

Maylis Orio

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/6853919/publications.pdf>

Version: 2024-02-01

109
papers

3,668
citations

159358

30
h-index

143772

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 molybdenum sulfide. <i>Nature Materials</i> , 2016, 15, 640-646.	13.3	490
2	Density functional theory. <i>Photosynthesis Research</i> , 2009, 102, 443-453.	1.6	282
3	Nickel-centred proton reduction catalysis in a model of [NiFe] hydrogenase. <i>Nature Chemistry</i> , 2016, 8, 1054-1060.	6.6	200
4	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, 4989-4992.	7.2	166
5	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, 5108-5123.	1.7	123
6	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.	1.3	121
7	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, 240-243.	7.2	121
8	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, 7251-7260.	1.9	107
9	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.	1.6	100
10	Ligand Contributions to the Electronic Structures of the Oxidized Cobalt(II) salen Complexes. <i>Inorganic Chemistry</i> , 2012, 51, 10557-10571.	1.9	80
11	Radical Localization in a Series of Symmetric Ni ^{II} Complexes with Oxidized Salen Ligands. <i>Chemistry - A European Journal</i> , 2012, 18, 14117-14127.	1.7	76
12	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.	1.9	66
13	One-Electron Oxidized Copper(II) Salophen Complexes: Phenoxyl versus Diiminobenzene Radical Species. <i>Chemistry - A European Journal</i> , 2012, 18, 1068-1072.	1.7	57
14	A Thiosemicarbazone-Nickel(II) Complex as Efficient Electrocatalyst for Hydrogen Evolution. <i>ChemCatChem</i> , 2017, 9, 2262-2268.	1.8	57
15	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, 10281-10288.	1.9	53
16	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.	1.7	50
17	Spin Interaction in Octahedral Zinc Complexes of Mono- and Diradical Schiff and Mannich Bases. <i>Inorganic Chemistry</i> , 2010, 49, 646-658.	1.9	47
18	Tuning Reactivity of Bioinspired [NiFe]-Hydrogenase Models by Ligand Design and Modeling the CO Inhibition Process. <i>ACS Catalysis</i> , 2018, 8, 10658-10667.	5.5	47

#	ARTICLE	IF	CITATIONS
19	Variation of Average g Values and Effective Exchange Coupling Constants among $[2\text{Fe}^{\text{II}}\text{S}]$ 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, 5394-5416.	1.9	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. <i>Inorganic Chemistry</i> , 2010, 49, 6399-6401.	1.9	43
21	Iminosemiquinone radical ligands enable access to a well-defined redox-active $\text{Cu}^{\text{II}}\text{CF}_3$ complex. <i>Chemical Communications</i> , 2014, 50, 10394-10397.	2.2	43
22	Redox Noninnocence of the Bridge in Copper(II) Salophen and Bis(oxamato) Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 9013-9026.	1.9	38
23	Reversible Double Oxidation and Protonation of the Non-Innocent Bridge in a Nickel(II) Salophen Complex. <i>Inorganic Chemistry</i> , 2012, 51, 12796-12804.	1.9	37
24	Understanding Ferroelectricity in the Pb-Free Perovskite-Like Metal-Organic Framework $[(\text{CH}_3)_2\text{NH}]_2\text{Zn}(\text{HCOO})_3$: Dielectric, 2D NMR, and Theoretical Studies. <i>Journal of Physical Chemistry C</i> , 2017, 121, 6314-6322.	1.5	36
25	Unsymmetrical one-electron oxidized Ni(II)-bis(salicylidene) complexes: a protonation-induced shift of the oxidation site. <i>Chemical Communications</i> , 2010, 46, 6765.	2.2	34
26	A Bio-Inspired Switch Based on Cobalt(II) Disulfide/Cobalt(III) Thiolate Interconversion. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 5318-5321.	7.2	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. <i>Inorganic Chemistry</i> , 2011, 50, 3707-3716.	1.9	33
28	Circumventing Intrinsic Metal Reactivity: Radical Generation with Redox-Active Ligands. <i>Chemistry - A European Journal</i> , 2017, 23, 15030-15034.	1.7	33
29	Molecular Electrocatalysts for the Hydrogen Evolution Reaction: Input from Quantum Chemistry. <i>ChemSusChem</i> , 2019, 12, 4905-4915.	3.6	33
30	Versatile Effects of Aurone Structure on Mushroom Tyrosinase Activity. <i>ChemBioChem</i> , 2012, 13, 559-565.	1.3	31
31	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, 10712-10716.	7.2	31
32	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, 509-525.	1.1	30
33	Stable Anilinyll Radicals Coordinated to Nickel: X-Ray Crystal Structure and Characterization. <i>Chemistry - A European Journal</i> , 2013, 19, 16707-16721.	1.7	30
34	Copper Complexes as Bioinspired Models for Lytic Polysaccharide Monooxygenases. <i>Inorganic Chemistry</i> , 2017, 56, 1023-1026.	1.9	30
35	A nickel dimethyl glyoximate complex to form nickel based nanoparticles for electrocatalytic H_2 production. <i>Chemical Communications</i> , 2014, 50, 13514-13516.	2.2	29
36	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, 11134-11137.	2.2	29

