

Maylis Orio

List of Publications by Year in Descending Order

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Version: 2024-04-26

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

108
papers

2,862
citations

28
h-index

50
g-index

114
ext. papers

3,261
ext. citations

5.4
avg, IF

5.08
L-index

#	Paper	IF	Citations
108	EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory. <i>Magnetochemistry</i> , 2022 , 8, 36	3.1	0
107	Quantum dynamics of Mn in dimethylammonium magnesium formate. <i>Journal of Chemical Physics</i> , 2021 , 154, 154201	3.9	0
106	Nickel Complexes and Carbon Dots for Efficient Light-Driven Hydrogen Production. <i>European Journal of Inorganic Chemistry</i> , 2021 , 2021, 3097-3103	2.3	1
105	Unraveling the catalytic mechanisms of H production with thiosemicarbazone nickel complexes.. <i>RSC Advances</i> , 2021 , 11, 5232-5238	3.7	5
104	Successes, challenges, and opportunities for quantum chemistry in understanding metalloenzymes for solar fuels research. <i>Chemical Communications</i> , 2021 , 57, 3952-3974	5.8	6
103	Electrochemical, Spectroscopic, and Computational Investigation of a Series of Polypyridyl Ruthenium(II) Complexes: Characterization of Reduced States. <i>European Journal of Inorganic Chemistry</i> , 2021 , 2021, 1263-1270	2.3	
102	Magnetic exchange coupling in Cu dimers studied with modern multireference methods and broken-symmetry coupled cluster theory. <i>Theoretical Chemistry Accounts</i> , 2021 , 140, 1	1.9	1
101	Self-assembled nickel cubanes as oxygen evolution catalysts. <i>Chemical Communications</i> , 2021 , 57, 8608-8611	5.1	0
100	Comparison of Density Functional and Correlated Wave Function Methods for the Prediction of Cu(II) Hyperfine Coupling Constants. <i>ChemPhysChem</i> , 2020 , 21, 2667-2679	3.2	8
99	Unexpected rapid aerobic transformation of 2,2,6,6-tetraethyl-4-oxo(piperidin-1-yloxy) radical by cytochrome P450 in the presence of NADPH: Evidence against a simple reduction of the nitroxide moiety to the hydroxylamine. <i>Free Radical Biology and Medicine</i> , 2020 , 156, 144-156	7.8	2
98	From non-innocent to guilty: on the role of redox-active ligands in the electro-assisted reduction of CO ₂ mediated by a cobalt(II)-polypyridyl complex. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 3668-3676	5.8	13
97	Ligand-based electronic effects on the electrocatalytic hydrogen production by thiosemicarbazone nickel complexes. <i>Dalton Transactions</i> , 2020 , 49, 5064-5073	4.3	10
96	Optimizing Group Transfer Catalysis by Copper Complex with Redox-Active Ligand in an Entatic State. <i>IScience</i> , 2020 , 23, 100955	6.1	5
95	Tuning Inner-Sphere Electron Transfer in a Series of Copper/Nitrosoarene Adducts. <i>Inorganic Chemistry</i> , 2020 , 59, 8678-8689	5.1	5
94	Neutral Lipophilic Palladium(II) Complexes and their Applications in Electrocatalytic Hydrogen Production and C-C Coupling Reactions. <i>European Journal of Inorganic Chemistry</i> , 2020 , 2020, 813-822	2.3	1
93	Role of the Metal Ion in Bio-Inspired Hydrogenase Models: Investigation of a Homodinuclear FeFe Complex vs Its Heterodinuclear NiFe Analogue. <i>ACS Catalysis</i> , 2020 , 10, 177-186	13.1	11
92	Catalytic Reduction of Oxygen by a Copper Thiosemicarbazone Complex. <i>European Journal of Inorganic Chemistry</i> , 2020 , 2020, 4549-4555	2.3	2

