Maylis Orio

List of Publications by Year
in descending order

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Version: 2024-02-01

109 papers	3,668 citations	159585 30 h-index	144013 57 g-index
114 all docs	114 docs citations	114 times ranked	4799 citing authors

#	Article	IF	Citations
1	Coordination polymer structure and revisited hydrogen evolution catalytic mechanism for amorphous molybdenumÂsulfide. Nature Materials, 2016, 15, 640-646.	27.5	490
2	Density functional theory. Photosynthesis Research, 2009, 102, 443-453.	2.9	282
3	Nickel-centred proton reduction catalysis in a model of [NiFe] hydrogenase. Nature Chemistry, 2016, 8, 1054-1060.	13.6	200
4	Xâ€Ray Structures of Copper(II) and Nickel(II) Radical Salen Complexes: The Preference of Galactose Oxidase for Copper(II). Angewandte Chemie - International Edition, 2010, 49, 4989-4992.	13.8	166
5	A New Quantum Chemical Approach to the Magnetic Properties of Oligonuclear Transitionâ€Metal Complexes: Application to a Model for the Tetranuclear Manganese Cluster of Photosystemâ€...II. Chemistry - A European Journal, 2009, 15, 5108-5123.	3.3	123
6	Structure of the oxygen-evolving complex of photosystem II: information on the S2 state through quantum chemical calculation of its magnetic properties. Physical Chemistry Chemical Physics, 2009, 11, 6788.	2.8	121
7	Pulsedâ€EPR Evidence of a Manganese(II) Hydroxycarbonyl Intermediate in the Electrocatalytic Reduction of Carbon Dioxide by a Manganese Bipyridyl Derivative. Angewandte Chemie - International Edition, 2014, 53, 240-243.	13.8	121
8	Magnetic and Spectroscopic Properties of Mixed Valence Manganese(III,IV) Dimers: A Systematic Study Using Broken Symmetry Density Functional Theory. Inorganic Chemistry, 2009, 48, 7251-7260.	4.0	107
9	Theoretical magnetochemistry of dinuclear manganese complexes: broken symmetry density functional theory investigation on the influence of bridging motifs on structure and magnetism. Dalton Transactions, 2010, 39, 4959.	3.3	100
10	Ligand Contributions to the Electronic Structures of the Oxidized Cobalt(II) salen Complexes. Inorganic Chemistry, 2012, 51, 10557-10571.	4.0	80
11	Radical Localization in a Series of Symmetric Ni^{II} Complexes with Oxidized Salen Ligands. Chemistry - A European Journal, 2012, 18, 14117-14127.	3.3	76
12	Copper(II) Complexes of Phenanthroline and Histidine Containing Ligands: Synthesis, Characterization and Evaluation of their DNA Cleavage and Cytotoxic Activity. Inorganic Chemistry, 2016, 55, 11801-11814.	4.0	66
13	Oneâ€Electron Oxidized Copper(II) Salophen Complexes: Phenoxyl versus Diiminobenzene Radical Species. Chemistry - A European Journal, 2012, 18, 1068-1072.	3.3	57
14	A Thiosemicarbazoneâ€“Nickel(II) Complex as Efficient Electrocatalyst for Hydrogen Evolution. ChemCatChem, 2017, 9, 2262-2268.	3.7	57
15	Trinuclear Terpyridine Frustrated Spin System with a Mn^{IV}₃O₄ Core: Synthesis, Physical Characterization, and Quantum Chemical Modeling of Its Magnetic Properties. Inorganic Chemistry, 2009, 48, 10281-10288.	4.0	53
16	Hydrogen Evolution Reactions Catalyzed by a Bis(thiosemicarbazone) Cobalt Complex: An Experimental and Theoretical Study. Chemistry - A European Journal, 2018, 24, 8779-8786.	3.3	50