#	ARTICLE	IF	CITATIONS
37	A {Cu ₂ S} ²⁺ Mixed-Valent Core Featuring a Cu ^{II} –Cu Bond. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 8249-8252.	7.2	28
38	Copper-Catalyzed Aziridination with Redox-Active Ligands: Molecular Spin Catalysis. <i>Chemistry - A European Journal</i> , 2018, 24, 5086-5090.	1.7	28
39	Influence of Confinement Effect on Electron Transfers Induced by <i>t</i> -Stilbene Sorption in Medium Pore Acidic Zeolites. <i>Journal of Physical Chemistry C</i> , 2012, 116, 1812-1825.	1.5	26
40	N ₂ O reduction at a dissymmetric {Cu ₂ S}-containing mixed-valent center. <i>Chemical Science</i> , 2014, 5, 4774-4784.	3.7	26
41	Vanadium Thiolate Complexes for Efficient and Selective Sulfoxidation Catalysis: A Mechanistic Investigation. <i>Inorganic Chemistry</i> , 2013, 52, 13424-13431.	1.9	24
42	Successes, challenges, and opportunities for quantum chemistry in understanding metalloenzymes for solar fuels research. <i>Chemical Communications</i> , 2021, 57, 3952-3974.	2.2	24
43	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.	1.0	23
44	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.	2.5	22
45	An Experimental and Theoretical Investigation on Pentacoordinated Cobalt(III) Complexes with an Intermediate <i>S</i> =1 Spin State: How Halide Ligands Affect their Magnetic Anisotropy. <i>Chemistry - A European Journal</i> , 2016, 22, 925-933.	1.7	21
46	Ligand-based electronic effects on the electrocatalytic hydrogen production by thiosemicarbazone nickel complexes. <i>Dalton Transactions</i> , 2020, 49, 5064-5073.	1.6	20
47	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.	5.5	19
48	Effect of the Metal on Disulfide/Thiolate Interconversion: Manganese versus Cobalt. <i>Chemistry - A European Journal</i> , 2015, 21, 18770-18778.	1.7	18
49	Efficient Light-Driven Hydrogen Evolution Using a Thiosemicarbazone-Nickel (II) Complex. <i>Frontiers in Chemistry</i> , 2019, 7, 405.	1.8	18
50	Geometric and Electronic Structures of Phenoxy Radicals Hydrogen Bonded to Neutral and Cationic Partners. <i>Chemistry - A European Journal</i> , 2012, 18, 5416-5429.	1.7	16
51	Multifrequency cw-EPR and DFT Studies of an Apparent Compressed Octahedral Cu(II) Complex. <i>Inorganic Chemistry</i> , 2016, 55, 1497-1504.	1.9	16
52	Indolino-Oxazolidine Acido- and Photochromic System Investigated by NMR and Density Functional Theory Calculations. <i>Journal of Organic Chemistry</i> , 2018, 83, 10409-10419.	1.7	16
53	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.	6.6	16
54	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.	1.0	16