91	Hydrogen evolution reaction mediated by an all-sulfur trinuclear nickel complex. <i>Chemical Communications</i> , 2020 , 56, 11106-11109	5.8	7
90	Electron Spin Resonance of Defects in Spin Chains (hbox {o}-(hbox {DMTTF})_2hbox {X}): A Versatile System Behaving Like Molecular Magnet. <i>Applied Magnetic Resonance</i> , 2020 , 51, 1307-1320	0.8	1
89	Efficient Light-Driven Hydrogen Evolution Using a Thiosemicarbazone-Nickel (II) Complex. <i>Frontiers in Chemistry</i> , 2019 , 7, 405	5	12
88	Influence of Copper Coordination Spheres on Nitrous Oxide Reductase (NOR) Activity of a Mixed-Valent Copper Complex Containing a {CuS} Core. <i>Inorganic Chemistry</i> , 2019 , 58, 11649-11655	5.1	4
87	When Light and Acid Play Tic-Tac-Toe with a Nine-State Molecular Switch. <i>Journal of the American Chemical Society</i> , 2019 , 141, 19151-19160	16.4	10
86	Molecular Electrocatalysts for the Hydrogen Evolution Reaction: Input from Quantum Chemistry. <i>ChemSusChem</i> , 2019 , 12, 4905-4915	8.3	16
85	Copper-Catalyzed Aziridination with Redox-Active Ligands: Molecular Spin Catalysis. <i>Chemistry - A European Journal</i> , 2018 , 24, 5086-5090	4.8	22
84	An Air-Stable Molybdenum-Based Precatalyst in Oxygen-Atom Transfer Reactions. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 1427-1434	2.3	2
83	Influence of the Metal Ion on the Electrocatalytic Hydrogen Production by a Thiosemicarbazone Palladium Complex. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 2259-2266	2.3	15
82	Tuning the locus of oxidation in Cu-diamido-diphenoxo complexes: From Cu(III) to Cu(II)-phenoxy radical. <i>Inorganica Chimica Acta</i> , 2018 , 481, 143-150	2.7	1
81	Indolino-Oxazolidine Acido- and Photochromic System Investigated by NMR and Density Functional Theory Calculations. <i>Journal of Organic Chemistry</i> , 2018 , 83, 10409-10419	4.2	8
80	Hydrogen Evolution Reactions Catalyzed by a Bis(thiosemicarbazone) Cobalt Complex: An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2018 , 24, 8779-8786	4.8	34
79	Superlattice Induced by Charge Order in the Organic Spin Chain (TMTTF)X (X = SbF, AsF, and PF) Revealed by High-Field Electron Paramagnetic Resonance. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 5598-5603	6.4	2
78	Measuring Motional Dynamics of [(CH ₃) ₂ NH ₂] ⁺ in the Perovskite-Like Metal-Organic Framework [(CH ₃) ₂ NH ₂][Zn(HCOO) ₃]: The Value of Low-Frequency Electron Paramagnetic Resonance. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 16431-16436	3.8	8
77	Valence Localization at a Bio-inspired Mixed-Valent {Cu S} Motif upon Solvation in Acetonitrile: Effect on Nitrous Oxide Reductase (NOR) Activity. <i>Chemistry - A European Journal</i> , 2018 , 24, 5060-5063	4.8	2
76	Magnetic resonance probing of ferroelectricity and magnetism in metal-organic frameworks. <i>Ferroelectrics</i> , 2018 , 534, 11-18	0.6	2
75	Magneto-Structural and Computational Study of a Tetranuclear Copper Complex Displaying Carbonyl-π Interactions. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 5037-5037	2.3	
74	Tuning Reactivity of Bioinspired [NiFe]-Hydrogenase Models by Ligand Design and Modeling the CO Inhibition Process. <i>ACS Catalysis</i> , 2018 , 8, 10658-10667	13.1	35