17	Spin Interaction in Octahedral Zinc Complexes of Mono- and Diradical Schiff and Mannich Bases. Inorganic Chemistry, 2010, 49, 646-658.	4.0	47
18	Tuning Reactivity of Bioinspired [NiFe]-Hydrogenase Models by Ligand Design and Modeling the CO Inhibition Process. ACS Catalysis, 2018, 8, 10658-10667.	11.2	47

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19	Variation of Average g Values and Effective Exchange Coupling Constants among [2Feâ^'2S] Clusters: A Density Functional Theory Study of the Impact of Localization (Trapping Forces) versus Delocalization (Double-Exchange) as Competing Factors. Inorganic Chemistry, 2008, 47, 5394-5416.	4.0	43
20	Reversible Apical Coordination of Imidazole between the Ni(III) and Ni(II) Oxidation States of a Dithiolate Complex: A Process Related to the Ni Superoxide Dismutase. Inorganic Chemistry, 2010, 49, 6399-6401.	4.0	43
21	Iminosemiquinone radical ligands enable access to a well-defined redox-active Cu^{II}â€"CF₃ complex. Chemical Communications, 2014, 50, 10394-10397.	4.1	43
22	Redox Noninnocence of the Bridge in Copper(II) Salophen and Bis(oxamato) Complexes. Inorganic Chemistry, 2015, 54, 9013-9026.	4.0	38
23	Reversible Double Oxidation and Protonation of the Non-Innocent Bridge in a Nickel(II) Salophen Complex. Inorganic Chemistry, 2012, 51, 12796-12804.	4.0	37
24	Understanding Ferroelectricity in the Pb-Free Perovskite-Like Metalâ€"Organic Framework [(CH₃)₂NH₂]Zn(HCOO)₃: Dielectric, 2D NMR, and Theoretical Studies. Journal of Physical Chemistry C, 2017, 121, 6314-6322.	3.1	36
25	Unsymmetrical one-electron oxidized Ni(ii)â€"bis(salicylidene) complexes: a protonation-induced shift of the oxidation site. Chemical Communications, 2010, 46, 6765.	4.1	34
26	A Bioâ€Inspired Switch Based on Cobalt(II) Disulfide/Cobalt(III) Thiolate Interconversion. Angewandte Chemie - International Edition, 2014, 53, 5318-5321.	13.8	34
27	Influence of Mixed Thiolate/Thioether versus Dithiolate Coordination on the Accessibility of the Uncommon +I and +III Oxidation States for the Nickel Ion: An Experimental and Computational Study. Inorganic Chemistry, 2011, 50, 3707-3716.	4.0	33
28	Circumventing Intrinsic Metal Reactivity: Radical Generation with Redoxâ€Active Ligands. Chemistry - A European Journal, 2017, 23, 15030-15034.	3.3	33
29	Molecular Electrocatalysts for the Hydrogen Evolution Reaction: Input from Quantum Chemistry. ChemSusChem, 2019, 12, 4905-4915.	6.8	33
30	Versatile Effects of Aurone Structure on Mushroom Tyrosinase Activity. ChemBioChem, 2012, 13, 559-565.	2.6	31
31	Câ^'N Bond Formation from a Masked Highâ€Valent Copper Complex Stabilized by Redox Nonâ€Innocent Ligands. Angewandte Chemie - International Edition, 2016, 55, 10712-10716.	13.8	31
32	Spectroscopic description of an unusual protonated ferryl species in the catalase from Proteus mirabilis and density functional theory calculations on related models. Consequences for the ferryl protonation state in catalase, peroxidase and chloroperoxidase. Journal of Biological Inorganic Chemistry, 2007, 12, 509-525.	2.6	30
33	Stable Anilinyl Radicals Coordinated to Nickel: Xâ€ray Crystal Structure and Characterization. Chemistry - A European Journal, 2013, 19, 16707-16721.	3.3	30
34	Copper Complexes as Bioinspired Models for Lytic Polysaccharide Monooxygenases. Inorganic Chemistry, 2017, 56, 1023-1026.	4.0	30
