

PUBLICATIONS

PUBLICATIONS DANS DES JOURNAUX INTERNATIONAUX

- 115.** M. Papadakis, G. Landrou, M. Giorgi, R. Hardré, K. Ladomenou, A. G. Coutsolelos, **M. Orio***
“A series of cobalt bis(thiosemicarbazone) catalysts for effective photocatalytic hydrogen evolution reaction.”
EurJIC, 2023, DOI: 10.1002/ejic.202300352.
- 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 [P₂V₃W₁₅O₅₉(trisDPA {Cu(OAc)})]⁵⁻ polyoxometalate and its use to photocatalytically generate CF₃ radical.”
J. Am. Chem. Soc., 2023. 145, 12136–12147.
- 112.** M. Papadakis, A. Barrozo, L. Delmotte, T. Straistari, S. Shova, S. Bertaina, M. Réglie, V. Krewald, R. Hardré, **M. Orio***
“How Nuclearity Impacts H₂ Production in Thiocarbonylhydrazones-based Complexes.”
Inorganics, 2023, 11, 149.
- 111.** A. Rančić, N. Babić, **M. Orio**, F. Peyrot
“Metabolic stability of nitroxides in rat liver microsomes. Special attention devoted to isoindoline nitroxide with tetraethyl-substitution: EPR, HPLC-HRMS and DFT study.”
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 (NO₂⁻) 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 CO₂ 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 H₂ 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
"Electron spins interaction in the spin-Peierls phase of the organic spin chain (*o*-DMTTF)₂X (X = Cl, Br, I)."
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.
"Synthesis and electronic structure of 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
“Studying magnetic exchange coupling in Cu dimers 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 CaCl₂ 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 Mn²⁺ 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 H₂ Production in Thiosemicarbazone Nickel Complexes."
RSC Adv., 2021, 11, 5232-5238.
- 93.** R. J. Gómez-Piñeiro, D. A. Pantazis, **M. Orio***
"Comparison of density functional and correlated wave function methods for the prediction of Cu(II) hyperfine coupling constants."
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
"Hydrogen evolution reaction mediated by a trinuclear nickel complex with an all sulfured coordination sphere."
Chem. Comm., 2020, **56**, 11106-11109.
- 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)₂X: 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***
"Ligand-Based Electronic Effects on the Electrocatalytic Hydrogen Production by Thiosemicarbazone Nickel Complexes."
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. Vanthuyn, 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
"Role of the metal ion in bio-inspired hydrogenase models: investigation of heterodinuclear FeFe vs NiFe complexes."
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***
"Molecular electrocatalysts for Hydrogen Evolution Reaction: The input from quantum chemistry."
Chem. Sus. Chem., 2019, 12, 4905-4915.
- 80.** C. Esmieu, **M. Orio**, S. Ménage, S. Torelli
"Influence of the copper coordination spheres on the N₂O_r activity by a mixed-valent copper complex containing a {Cu₂S} core."
Inorg. Chem., 2019, 58, 11649-11655.
- 79.** **M. Orio***, S. Blanchard
"Un duo gagnant pour la catalyse rédox."
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)₂X (X = SbF₆, AsF₆ and PF₆) revealed by high field EPR."
J. Phys. Chem. Lett., 2018, 9, 5598–5603.
- 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***
"Experimental and theoretical studies of a thiosemicarbazone cobalt electrocatalyst for proton reduction."
Chem. Eur. J., 2018, 24, 8779-8786.
Highlight dans "En direct des laboratoires de l'institut de Chimie".
- 71.** M. Eckshtain-Levi, R. Lavi, **M. Orio***, L. Benisvy
"Tuning the locus of oxidation in Cu-diamido-diphenoxo complexes: from Cu(III) to Cu(II)-phenoxyl radical."
Inorg. Chim. Acta, 2018, 481, 143-150.
- 70.** S. Bertaina, N. Abhyankar, **M. Orio**, N. Dalal
"Measuring Motional Dynamics of (CH₃)₂NH₂⁺ in the Perovskite-like Metal-Organic Framework [(CH₃)₂NH₂] [Zn(HCOO)₃]: The Value of Low-Frequency EPR."
J. Phys. Chem. C, 2018, 122, 16431-16436.

69. G. Charalampidis, S. Das, A. Trapali, A. Quaranta, **M. Orio**, Z. Halime, P. Fertey, R. Guillot, A. Coutsolelos, W. Leibl, A. Aukauloo, M. Sircoglou.