73	Magneto-Structural and Computational Study of a Tetranuclear Copper Complex Displaying Carbonyl π Interactions. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 5039-5046	2.3	3
72	Water Molecules Gating a Photoinduced One-Electron Two-Protons Transfer in a Tyrosine/Histidine (Tyr/His) Model of Photosystem II. <i>Angewandte Chemie</i> , 2018 , 130, 9151-9155	3.6	3
71	Water Molecules Gating a Photoinduced One-Electron Two-Protons Transfer in a Tyrosine/Histidine (Tyr/His) Model of Photosystem II. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 9013-9017	16.4	12
70	Copper Complexes as Bioinspired Models for Lytic Polysaccharide Monooxygenases. <i>Inorganic Chemistry</i> , 2017 , 56, 1023-1026	5.1	19
69	Understanding Ferroelectricity in the Pb-Free Perovskite-Like MetalOrganic Framework [(CH ₃) ₂ NH ₂]Zn(HCOO) ₃ : Dielectric, 2D NMR, and Theoretical Studies. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 6314-6322	3.8	29
68	Characterization of a Dinuclear Copper(II) Complex and Its Fleeting Mixed-Valent Copper(II)/Copper(III) Counterpart. <i>ChemPlusChem</i> , 2017 , 82, 615-624	2.8	8
67	Characterization of Cu(II)-reconstituted ACC Oxidase using experimental and theoretical approaches. <i>Archives of Biochemistry and Biophysics</i> , 2017 , 623-624, 31-41	4.1	6
66	Circumventing Intrinsic Metal Reactivity: Radical Generation with Redox-Active Ligands. <i>Chemistry - A European Journal</i> , 2017 , 23, 15030-15034	4.8	28
65	Fusion of Ultraviolet-Visible and Infrared Transient Absorption Spectroscopy Data to Model Ultrafast Photoisomerization. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 3530-3535	6.4	5
64	A ThiosemicarbazoneNickel(II) Complex as Efficient Electrocatalyst for Hydrogen Evolution. <i>ChemCatChem</i> , 2017 , 9, 2262-2268	5.2	43
63	Nickel-centred proton reduction catalysis in a model of [NiFe] hydrogenase. <i>Nature Chemistry</i> , 2016 , 8, 1054-1060	17.6	152
62	Oxidative DNA Cleavage Promoted by a Phenoxy-Radical Copper(II) Complex. <i>European Journal of Inorganic Chemistry</i> , 2016 , 2016, 5575-5584	2.3	2
61	Copper(II) Complexes of Phenanthroline and Histidine Containing Ligands: Synthesis, Characterization and Evaluation of their DNA Cleavage and Cytotoxic Activity. <i>Inorganic Chemistry</i> , 2016 , 55, 11801-11814	5.1	48
60	Electronic and magnetic interactions in diporphyrinylamines. <i>Journal of Porphyrins and Phthalocyanines</i> , 2016 , 20, 1233-1243	1.8	2
59	Redox-Innocent Metal-Assisted Cleavage of S-S Bond in a Disulfide-Containing Ligand. <i>Inorganic Chemistry</i> , 2016 , 55, 6208-17	5.1	5
58	An Experimental and Theoretical Investigation on Pentacoordinated Cobalt(III) Complexes with an Intermediate S=1 Spin State: How Halide Ligands Affect their Magnetic Anisotropy. <i>Chemistry - A European Journal</i> , 2016 , 22, 925-33	4.8	18
57	Multifrequency cw-EPR and DFT Studies of an Apparent Compressed Octahedral Cu(II) Complex. <i>Inorganic Chemistry</i> , 2016 , 55, 1497-504	5.1	13
56	Coordination polymer structure and revisited hydrogen evolution catalytic mechanism for amorphous molybdenumSulfide. <i>Nature Materials</i> , 2016 , 15, 640-6	27	379

55	Cu-N Bond Formation from a Masked High-Valent Copper Complex Stabilized by Redox Non-Innocent Ligands. <i>Angewandte Chemie</i> , 2016 , 128, 10870-10874	3.6	8
54	C-N Bond Formation from a Masked High-Valent Copper Complex Stabilized by Redox Non-Innocent Ligands. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 10712-6	16.4	23
53	Changing the chemical and physical properties of high valent heterobimetallic bis-(η^2 -oxido) Cu-Ni complexes by ligand effects. <i>Dalton Transactions</i> , 2016 , 45, 15994-16000	4.3	8
52	Dinuclear iridium and rhodium complexes with bridging arylimidazolide-N(3),C(2) ligands: synthetic, structural, reactivity, electrochemical and spectroscopic studies. <i>Dalton Transactions</i> , 2015 , 44, 17030-44	4.3	14
51	Controlled nitrene transfer from a tyrosinase-like arylnitroso-copper complex. <i>Chemical Communications</i> , 2015 , 51, 11206-9	5.8	14
50	Side-on cupric-superoxo triplet complexes as competent agents for H-abstraction relevant to the active site of PHM. <i>Chemical Communications</i> , 2015 , 51, 11134-7	5.8	25
49	X-ray structure of a Ni(II)-tri-phenoxy radical complex. <i>Dalton Transactions</i> , 2015 , 44, 17924-6	4.3	4
48	Redox noninnocence of the bridge in copper(II) salophen and bis(oxamato) complexes. <i>Inorganic Chemistry</i> , 2015 , 54, 9013-26	5.1	30
47	Charge-ordering induces magnetic axes rotation in organic materials (TMTTF) ₂ X (with X = SbF ₆ , AsF ₆ , and PF ₆). <i>Low Temperature Physics</i> , 2015 , 41, 942-944	0.7	3
46	Monoanionic DipyrrinPyridine Ligands: Synthesis, Structure and Photophysical Properties. <i>European Journal of Inorganic Chemistry</i> , 2015 , 2015, 5405-5410	2.3	12
45	Effect of the Metal on Disulfide/Thiolate Interconversion: Manganese versus Cobalt. <i>Chemistry - A European Journal</i> , 2015 , 21, 18770-8	4.8	15
44	Pulsed-EPR evidence of a manganese(II) hydroxycarbonyl intermediate in the electrocatalytic reduction of carbon dioxide by a manganese bipyridyl derivative. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 240-3	16.4	102
43	N ₂ O reduction at a dissymmetric {Cu ₂ S}-containing mixed-valent center. <i>Chemical Science</i> , 2014 , 5, 4774-4784	9.4	23
42	A nickel dimethyl glyoximato complex to form nickel based nanoparticles for electrocatalytic H ₂ production. <i>Chemical Communications</i> , 2014 , 50, 13514-6	5.8	26
41	Iminosemiquinone radical ligands enable access to a well-defined redox-active Cu(II)-CF ₃ complex. <i>Chemical Communications</i> , 2014 , 50, 10394-7	5.8	35
40	A multifunctional photoswitch: 6 π electrocyclization versus ESIPT and metalation. <i>Chemistry - A European Journal</i> , 2014 , 20, 12279-88	4.8	6
39	A bio-inspired switch based on cobalt(II) disulfide/cobalt(III) thiolate interconversion. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 5318-21	16.4	24
38	A Bio-Inspired Switch Based on Cobalt(II) Disulfide/Cobalt(III) Thiolate Interconversion. <i>Angewandte Chemie</i> , 2014 , 126, 5422-5425	3.6	8