35	A nickel dimethyl glyoximato complex to form nickel based nanoparticles for electrocatalytic H₂ production. Chemical Communications, 2014, 50, 13514-13516.	4.1	29
36	Side-on cupricâ€"superoxo triplet complexes as competent agents for H-abstraction relevant to the active site of PHM. Chemical Communications, 2015, 51, 11134-11137.	4.1	29

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37	A {Cu₂S}²⁺ Mixedâ€Valent Core Featuring a Cuï£¿Cu Bond. Angewandte Chemie - International Edition, 2010, 49, 8249-8252.	13.8	28
38	Copperâ€Catalyzed Aziridination with Redoxâ€Active Ligands: Molecular Spin Catalysis. Chemistry - A European Journal, 2018, 24, 5086-5090.	3.3	28
39	Influence of Confinement Effect on Electron Transfers Induced by t-Stilbene Sorption in Medium Pore Acidic Zeolites. Journal of Physical Chemistry C, 2012, 116, 1812-1825.	3.1	26
40	N₂O reduction at a dissymmetric {Cu₂S}-containing mixed-valent center. Chemical Science, 2014, 5, 4774-4784.	7.4	26
41	Vanadium Thiolate Complexes for Efficient and Selective Sulfoxidation Catalysis: A Mechanistic Investigation. Inorganic Chemistry, 2013, 52, 13424-13431.	4.0	24
42	Successes, challenges, and opportunities for quantum chemistry in understanding metalloenzymes for solar fuels research. Chemical Communications, 2021, 57, 3952-3974.	4.1	24
43	Influence of the Metal Ion on the Electrocatalytic Hydrogen Production by a Thiosemicarbazone Palladium Complex. European Journal of Inorganic Chemistry, 2018, 2018, 2259-2266.	2.0	23
44	From non-innocent to guilty: on the role of redox-active ligands in the electro-assisted reduction of CO₂ mediated by a cobalt(<scp>ii</scp>)-polypyridyl complex. Sustainable Energy and Fuels, 2020, 4, 3668-3676.	4.9	22
45	An Experimental and Theoretical Investigation on Pentacoordinated Cobalt(III) Complexes with an Intermediate S=1 Spin State: How Halide Ligands Affect their Magnetic Anisotropy. Chemistry - A European Journal, 2016, 22, 925-933.	3.3	21
46	Ligand-based electronic effects on the electrocatalytic hydrogen production by thiosemicarbazone nickel complexes. Dalton Transactions, 2020, 49, 5064-5073.	3.3	20
47	Role of the Metal Ion in Bio-Inspired Hydrogenase Models: Investigation of a Homodinuclear FeFe Complex vs Its Heterodinuclear NiFe Analogue. ACS Catalysis, 2020, 10, 177-186.	11.2	19
48	Effect of the Metal on Disulfide/Thiolate Interconversion: Manganese versus Cobalt. Chemistry - A European Journal, 2015, 21, 18770-18778.	3.3	18
49	Efficient Light-Driven Hydrogen Evolution Using a Thiosemicarbazone-Nickel (II) Complex. Frontiers in Chemistry, 2019, 7, 405.	3.6	18
50	Geometric and Electronic Structures of Phenoxyl Radicals Hydrogen Bonded to Neutral and Cationic Partners. Chemistry - A European Journal, 2012, 18, 5416-5429.	3.3	16
51	Multifrequency cw-EPR and DFT Studies of an Apparent Compressed Octahedral Cu(II) Complex. Inorganic Chemistry, 2016, 55, 1497-1504.	4.0	16
52	Indolino-Oxazolidine Acido- and Photochromic System Investigated by NMR and Density Functional Theory Calculations. Journal of Organic Chemistry, 2018, 83, 10409-10419.	3.2	16
53	When Light and Acid Play Tic-Tac-Toe with a Nine-State Molecular Switch. Journal of the American Chemical Society, 2019, 141, 19151-19160.	13.7	16
