

## PUBLICATIONS

PUBLICATIONS DANS DES JOURNAUX INTERNATIONAUX

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- 120.** J. Mangué, I. Wehrung, J. Pécaut, S. Ménage, **M. Orio\***, S. Torelli  
"Copper complexes with Cu<sub>2</sub>S cores: Structure and Solvent Effects on Oxygen Reduction Reactions."  
*Dalton Trans.*, 2024, DOI: 10.1039/d4dt01629g.
- 119.** T. Caradec, C. Ple, G. Sicoli, R. Petrov, E. Pradel, C. Sobieski, R. Antoine, **M. Orio**, A. Herledan, N. Willand, R. C. Hartkoorn  
"Small molecule MarR modulators potentiate metronidazole antibiotic activity in aerobic *E. coli* by inducing activation by the nitroreductase NfsA."  
*J. Biol. Chem.*, 2024, 300(7) 107431.
- 118.** A. Munzone, M. Pujol, A. Tamhankar, C. Joseph, I. Mazurenko, S. A. V. Jannuzzi, M. Réglier, A. Royant, G. Sicoli, S. DeBeer, **M. Orio\***, A. J. Simaan, C. Decroos  
"Integrated experimental and theoretical investigation of copper active site properties of Lytic Polysaccharide monooxygenase (LPMO) from *Serratia marcescens*."  
*Inorg. Chem.*, 2024, 63, 11063–11078.
- 117.** M. Papadakis, J. Mehrez, I. Wehrung, L. Delmotte, M. Giorgi, R. Hardré, **M. Orio\***  
"Stereochemical tailoring of nickel-based electrocatalysts for hydrogen evolution reaction."  
*Chem. Cat. Chem.*, 2024, e202400426.
- 116.** S. Chandra Dantu, M. Khalil, M. Bria, C. Saint-Pierre, **M. Orio**, D. Gasparutto, G. Sicoli  
"Cleaving DNA with DNA: cooperative tuning of structure and reactivity driven by copper ions."  
*Adv. Sci.*, 2024, 2306710.
- 115.** M. Papadakis, G. Landrou, M. Poisson, L. Delmotte, K. Achileos, S. Bertaina, R. Hardré, K. Ladomenou, A. G. Coutsolelos, **M. Orio\***  
"A series of cobalt bis(thiosemicarbazone) catalysts for effective photocatalytic hydrogen evolution reaction."  
*EurJIC*, 2023, e202300352.
- 114.** M.-A. Carvalho, K. Merahi, J. Haumesser, N. Parizel, **M. Orio**, J.-P. Gisselbrecht, L. Ruhlmann, J. Weiss, S. Choua, R. Ruppert  
"Synthesis, electrochemical and EPR studies of porphyrins functionalized with bulky donors."  
*Molecules*, 2023, 28, 4405.
- 113.** W. Wang, L.-M. Chamoreau, G. Izzet, A. Proust, **M. Orio\***, S. Blanchard  
"Visible light photoaccumulation of 3 electrons by the hybrid [P<sub>2</sub>V<sub>3</sub>W<sub>15</sub>O<sub>59</sub>(trisDPA {Cu(OAc)})]<sup>5-</sup> polyoxometalate and its use to photocatalytically generate CF<sub>3</sub> radical."  
*J. Am. Chem. Soc.*, 2023, 145, 12136–12147.
- 112.** M. Papadakis, A. Barrozo, L. Delmotte, T. Straistari, S. Shova, S. Bertaina, M. Réglier, V. Krewald, R. Hardré, **M. Orio\***  
"How Nuclearity Impacts H<sub>2</sub> Production in Thiocarbonylhydrazones-based Complexes."  
*Inorganics*, 2023, 11, 149.