#	ARTICLE	IF	CITATIONS
55	Insights into the recombination of radical pairs in hexaarylbiimidazoles. <i>Chemical Communications</i> , 2013, 49, 5841.	2.2	15
56	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, 17030-17044.	1.6	15
57	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.	7.2	15
58	Redox-switchable tetra-copper assembly of N,N-, N,O-phenolate-phenanthroimidazolate bridging ligands. <i>Dalton Transactions</i> , 2013, 42, 2358.	1.6	14
59	Monoanionic Dipyrrin-Pyridine Ligands: Synthesis, Structure and Photophysical Properties. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 5405-5410.	1.0	14
60	Controlled nitrene transfer from a tyrosinase-like arylnitroso-copper complex. <i>Chemical Communications</i> , 2015, 51, 11206-11209.	2.2	14
61	Optimizing Group Transfer Catalysis by Copper Complex with Redox-Active Ligand in an Entatic State. <i>IScience</i> , 2020, 23, 100955.	1.9	14
62	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.	0.5	13
63	Electropolymerized biotinylated poly (pyrrole-viologen) film as platform for the development of reagentless impedimetric immunosensors. <i>Electrochemistry Communications</i> , 2010, 12, 311-314.	2.3	12
64	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, 13482-13494.	1.7	12
65	Nickel(III) complexes of di-amidato-di-phenolato ligands: effect of H-bonding. <i>Dalton Transactions</i> , 2013, 42, 13323.	1.6	11
66	Changing the chemical and physical properties of high valent heterobimetallic bis-(μ -oxido) Cu-Ni complexes by ligand effects. <i>Dalton Transactions</i> , 2016, 45, 15994-16000.	1.6	10
67	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.	1.5	10
68	Unraveling the catalytic mechanisms of H ₂ production with thiosemicarbazone nickel complexes. <i>RSC Advances</i> , 2021, 11, 5232-5238.	1.7	10
69	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.	1.6	9
70	A Multifunctional Photoswitch: μ -Electrocyclization versus ESIPT and Metalation. <i>Chemistry - A European Journal</i> , 2014, 20, 12279-12288.	1.7	9
71	Characterization of a Dinuclear Copper(II) Complex and Its Fleeting Mixed-Valent Copper(II)/Copper(III) Counterpart. <i>ChemPlusChem</i> , 2017, 82, 615-624.	1.3	9
72	Characterization of Cu(II)-reconstituted ACC Oxidase using experimental and theoretical approaches. <i>Archives of Biochemistry and Biophysics</i> , 2017, 623-624, 31-41.	1.4	9

#	ARTICLE	IF	CITATIONS
73	CâˆN Bond Formation from a Masked Highâ€Valent Copper Complex Stabilized by Redox Nonâ€Innocent Ligands. <i>Angewandte Chemie</i> , 2016, 128, 10870-10874.	1.6	8
74	Redox-Innocent Metal-Assisted Cleavage of Sâ€S Bond in a Disulfide-Containing Ligand. <i>Inorganic Chemistry</i> , 2016, 55, 6208-6217.	1.9	8
75	Hydrogen evolution reaction mediated by an all-sulfur trinuclear nickel complex. <i>Chemical Communications</i> , 2020, 56, 11106-11109.	2.2	8
76	A novel di-compartmental bis-(2-hydroxyisophtalamide) macrocyclic ligand and its mononuclear Cu(ii) and Ni(ii) complexes. <i>Dalton Transactions</i> , 2012, 41, 12457.	1.6	7
77	Fusion of Ultravioletâ€Visible and Infrared Transient Absorption Spectroscopy Data to Model Ultrafast Photoisomerization. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3530-3535.	2.1	7
78	Tuning the locus of oxidation in Cu-diamido-diphenoxo complexes: From Cu(III) to Cu(II)-phenoxyl radical. <i>Inorganica Chimica Acta</i> , 2018, 481, 143-150.	1.2	7
79	Catalytic Reduction of Oxygen by a Copper Thiosemicarbazone Complex. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 4549-4555.	1.0	7
80	Quantum dynamics of Mn ²⁺ in dimethylammonium magnesium formate. <i>Journal of Chemical Physics</i> , 2021, 154, 154201.	1.2	7
81	EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory. <i>Magnetochemistry</i> , 2022, 8, 36.	1.0	7
82	Tuning Inner-Sphere Electron Transfer in a Series of Copper/Nitrosoarene Adducts. <i>Inorganic Chemistry</i> , 2020, 59, 8678-8689.	1.9	6
83	Nickel Complexes and Carbon Dots for Efficient Lightâ€Driven Hydrogen Production. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3097-3103.	1.0	6
84	Cellulose Depolymerization with LPMOâ€Inspired Cu Complexes. <i>ChemCatChem</i> , 2021, 13, 4700-4704.	1.8	6
85	Structure and Dynamics of the Excited States of 1,3â€Diarylisobenzofurans: An Experimental and Theoretical Study. <i>Photochemistry and Photobiology</i> , 2012, 88, 633-638.	1.3	5
86	Influence of Copper Coordination Spheres on Nitrous Oxide Reductase (N ₂ O _r) Activity of a Mixed-Valent Copper Complex Containing a {Cu ₂ S} Core. <i>Inorganic Chemistry</i> , 2019, 58, 11649-11655.	1.9	5
87	Self-assembled nickel cubanes as oxygen evolution catalysts. <i>Chemical Communications</i> , 2021, 57, 8608-8611.	2.2	5
88	Radicals of Free and Zinc(II)-Coordinated Î±-Azophenols. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 45-48.	1.0	4
89	X-ray structure of a Ni(ii)â€tri-phenoxyl radical complex. <i>Dalton Transactions</i> , 2015, 44, 17924-17926.	1.6	4
90	Oxidative DNA Cleavage Promoted by a Phenoxyl-Radical Copper(II) Complex. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5575-5584.	1.0	4