54	Comparison of Density Functional and Correlated Wave Function Methods for the Prediction of Cu(II) Hyperfine Coupling Constants. ChemPhysChem, 2020, 21, 2667-2679.	2.1	16

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55	Insights into the recombination of radical pairs in hexaarylbiimidazoles. Chemical Communications, 2013, 49, 5841.	4.1	15
56	Dinuclear iridium and rhodium complexes with bridging arylimidazolide-N³,C² ligands: synthetic, structural, reactivity, electrochemical and spectroscopic studies. Dalton Transactions, 2015, 44, 17030-17044.	3.3	15
57	Water Molecules Gating a Photoinduced Oneâ€Electron Twoâ€Protons Transfer in a Tyrosine/Histidine (Tyr/His) Model of Photosystemâ€...II. Angewandte Chemie - International Edition, 2018, 57, 9013-9017.	13.8	15
58	Redox-switchable tetra-copper assembly of N,N-, N,O-phenolate-phenanthroimidazolate bridging ligands. Dalton Transactions, 2013, 42, 2358.	3.3	14
59	Monoanionic Dipyrrinâ€“Pyridine Ligands: Synthesis, Structure and Photophysical Properties. European Journal of Inorganic Chemistry, 2015, 2015, 5405-5410.	2.0	14
60	Controlled nitrene transfer from a tyrosinase-like arylnitrosoâ€“copper complex. Chemical Communications, 2015, 51, 11206-11209.	4.1	14
61	Optimizing Group Transfer Catalysis by Copper Complex with Redox-Active Ligand in an Entatic State. IScience, 2020, 23, 100955.	4.1	14
62	Magnetic exchange coupling in Cu dimers studied with modern multireference methods and broken-symmetry coupled cluster theory. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	13
63	Electropolymerized biotinylated poly (pyrroleâ€“viologen) film as platform for the development of reagentless impedimetric immunosensors. Electrochemistry Communications, 2010, 12, 311-314.	4.7	12
64	The Versatile Binding Mode of Transitionâ€State Analogue Inhibitors of Tyrosinase towards Dicopper(II) Model Complexes: Experimental and Theoretical Investigations. Chemistry - A European Journal, 2011, 17, 13482-13494.	3.3	12
65	Nickel(iii) complexes of di-amidato-di-phenolato ligands: effect of H-bonding. Dalton Transactions, 2013, 42, 13323.	3.3	11
66	Changing the chemical and physical properties of high valent heterobimetallic bis-(Î¼-oxido) Cuâ€“Ni complexes by ligand effects. Dalton Transactions, 2016, 45, 15994-16000.	3.3	10
67	Measuring Motional Dynamics of [(CH3)2NH2]+ in the Perovskite-Like Metalâ€“Organic Framework [(CH3)2NH2][Zn(HCOO)3]: The Value of Low-Frequency Electron Paramagnetic Resonance. Journal of Physical Chemistry C, 2018, 122, 16431-16436.	3.1	10
68	Unraveling the catalytic mechanisms of H₂ production with thiosemicarbazone nickel complexes. RSC Advances, 2021, 11, 5232-5238.	3.6	10
69	Structural, spectroscopic and redox properties of a mononuclear CoII thiolate complex â€“ the reactivity toward S-alkylation: an experimental and theoretical study. Dalton Transactions, 2012, 41, 12586.	3.3	9
70	A Multifunctional Photoswitch: 6Ï€ Electrocyclization versus ESIPT and Metalation. Chemistry - A European Journal, 2014, 20, 12279-12288.	3.3	9
71	Characterization of a Dinuclear Copper(II) Complex and Its Fleeting Mixedâ€Valent Copper(II)/Copper(III) Counterpart. ChemPlusChem, 2017, 82, 615-624.	2.8	9