- 111.** A. Rančić, N. Babić, **M. Orio**, F. Peyrot  
“32. Structural Features Governing the Metabolic Stability of Tetraethyl-Substituted Nitroxides in Rat Liver Microsomes.”  
*Antioxidants*, 2023, 12, 402.
- 110.** L. Soriano, **M. Orio**, O. Pilone, O. Jeannin, E. Reinheimer, N. Quéméré, P. Auban-Senzier, M. Fourmigué, S. Bertaina  
“A tetrathiafulvalene salt of the nitrite (NO<sub>2</sub><sup>-</sup>) anion: investigations of the spin-Peierls phase”  
*J. Mat. Chem. C*, 2023, 11, 8170–8177.
- 109.** A. Stoumpidi, A. Trapali, M. Poisson, A. Barrozo, S. Bertaina, **M. Orio\***, G. Charalambidis, A. G. Coutsolelos  
“Highly Efficient Light-Driven CO<sub>2</sub> to CO reduction by an Appropriately Decorated Iron Porphyrin Molecular Catalyst.”  
*ChemCatChem.*, 2023, e202200856.
- 108.** S. Gamboa, B. Faure, M. Réglie, A. J. Simaan, **M. Orio\***  
“Computational investigation of Cu-promoted intramolecular stereoselective O-atom transfer reaction with tridentate ligands.”  
*Chem. Eur. J.*, 2022, e202202206.
- 107.** L. Rulišek, M. Gruden, **M. Orio\***, R. J. Deeth  
“Quantum Bio-Inorganic Chemistry (QBIC) Society Special Collection.”  
*Chem. Eur. J.*, 2022, 28, e202202185.
- 106.** R. J. Gómez-Piñeiro, M. Drosou, C. Decroos, A. J. Simaan, D.A. Pantazis, **M. Orio\***  
“Decoding the ambiguous EPR signal in PIAA10 LPMO enzyme: A computational investigation.”  
*Inorg. Chem.*, 2022, 61, 8022–8035.
- 105.** M. Drosou, C.A. Mitsopoulou, **M. Orio**, D. A. Pantazis  
“EPR spectroscopy of Cu(II) complexes: prediction of *g*-tensors using double-hybrid density functional theory.”  
*Magnetochemistry*, 2022, 8, 36.
- 104.** A. Barrozo, **M. Orio\***  
“From ligand- to metal-centered reactivity: Metal substitution effect in thiosemicarbazone-based complexes for H<sub>2</sub> production .”  
*Chem. Phys. Chem.*, 2022, 23, e202200056.
- 103.** L. Soriano, O. Pilone, M.D. Kuz'min, H. Vezin, O. Jeannin, M. Fourmigué, **M. Orio**, S. Bertaina  
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*Phys. Rev. B*, 2022, 105, 064434.

**102.** A. Das, H. Jobelius, J. Schleinitz, S. Gamboa-Ramirez, G. Creste, G. Kervern, J. Raya, N. Le Breton, A. Guénet, Z. Boubegtiten-Fezoua, L. Grimaud, **M. Orio**, G. Rogez, P. Hellwig, S. Choua, S. Ferlay, M. Desage-El Murr.

"A hybrid bioinspired catechol-alloxazine triangular nickel complex stabilizing protons and electrons."

*Inorg. Chem. Front.*, 2021, 8, 5286-5298.

**101.** I. Castillo, A. P. Torres-Flores, D. F. Abad-Aguilar, A. Berlanga-Vázquez, **M. Orio**, D. Martínez-Otero

"Cellulose Depolymerization with LPMO-inspired Cu Complexes."

*ChemCatChem.*, 2021, 13, 4700-4704.

**100.** G. Singh, S. Gamboa, **M. Orio\***, D.A. Pantazis, M. Roemelt

"Magnetic exchange coupling in Cu dimers studied with modern multireference methods and broken-symmetry coupled cluster theory."

*Theo. Chem. Acc.*, 2021, 140, 139.

**99.** A. C. García-Álvarez, S. Gamboa-Ramírez, D. Martínez-Otero, **M. Orio\***, I. Castillo

"Enhanced oxygen evolution electrocatalysis by self-assembled nickel cubanes with CaCl<sub>2</sub> as electrolyte."

*Chem. Comm.*, 2021, 57, 8608-8611.

**98.** K. Ladomenou, M. Papadakis, G. Landrou, M. Giorgi, C. Drivas, S. Kennou, R. Hardré, J. Massin, A. G. Coutsolelos, **M. Orio\***

"Nickel complexes and carbon dots for efficient light-driven hydrogen production."

*EurJIC*, 2021, 30, 3097-3103.

**97.** **M. Orio\***, J. Kaur, J. vanTol, M. Giorgi, N. Dalal, S. Bertaina

"Quantum dynamic of Mn<sup>2+</sup> in dimethylammonium magnesium formate."

*J. Chem. Phys.*, 2021, 154, 154201.