37	Nickel(III) complexes of di-amidato-di-phenolato ligands: effect of H-bonding. <i>Dalton Transactions</i> , 2013 , 42, 13323-6	4.3	10
36	Vanadium thiolate complexes for efficient and selective sulfoxidation catalysis: a mechanistic investigation. <i>Inorganic Chemistry</i> , 2013 , 52, 13424-31	5.1	20
35	Redox-switchable tetra-copper assembly of N,N-, N,O-phenolate-phenanthroimidazolate bridging ligands. <i>Dalton Transactions</i> , 2013 , 42, 2358-61	4.3	10
34	Insights into the recombination of radical pairs in hexaarylbiimidazoles. <i>Chemical Communications</i> , 2013 , 49, 5841-3	5.8	14
33	Stable aniliny radical coordinated to nickel: X-ray crystal structure and characterization. <i>Chemistry - A European Journal</i> , 2013 , 19, 16707-21	4.8	27
32	Structure and dynamics of the excited states of 1,3-diarylisobenzofurans: an experimental and theoretical study. <i>Photochemistry and Photobiology</i> , 2012 , 88, 633-8	3.6	3
31	Versatile effects of aurone structure on mushroom tyrosinase activity. <i>ChemBioChem</i> , 2012 , 13, 559-65	3.8	24
30	One-electron oxidized copper(II) salophen complexes: phenoxyl versus diiminobenzene radical species. <i>Chemistry - A European Journal</i> , 2012 , 18, 1068-72	4.8	52
29	Reversible double oxidation and protonation of the non-innocent bridge in a nickel(II) salophen complex. <i>Inorganic Chemistry</i> , 2012 , 51, 12796-804	5.1	33
28	Geometric and electronic structures of phenoxyl radicals hydrogen bonded to neutral and cationic partners. <i>Chemistry - A European Journal</i> , 2012 , 18, 5416-29	4.8	13
27	A novel di-compartmental bis-(2-hydroxyisophthalamide) macrocyclic ligand and its mononuclear Cu(II) and Ni(II) complexes. <i>Dalton Transactions</i> , 2012 , 41, 12457-67	4.3	6
26	Structural, spectroscopic and redox properties of a mononuclear Co(II) thiolate complex--the reactivity toward S-alkylation: an experimental and theoretical study. <i>Dalton Transactions</i> , 2012 , 41, 12586-94	4.3	8
25	Ligand contributions to the electronic structures of the oxidized cobalt(II) salen complexes. <i>Inorganic Chemistry</i> , 2012 , 51, 10557-71	5.1	67
24	Radical localization in a series of symmetric Ni(II) complexes with oxidized salen ligands. <i>Chemistry - A European Journal</i> , 2012 , 18, 14117-27	4.8	67
23	Influence of Confinement Effect on Electron Transfers Induced by t-Stilbene Sorption in Medium Pore Acidic Zeolites. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 1812-1825	3.8	23
22	Radicals of Free and Zinc(II)-Coordinated β -Azophenols. <i>European Journal of Inorganic Chemistry</i> , 2011 , 2011, 45-48	2.3	4
21	The versatile binding mode of transition-state analogue inhibitors of tyrosinase towards dicopper(II) model complexes: experimental and theoretical investigations. <i>Chemistry - A European Journal</i> , 2011 , 17, 13482-94	4.8	8
20	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. <i>Inorganic Chemistry</i> , 2011 , 50, 3707-16	5.1	30

