrough spectroscopic and theoretical approach. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 5929-5938.	2.8	10
16	Efficient alkene hydrosilylation with bis(8-quinolyl)phosphine (NPN) nickel catalysts. The dominant role of silyl-over hydrido-nickel catalytic intermediates. <i>Chemical Science</i> , 2020, 11, 5043-5051.	7.4	7
17	Can aluminum, a non-redox metal, alter the thermodynamics of key biological redox processes? The DPPH-QH2 radical scavenging reaction as a test case. <i>Free Radical Biology and Medicine</i> , 2022, 179, 200-207.	2.9	2