**96.** **M. Orio\***, D. A. Pantazis

"Challenges and opportunities for theory in understanding metalloenzymes."

*Chem. Comm.*, 2021, 57, 3952-3974.

**95.** N. Queyriaux, C. Esmieu, A. K. Gupta, L. Vendier, S. Ott, **M. Orio**, L. Hammarström

"Electrochemical, spectroscopic and computational investigations of a series of polypyridyl ruthenium(II) complexes: reduced states characterizations."

*EurJIC*, 2021, 1263-1270.

**94.** A. Barrozo, **M. Orio\***

"Unraveling the Catalytic Mechanisms of H<sub>2</sub> Production in Thiosemicarbazone Nickel Complexes."

*RSC Adv.*, 2021, 11, 5232-5238.

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*Chem. Phys. Chem.*, 2020, 21, 2667-2679.

- 92.** T. Straistari, A. Morozan, S. Sergiu, M. Réglie, **M. Orio\***, V Artero  
"Catalytic reduction of oxygen by copper thiosemicarbazone systems."  
*EurJIC*, 2020, 48, 4549-4555.
- 91.** C. Pieri, A. Bhattacharjee, A. Barrozo, B. Faure, M. Giorgi, J. Fize, M. Réglie, M. Field, **M. Orio\***, V. Artero, R. Hardré  
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- 90.** L. Soriano, J. Zeisner, V. Kataev, O. Pilone, M. Fourmigué, H. Vezin, **M. Orio**, S. Bertaina  
"Electron Spin Resonance of Defects in Spin Chains. o-(DMTTF)<sub>2</sub>X: a versatile system behaving like molecular magnet."  
*Appl. Magn. Res.*, 2020, 51, 1307–1320.
- 89.** N. Babić, **M. Orio**, F. Peyrot  
"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."  
*Free Radical Biology and Medicine*, 2020, 156, 144-156.
- 88.** N. Queyriaux, K. Abel, J. Fize, J. Pécaut, **M. Orio\***, L. Hammarström  
"Carbon Dioxide Reduction Catalyzed by a Cobalt(II)-Polypyridyl Complex: An Experimental and Theoretical Study."  
*Sustainable Energy & Fuels*, 2020, 4, 3668-3676.
- 87.** M. Papadakis, A. Barrozo, T. Straistari, N. Queyriaux, A. Putri, J. Fize, M. Giorgi, M. Réglie, J. Massin, R. Hardré, **M. Orio\***  
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*Dalton Trans.*, 2020, 49, 5064-5073.
- 86.** O. Cuzan-Munteanu, D. Sirbu, M. Giorgi, S. Shova, E. A. Gibson, M. Réglie, **M. Orio**, L. M. D. R. S. Martins, A. C. Benniston  
"Neutral Lipophilic Palladium(II) Complexes and their Applications in Electrocatalytic Hydrogen Production and C-C Coupling Reactions."  
*EurJIC*, 2020, 10, 813-822.
- 85.** M. S. Askari, F. Effaty, F. Gennarini, **M. Orio**, N. Le Poul, X. Ottenwaelde  
"Sequential Inner-Sphere Electron Transfers in a Family of Copper-Nitrosoarene Adducts."  
*Inorg. Chem.*, 2020, 59, 8678-8689.
- 84.** Y. Ren, R. Forté, K. Cheaib, N. Vanthuynne, L. Fensterbank, H. Vezin, **M. Orio**, S. Blanchard, M. Desage-El Murr.  
"High-performance group transfer catalysis by copper complex with redox-active ligand in an entatic state."  
*iScience*, 2020, 23, 100955.