19	Separation of geometric isomers of a dicopper complex by using a (19)F-labeled ligand: dynamics, structures, and DFT calculations. <i>Inorganic Chemistry</i> , 2010 , 49, 7832-40	5.1	2
18	Unsymmetrical one-electron oxidized Ni(II)-bis(salicylidene) complexes: a protonation-induced shift of the oxidation site. <i>Chemical Communications</i> , 2010 , 46, 6765-7	5.8	32
17	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. <i>Inorganic Chemistry</i> , 2010 , 49, 6399-401	5.1	33
16	Spin interaction in octahedral zinc complexes of mono- and diradical Schiff and mannich bases. <i>Inorganic Chemistry</i> , 2010 , 49, 646-58	5.1	43
15	Theoretical magnetochemistry of dinuclear manganese complexes: broken symmetry density functional theory investigation on the influence of bridging motifs on structure and magnetism. <i>Dalton Transactions</i> , 2010 , 39, 4959-67	4.3	93
14	X-Ray Structures of Copper(II) and Nickel(II) Radical Salen Complexes: The Preference of Galactose Oxidase for Copper(II). <i>Angewandte Chemie</i> , 2010 , 122, 5109-5112	3.6	35
13	A {Cu ₂ S} ₂ ⁺ Mixed-Valent Core Featuring a Cu-Cu Bond. <i>Angewandte Chemie</i> , 2010 , 122, 8425-8428	3.6	7
12	X-ray structures of copper(II) and nickel(II) radical salen complexes: the preference of galactose oxidase for copper(II). <i>Angewandte Chemie - International Edition</i> , 2010 , 49, 4989-92	16.4	150
11	A {Cu ₂ S} ₂ ⁺ mixed-valent core featuring a Cu-Cu bond. <i>Angewandte Chemie - International Edition</i> , 2010 , 49, 8249-52	16.4	21
10	Electropolymerized biotinylated poly (pyrrole-co-phenol) film as platform for the development of reagentless impedimetric immunosensors. <i>Electrochemistry Communications</i> , 2010 , 12, 311-314	5.1	12
9	A new quantum chemical approach to the magnetic properties of oligonuclear transition-metal complexes: application to a model for the tetranuclear manganese cluster of photosystem II. <i>Chemistry - A European Journal</i> , 2009 , 15, 5108-23	4.8	106
8	Density functional theory. <i>Photosynthesis Research</i> , 2009 , 102, 443-53	3.7	174
7	Magnetic and spectroscopic properties of mixed valence manganese(III,IV) dimers: a systematic study using broken symmetry density functional theory. <i>Inorganic Chemistry</i> , 2009 , 48, 7251-60	5.1	98
6	Trinuclear terpyridine frustrated spin system with a Mn(IV) ₃ O ₄ core: synthesis, physical characterization, and quantum chemical modeling of its magnetic properties. <i>Inorganic Chemistry</i> , 2009 , 48, 10281-8	5.1	50
5	Structure of the oxygen-evolving complex of photosystem II: information on the S(2) state through quantum chemical calculation of its magnetic properties. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 6788-98	3.6	114
4	Variation of average g values and effective exchange coupling constants among [2Fe-2S] clusters: a density functional theory study of the impact of localization (trapping forces) versus delocalization (double-exchange) as competing factors. <i>Inorganic Chemistry</i> , 2008 , 47, 5394-416	5.1	37
3	Spectroscopic description of an unusual protonated ferryl species in the catalase from <i>Proteus mirabilis</i> and density functional theory calculations on related models. Consequences for the ferryl protonation state in catalase, peroxidase and chloroperoxidase. <i>Journal of Biological Inorganic Chemistry</i> , 2007 , 12, 509-25	3.7	28
2	A hybrid bioinspired catechol-alloxazine triangular nickel complex stabilizing protons and electrons. <i>Inorganic Chemistry Frontiers</i> ,	6.8	1

1 Cellulose Depolymerization with LPMO-inspired Cu Complexes. *ChemCatChem*,

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