#	ARTICLE	IF	CITATIONS
91	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.	1.3	4
92	Electron-spin interaction in the spin-Peierls phase of the organic spin chain (TMTTF) ₂ X (with X = SbF ₆ , AsF ₆). <i>Physical Review B</i> , 2022, 105, .	1.1	4
93	Decoding the Ambiguous Electron Paramagnetic Resonance Signals in the Lytic Polysaccharide Monoxygenase from <i>Photorhabdus luminescens</i> . <i>Inorganic Chemistry</i> , 2022, 61, 8022-8035.	1.9	4
94	Charge-ordering induces magnetic axes rotation in organic materials (TMTTF) ₂ X (with X = SbF ₆ , AsF ₆). <i>Physical Review B</i> , 2022, 105, .	0.2	3
95	Electronic and magnetic interactions in diporphyrinylamines. <i>Journal of Porphyrins and Phthalocyanines</i> , 2016, 20, 1233-1243.	0.4	3
96	An Air-Stable Molybdenum-Based Precatalyst in Oxygen-Atom Transfer Reactions. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 1427-1434.	1.0	3
97	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.	1.0	3
98	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.	1.6	3
99	Superlattice Induced by Charge Order in the Organic Spin Chain (TMTTF) ₂ X (X =) Resonance. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5598-5603.	2.1	3
100	Electron Spin Resonance of Defects in Spin Chains (TMTTF) ₂ X: A Versatile System Behaving Like Molecular Magnet. <i>Applied Magnetic Resonance</i> , 2020, 51, 1307-1320.	0.6	3
101	From Ligand-to Metal-Centered Reactivity: Metal Substitution Effect in Thiosemicarbazone-based Complexes for H ₂ Production. <i>ChemPhysChem</i> , 2022, 23, .	1.0	3
102	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, 7832-7840.	1.9	2
103	Valence Localization at a Bio-Inspired Mixed-Valent {Cu ₂ S} ₂₊ Motif upon Solvation in Acetonitrile: Effect on Nitrous Oxide Reductase (N ₂ O) Activity. <i>Chemistry - A European Journal</i> , 2018, 24, 5060-5063.	1.7	2
104	Magnetic resonance probing of ferroelectricity and magnetism in metal-organic frameworks. <i>Ferroelectrics</i> , 2018, 534, 11-18.	0.3	2
105	A hybrid bioinspired catechol-alloxazine triangular nickel complex stabilizing protons and electrons. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 5286-5298.	3.0	2
106	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.	1.0	1
107	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.	1.0	0
108	Frontispiece: Hydrogen Evolution Reactions Catalyzed by a Bis(thiosemicarbazone) Cobalt Complex: An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2018, 24, .	1.7	0

#	ARTICLE	IF	CITATIONS
109	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.	1.0	0