- 83.** L. Wang, M. Gennari, A. Barrozo, J. Fize, A. Barrozo, C. Philouze, S. Demeshko, F. Meyer, **M. Orio**, V. Artero, C. Duboc  
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*ACS Catal.*, 2020, 10, 1, 177-186.
- 82.** C. Guerrin, Y. Aidibi, L. Sanguinet, P. Leriche, S. Aloise, **M. Orio**, S. Delbaere  
"Indolino-oxazolidine dyads: multiresponsive and multiaddressable molecular switches under NMR investigations."  
*J. Am. Chem. Soc.*, 2019, 141, 19151-19160.
- 81.** A. Barrozo, **M. Orio\***  
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*Chem. Sus. Chem.*, 2019, 12, 4905-4915.
- 80.** C. Esmieu, **M. Orio**, S. Ménage, S. Torelli  
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- 79.** **M. Orio\***, S. Blanchard  
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*Act. Chim.*, 2019, 443, 20-24.
- 78.** S. Panagiotakis, G. Landrou, V. Nikolaou, A. Putri, R. Hardré, J. Massin, G. Charalambidis, A. G. Coutsolelos, **M. Orio\***  
"Efficient light-driven hydrogen evolution using a thiosemicarbazone-nickel (II) complex."  
*Front. Chem.*, 2019, 7, 405.
- 77.** N. Abhyankar, S. Bertaina, **M. Orio**, N. Dalal  
"Magnetic resonance probing of ferroelectricity and magnetism in metal-organic frameworks."  
*Ferroelectrics*, 2018, 534, 11-18.
- 76.** D. Brazzolotto, L. Wang, H. Tang, M. Gennari, N. Queyriaux, C. Philouze, S. Demeshko, F. Meyer, **M. Orio**, V. Artero, M. B. Hall, C. Duboc  
"Tuning catalytic reactivity of [NiFe] hydrogenase models by ligand design and mimicking the CO inhibition process."  
*ACS Catal.*, 2018, 8, 10658-10667.
- 75.** A. Kochem, B. Faure, S. Bertaina, E. Rivière, M. Giorgi, M. Réglie, **M. Orio\***, J. Simaan  
"Original pacman shape tetranuclear copper complex: a magneto-structural and computational study."  
*EurJIC*, 2018, 47, 5039-5046.
- 74.** C.-E. Dutoit, A. Stepanov, J. van Tol, **M. Orio**, S. Bertaina  
"Superlattice induced by charge order in the organic spin chain (TMTTF)<sub>2</sub>X (X = SbF<sub>6</sub>, AsF<sub>6</sub> and PF<sub>6</sub>) revealed by high field EPR."  
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- 73.** C. Guerrin, G. Szalóki, J. Berthet, L. Sanguinet, **M. Orio\***, S. Delbaere  
"Indolino-oxazolidine Acido and Photochromic System – Insights by NMR and DFT Calculations."  
*J. Org. Chem.*, 2018, 83, 10409-10419.
- 72.** T. Straistari, R. Hardré, J. Fize, S. Shova, M. Réglie, V. Artero, **M. Orio\***  
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*Inorg. Chim. Acta*, 2018, 481, 143-150.
- 70.** S. Bertaina, N. Abhyankar, **M. Orio**, N. Dalal  
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- 66.** E. Oheix, **M. Orio**, M. Réglie, O. Iranzo, R. Hardré  
"An air stable molybdenum based pre-catalyst in oxygen-atom transfer"  
*EurJIC*, 2018, 1427–1434.
- 65.** C. Esmieu, **M. Orio**, E. Tirel, J. Mangué, J. Pécaut, S. Ménage, S. Torelli  
"An unusual behavior for a mixed valent complex containing a  $\{\text{Cu}_2\text{S}\}$  motif. Toward a rationale for bio-inspired  $\text{N}_2\text{O}$ -reductase activity."  
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- 63.** B. Debus, **M. Orio**, J. Rehaut, G. Burdzinski, C. Ruckebusch, M. Sliwa  
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- 62.** T. Straistari, J. Fize, S. Shova, M. Réglie, V. Artero, **M. Orio\***  
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- 61.** N. El Bakkali-Tahéri, S. Tachon, **M. Orio**, S. Bertaina, M. Marthino, V. Robert, M. Réglie, T. Tron, P. Dorlet, A. J. Simaan  
"Replacement of the non-heme Fe(II) by Cu(II) in ACC Oxidase: characterization and mutational analysis."  
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- 60.** A. Kochem, F. Gennarini, M. Yemloul, **M. Orio**, N. Le Poul, E. Rivière, M. Giorgi, B. Faure, Y. Le Mest, M. Réglie, A. J. Simaan  
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"Copper(II) Complexes of Phenanthroline and Histidine Containing Ligands: Synthesis, Characterization and Evaluation of their DNA Cleavage and Cytotoxic Activity."  
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- 55.** K. Merahi, A. M. V. M. Pereira, C. Jeandon, L. Ruhlmann, J. A. S. Cavaleiro, M. G. P. M. S. Neves, **M. Orio**, P. Turek, S. Choua, R. Ruppert  
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