72	Characterization of Cu(II)-reconstituted ACC Oxidase using experimental and theoretical approaches. Archives of Biochemistry and Biophysics, 2017, 623-624, 31-41.	3.0	9

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73	Câ^'N Bond Formation from a Masked Highâ€Valent Copper Complex Stabilized by Redox Nonâ€Innocent Ligands. Angewandte Chemie, 2016, 128, 10870-10874.	2.0	8
74	Redox-Innocent Metal-Assisted Cleavage of Sâ€“S Bond in a Disulfide-Containing Ligand. Inorganic Chemistry, 2016, 55, 6208-6217.	4.0	8
75	Hydrogen evolution reaction mediated by an all-sulfur trinuclear nickel complex. Chemical Communications, 2020, 56, 11106-11109.	4.1	8
76	A novel di-compartmental bis-(2-hydroxyisophtalamide) macrocyclic ligand and its mononuclear Cu(ii) and Ni(ii) complexes. Dalton Transactions, 2012, 41, 12457.	3.3	7
77	Fusion of Ultravioletâ€“Visible and Infrared Transient Absorption Spectroscopy Data to Model Ultrafast Photoisomerization. Journal of Physical Chemistry Letters, 2017, 8, 3530-3535.	4.6	7
78	Tuning the locus of oxidation in Cu-diamido-diphenoxo complexes: From Cu(III) to Cu(II)-phenoxyl radical. Inorganica Chimica Acta, 2018, 481, 143-150.	2.4	7
79	Catalytic Reduction of Oxygen by a Copper Thiosemicarbazone Complex. European Journal of Inorganic Chemistry, 2020, 2020, 4549-4555.	2.0	7
80	Quantum dynamics of Mn2+ in dimethylammonium magnesium formate. Journal of Chemical Physics, 2021, 154, 154201.	3.0	7
81	EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory. Magnetochemistry, 2022, 8, 36.	2.4	7
82	Tuning Inner-Sphere Electron Transfer in a Series of Copper/Nitrosoarene Adducts. Inorganic Chemistry, 2020, 59, 8678-8689.	4.0	6
83	Nickel Complexes and Carbon Dots for Efficient Lightâ€Driven Hydrogen Production. European Journal of Inorganic Chemistry, 2021, 2021, 3097-3103.	2.0	6
84	Cellulose Depolymerization with LPMOâ€inspired Cu Complexes. ChemCatChem, 2021, 13, 4700-4704.	3.7	6
85	Structure and Dynamics of the Excited States of 1,3â€Diarylisobenzofurans: An Experimental and Theoretical Study. Photochemistry and Photobiology, 2012, 88, 633-638.	2.5	5
86	Influence of Copper Coordination Spheres on Nitrous Oxide Reductase (N₂Or) Activity of a Mixed-Valent Copper Complex Containing a {Cu₂S} Core. Inorganic Chemistry, 2019, 58, 11649-11655.	4.0	5
87	Self-assembled nickel cubanes as oxygen evolution catalysts. Chemical Communications, 2021, 57, 8608-8611.	4.1	5
88	Radicals of Free and Zinc(II)-Coordinated Î±-Azophenols. European Journal of Inorganic Chemistry, 2011, 2011, 45-48.	2.0	4
89	X-ray structure of a Ni(ii)â€“tri-phenoxyl radical complex. Dalton Transactions, 2015, 44, 17924-17926.	3.3	4
90	Oxidative DNA Cleavage Promoted by a Phenoxyl-Radical Copper(II) Complex. European Journal of Inorganic Chemistry, 2016, 2016, 5575-5584.	2.0	4

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91	Unexpected rapid aerobic transformation of 2,2,6,6-tetraethyl-4-oxo(piperidin-1-yloxyl) radical by cytochrome P450 in the presence of NADPH: Evidence against a simple reduction of the nitroxide moiety to the hydroxylamine. Free Radical Biology and Medicine, 2020, 156, 144-156.	2.9	4
92	Electron-spin interaction in the spin-Peierls phase of the organic spin chain (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub><mml:mi>X</mml:mi></mml:mrow></mml:math> (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 722 Td (x	3.2	4
