Marius Retegan

List of Publications by Year
in descending order

39 papers	2,126 citations	293460 24 h-index	355658 38 g-index
39 all docs	39 docs citations	39 times ranked	2833 citing authors

#	Article	IF	Citations
1	XAS and XMCD Reveal a Cobalt(II) Imide Undergoes High-Pressure-Induced Spin Crossover. Journal of Physical Chemistry C, 2022, 126, 5784-5792.	1.5	4
2	2p x-ray absorption spectroscopy of 3d transition metal systems. Journal of Electron Spectroscopy and Related Phenomena, 2021, 249, 147061.	0.8	44
3	Demethylation of Methylmercury in Bird, Fish, and Earthworm. Environmental Science & Technology, 2021, 55, 1527-1534.	4.6	61
4	Probing the Local Coordination of Hexavalent Uranium and the Splitting of 5f Orbitals Induced by Chemical Bonding. Inorganic Chemistry, 2021, 60, 16286-16293.	1.9	12
5	New reflections on hard X-ray photon-in/photon-out spectroscopy. Nanoscale, 2020, 12, 16270-16284.	2.8	21
6	Chemical Sensitivity of KÎ² and KÎ± X-ray Emission from a Systematic Investigation of Iron Compounds. Inorganic Chemistry, 2020, 59, 12518-12535.	1.9	55
7	Enhanced Sorption of Radionuclides by Defect-Rich Graphene Oxide. ACS Applied Materials & Interfaces, 2020, 12, 45122-45135.	4.0	50
8	From an Enhanced Understanding to Commercially Viable Electrodes: The Case of PTCLi₄ as Sustainable Organic Lithiumâ€ion Anode Material. Advanced Sustainable Systems, 2017, 1, 1600032.	2.7	31
9	Multilevel Approaches within the Local Pair Natural Orbital Framework. Journal of Chemical Theory and Computation, 2017, 13, 3198-3207.	2.3	38
10	A Highâ€Valent Nonâ€Heme Î¼â€Oxo Manganese(IV) Dimer Generated from a Thiolateâ€Bound Manganese(II) Complex and Dioxygen. Angewandte Chemie - International Edition, 2017, 56, 8211-8215.	7.2	29
11	Differences in the Active Site of Water Oxidation among Photosynthetic Organisms. Journal of the American Chemical Society, 2017, 139, 14340-14343.	6.6	31
12	Time-Resolved Electron Paramagnetic Resonance and Theoretical Investigations of Metal-Free Room-Temperature Triplet Emitters. Journal of the American Chemical Society, 2017, 139, 12968-12975.	6.6	24
13	A Highâ€Valent Nonâ€Heme Î¼â€Oxo Manganese(IV) Dimer Generated from a Thiolateâ€Bound Manganese(II) Complex and Dioxygen. Angewandte Chemie, 2017, 129, 8323-8327.	1.6	10
14	Possibility to realize spin-orbit-induced correlated physics in iridium fluorides. Physical Review B, 2017, 95, .	1.1	15
15	Interaction of methanol with the oxygen-evolving complex: atomistic models, channel identification, species dependence, and mechanistic implications. Chemical Science, 2016, 7, 6463-6476.	3.7	47
16	Effect of Conjugation Pathway in Metal-Free Room-Temperature Dual Singletâ€“Triplet Emitters for Organic Light-Emitting Diodes. Journal of Physical Chemistry Letters, 2016, 7, 4802-4808.	2.1	42
17	A realistic in silico model for structure/function studies of molybdenumâ€“copper CO dehydrogenase. Journal of Biological Inorganic Chemistry, 2016, 21, 491-499.	1.1	21
18	A five-coordinate Mn(<scp>iv</scp>) intermediate in biological water oxidation: spectroscopic signature and a pivot mechanism for water binding. Chemical Science, 2016, 7, 72-84.	3.7	158