"Water Molecules Gating a Photoinduced One Electron Two Protons Transfer in a Tyr/His model of Photosystem II."

Angew. Chem., 2018, 57, 9013-9017.

Highlight dans "En direct des laboratoires de l'institut de Chimie".

68. T. Straistari, R. Hardré, J. Massin, M. Attolini, B. Faure, M. Giorgi, M. Réglie, **M. Orio***

"Influence of the metal ion on the electrocatalytic hydrogen production by a thiosemicarbazone palladium complex."

EurJIC, 2018, 2259-2266.

67. Y. Ren, K. Cheaib, J. Jacquet, H. Vezin, L. Fensterbank, **M. Orio**, S. Blanchard, M. Desage-El Murr.

"Copper-catalyzed aziridination with redox-active ligands: molecular spin catalysis."

Chem. Eur. J., 2018, 24, 5086 – 5090.

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 {Cu₂S} motif. Toward a rationale for bio-inspired N₂O-reductase activity."

Chem. Eur. J., 2018, 24, 5060 – 5063.

64. J. Jacquet, K. Cheaib, Y. Ren, H. Vezin, **M. Orio**, S. Blanchard, L. Fensterbank, M. Desage-El Murr.

"Overriding metallic intrinsic reactivity: radical generation with redox-active ligands."

Chem. Eur. J., 2017, 23, 15030–15033.

63. B. Debus, **M. Orio**, J. Rehaut, G. Burdzinski, C. Ruckebusch, M. Sliwa

"Fusion of UV-vis and IR Transient Absorption Data to Model Ultrafast Photo-Isomerization in Transient Absorption Spectroscopy."

J. Phys. Chem. Lett., 2017, 8, 3530–3535.

62. T. Straistari, J. Fize, S. Shova, M. Réglie, V. Artero, **M. Orio***

"A thiosemicarbazone-nickel(II) complex as efficient electrocatalyst for hydrogen evolution."

Chem. Cat. Chem., 2017, 9, 2262 –2268.

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."

Archiv. of Biochem. and Biophys., 2017, 623-624, 31-41.

- 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
"Characterization of a butterfly flapping dinuclear copper(II) complex and its fleeting mixed-valent Cu(II)Cu(III) counterpart."
Chem. Plus Chem., 2017, 82, 615-624.
- 59.** N. Abhyankar, J. J. Kweon, **M. Orio**, S. Bertaina, M. Lee, E. S. Choi, R. Fu, N. Dalal
"Understanding Ferroelectricity in the Pb-Free Perovskite-Like Metal-Organic Framework [(CH₃)₂NH₂]Zn(HCOO)₃: 2D NMR and Theoretical Studies."
J. Phys. Chem. C, 2017, 121, 6314-6322.
- 58.** A. L. Concia, M. R. Beccia, **M. Orio**, F. Terra Ferre, M. Scarpellini, F. Biaso, B. Guigliarelli, M. Réglie, A. J. Simaan
"Copper complexes as structural and functional models for Lytic Polysaccharide Monooxygenases."
Inorg. Chem., 2017, 56, 1023-26.
- 57.** O. Cuzan, A. Kochem, A. J. Simaan, B. Faure, V. Robert, S. Bertaina, M. Giorgi, S. Shova, M. Maffei, M. Réglie, **M. Orio***
"Oxydative DNA Cleavage Promoted by Phenoxyl-Radical Copper(II) Complex."
EurJIC, 2016, 5575-5584.
- 56.** S. M. G. Leite, L. M. P. Lima, S. Gama, F. Mendes, **M. Orio**, I. Bento, A. Paulo, R. Delgado, O. Iranzo
"Copper(II) Complexes of Phenanthroline and Histidine Containing Ligands: Synthesis, Characterization and Evaluation of their DNA Cleavage and Cytotoxic Activity."
Inorg. Chem., 2016, 55, 11801-11814.
- 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
"Electronic and magnetic interactions in diporphyrinylamine."
J. Phtalo.Porph., 2016, 20, 1-11.
- 54.** M.-C. Kafentzi, **M. Orio**, M. Réglie, S. Yao, U. Kuhlmann, P. Hildebrandt, M. Driess, J. Simaan, K. Ray
"Changing the chemical and physical properties of high valent heterobimetallic bis-(μ -oxido) Cu–Ni complexes by ligand effects."
Dalton Trans., 2016, 45, 15994-16000.
- 53.** J. Jacquet, P. Chaumont, G. Gontard, **M. Orio**, H. Vezin, S. Blanchard, M. Desage-El Murr, L. Fensterbank
"C–N bond formation from a masked high-valent copper complex stabilized by redox non-innocent ligands."
Angew. Chem. Int. Ed., 2016, 55, 10712-10716.
- 52.** D. Brazzolotto, M. Gennari, N. Queyriaux, T. Simmons, J. Pécaut, S. Demeshko, F. Meyer, **M. Orio**, V. Artero, C. Duboc
"A structural and functional mimic of the NiFe hydrogenase with unprecedented Ni-centered chemistry."
Nat. Chem., 2016, 8, 1054–1060.
Highlight dans "En direct des laboratoires de l'institut de Chimie".