93	Physical Review B, 2022, 105, . Decoding the Ambiguous Electron Paramagnetic Resonance Signals in the Lytic Polysaccharide Monooxygenase from Photorhabdus luminescens. Inorganic Chemistry, 2022, 61, 8022-8035.	4.0	4
94	Charge-ordering induces magnetic axes rotation in organic materials (TMTTF)2X (with X = SbF6, AsF6,) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.6	3
95	Electronic and magnetic interactions in diporphyrinylamines. Journal of Porphyrins and Phthalocyanines, 2016, 20, 1233-1243.	0.8	3
96	An Air-Stable Molybdenum-Based Precatalyst in Oxygen-Atom Transfer Reactions. European Journal of Inorganic Chemistry, 2018, 2018, 1427-1434.	2.0	3
97	Magneto-Structural and Computational Study of a Tetranuclear Copper Complex Displaying Carbonyl-Ï€ Interactions. European Journal of Inorganic Chemistry, 2018, 2018, 5039-5046.	2.0	3
98	Water Molecules Gating a Photoinduced Oneâ€Electron Twoâ€Protons Transfer in a Tyrosine/Histidine (Tyr/His) Model of Photosystemâ€...II. Angewandte Chemie, 2018, 130, 9151-9155.	2.0	3
99	Superlattice Induced by Charge Order in the Organic Spin Chain (TMTTF)₂X (X =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Resonance. Journal of Physical Chemistry Letters, 2018, 9, 5598-5603.	4.6	3
100	Electron Spin Resonance of Defects in Spin Chainsâ€”$$hbox {o}-(hbox {DMTTF})_2hbox {X}$$: A Versatile System Behaving Like Molecular Magnet. Applied Magnetic Resonance, 2020, 51, 1307-1320.	1.2	3
101	From Ligandâ€•to Metalâ€•centered Reactivity: Metal Substitution Effect in Thiosemicarbazoneâ€based Complexes for H₂ Production. ChemPhysChem, 2022, 23, .	2.1	3
102	Separation of Geometric Isomers of a Dicopper Complex by Using a ¹⁹F-Labeled Ligand: Dynamics, Structures, and DFT Calculations. Inorganic Chemistry, 2010, 49, 7832-7840.	4.0	2
103	Valence Localization at a Bioâ€inspired Mixedâ€Valent {Cu₂S}²⁺ Motif upon Solvation in Acetonitrile: Effect on Nitrous Oxide Reductase (N₂Or) Activity. Chemistry - A European Journal, 2018, 24, 5060-5063.	3.3	2
104	Magnetic resonance probing of ferroelectricity and magnetism in metal-organic frameworks. Ferroelectrics, 2018, 534, 11-18.	0.6	2
105	A hybrid bioinspired catechol-alloxazine triangular nickel complex stabilizing protons and electrons. Inorganic Chemistry Frontiers, 2021, 8, 5286-5298.	6.0	2
106	Neutral Lipophilic Palladium(II) Complexes and their Applications in Electrocatalytic Hydrogen Production and Câ€C Coupling Reactions. European Journal of Inorganic Chemistry, 2020, 2020, 813-822.	2.0	1
107	Magneto-Structural and Computational Study of a Tetranuclear Copper Complex Displaying Carbonyl-Ï€ Interactions. European Journal of Inorganic Chemistry, 2018, 2018, 5037-5037.	2.0	0
108	Frontispiece: Hydrogen Evolution Reactions Catalyzed by a Bis(thiosemicarbazone) Cobalt Complex: An Experimental and Theoretical Study. Chemistry - A European Journal, 2018, 24, .	3.3	0

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109	Electrochemical, Spectroscopic, and Computational Investigation of a Series of Polypyridyl Ruthenium(II) Complexes: Characterization of Reduced States. European Journal of Inorganic Chemistry, 2021, 2021, 1263-1270.	2.0	0