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19	Spin State as a Marker for the Structural Evolution of Natureâ€™s Water-Splitting Catalyst. Inorganic Chemistry, 2016, 55, 488-501.	1.9	87
20	Metal oxidation states in biological water splitting. Chemical Science, 2015, 6, 1676-1695.	3.7	275
21	Dioxygen Activation and Catalytic Reduction to Hydrogen Peroxide by a Thiolate-Bridged Dimanganese(II) Complex with a Pendant Thiol. Journal of the American Chemical Society, 2015, 137, 8644-8653.	6.6	56
22	Principles of Natural Photosynthesis. Topics in Current Chemistry, 2015, 371, 23-48.	4.0	51
23	Toward Atomistic Resolution Structure of Phosphatidylcholine Headgroup and Glycerol Backbone at Different Ambient Conditions. Journal of Physical Chemistry B, 2015, 119, 15075-15088.	1.2	109
24	The ironâ€“sulfur core in Rieske proteins is not symmetric. Journal of Biological Inorganic Chemistry, 2014, 19, 1287-1293.	1.1	4
25	Structure, ligands and substrate coordination of the oxygen-evolving complex of photosystem II in the S2 state: a combined EPR and DFT study. Physical Chemistry Chemical Physics, 2014, 16, 11877.	1.3	77
26	The first tyrosyl radical intermediate formed in the S2â€“S3 transition of photosystem II. Physical Chemistry Chemical Physics, 2014, 16, 11901.	1.3	68
27	A First-Principles Approach to the Calculation of the on-Site Zero-Field Splitting in Polynuclear Transition Metal Complexes. Inorganic Chemistry, 2014, 53, 11785-11793.	1.9	32
28	Electronic structure of the oxygen-evolving complex in photosystem II prior to O-O bond formation. Science, 2014, 345, 804-808.	6.0	432
29	Convergence of QM/MM and Cluster Models for the Spectroscopic Properties of the Oxygen-Evolving Complex in Photosystem II. Journal of Chemical Theory and Computation, 2013, 9, 3832-3842.	2.3	54
30	A combined high-field EPR and quantum chemical study on a weakly ferromagnetically coupled dinuclear Mn(<scp>iii</scp>) complex. A complete analysis of the EPR spectrum beyond the strong coupling limit. Physical Chemistry Chemical Physics, 2013, 15, 223-234.	1.3	21
31	Azurin as a Protein Scaffold for a Low-coordinate Nonheme Iron Site with a Small-molecule Binding Pocket. Journal of the American Chemical Society, 2012, 134, 19746-19757.	6.6	33
32	Visibleâ€Lightâ€Driven Generation of Highâ€Valent Oxoâ€Bridged Dinuclear and Tetranuclear Manganese Terpyridine Entities Linked to Photoactive Ruthenium Units of Relevance to Photosystem II. European Journal of Inorganic Chemistry, 2012, 2012, 5485-5499.	1.0	6
33	Redoxâ€Responsive Porphyrinâ€Based Molecular Tweezers. Chemistry - A European Journal, 2012, 18, 7648-7653.	1.7	48
34	Experimental and Computational Investigation of Thiolate Alkylation in Ni^{II} and Zn^{II} Complexes: Role of the Metal on the Sulfur Nucleophilicity. Inorganic Chemistry, 2011, 50, 10047-10055.	1.9	22
35	Electrochemical formation of bi- versus tetranuclear Î¼-oxo terpyridine manganese complexes in CH3CN. Influence of the terpyridine substituents. Inorganica Chimica Acta, 2011, 374, 187-196.	1.2	6
36	MESP: An efficient method to validate an ONIOM partition for the modelization of phosphine ligands commonly used in the Pausonâ€“Khand reaction. Computational and Theoretical Chemistry, 2011, 965, 231-235.	1.1	0

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37	Comparative Theoretical Studies of the Phosphomonoester Hydrolysis Mechanism by Purple Acid Phosphatases. Journal of Physical Chemistry A, 2010, 114, 7110-7116.	1.1	6
38	Free energy calculations using dual-level Bornâ€“Oppenheimer molecular dynamics. Journal of Chemical Physics, 2010, 133, 064103.	1.2	22
39	Exploring the Binding of Inhibitors Derived from Tetrabromobenzimidazole to the CK2 Protein Using a QM/MM-PB/SA Approach. Journal of Chemical Information and Modeling, 2009, 49, 963-971.	2.5	24