- 51.** C. Esmieu, **M. Orio**, L. Le Pape, C. Lebrun, J. Pécaut, S. Ménage, S. Torelli
"Redox-Innocent Metal-Assisted Cleavage of S–S Bond in a Disulfide-Containing Ligand."
Inorg. Chem., 2016, 55, 6208–62179.
- 50.** P. D. Tran, T. V. Tran, **M. Orio**, S. Torelli, D. Q. Truong, K. Nayuki, Y. Sasaki, S. Y. Chiam, R. Yi, I. Honma, J. Barber, V. Artero
"Coordination polymer structure and revisited hydrogen evolution catalytic mechanism for amorphous molybdenum sulfide."
Nat. Mat., 2016, 15, 640–646.
Highlight dans "En direct des laboratoires de l'institut de Chimie".
- 49.** N. Hall, **M. Orio**, M. Gennari, C. Wills, F. Molton, C. Philouze, M. A. Halcrow, C. Duboc, A. G. Blackman
"Multifrequency *cw*-EPR and DFT studies of an apparent compressed Jahn-Teller effect in a mononuclear Cu(II) complex."
Inorg. Chem., 2016, 55, 1497-1504.
- 48.** D. Brazzolotto, M. Gennari, S. Yu, J. Pécaut, M. Rouzières, R. Clérac, **M. Orio***, C. Duboc
"An Experimental and Theoretical Investigation on Intermediate Spin Pentacoordinated Cobalt(III) complexes: How Halide Ligands Affect the Zero Field Splitting."
Chem. Eur. J., 2016, 22, 925-933.
Highlight dans "En direct des laboratoires de l'institut de Chimie".
- 47.** M. Gennari, D. Brazzolotto, S. Yu, J. Pécaut, C. Philouze, M. Rouzières, R. Clérac, **M. Orio**, C. Duboc
"Effect of the metal on disulphide/thiolate interconversion: manganese vs cobalt."
Chem. Eur. J., 2015, 51, 18770-18778.
- 46.** C. Duclouset, P. Jouin, E. Paredes, R. Guillot, M. Sircoglou, **M. Orio**, W. Leiblb, A. Aukauloo
"Monoanionic DiPyrin Pyridine Ligand. Synthesis, Structure and Photophysical Properties."
EurJIC, 2015, 32, 5405–5410.
- 45.** C.-E. Dutoit, S. Bertaina, **M. Orio**, M. Dressel, A. Stepanov
"Charge-Ordering Induces Magnetic Axes Rotation in Organic Materials (TMTTF)₂X (with X=SbF₆, AsF₆ and PF₆)."
J. Low Temp. Phys., 2015, 41, 11, 1206-1208.
- 44.** L. Benisvy, G. M. Zats, O. Fleker, **M. Orio**, D. S. Yufit, G. Romanenko, V. Ovcharenko
"X-ray Structure of a Ni(II)-Tri-Phenoxyl Radical Complex."
Dalton Trans., 2015, 44, 17924–17926.
- 43.** D. de Bellefeuille, **M. Orio**, A.-L. Barra, A. Aukauloo, Y. Journaux, C. Philouze, X. Ottenwaelder, F. Thomas
"Redox Non-Innocence of the Bridge in Copper(II) Salophen and bis-Oxamato Complexes."
Inorg. Chem., 2015, 54, 9013–9026.

- 42.** F. He, L. Ruhlmann, J.-P. Gisselbrecht, S. Choua, **M. Orio**, M. Wesolek, A. A. Danopoulos, P. Braunstein
"Dinuclear iridium and rhodium complexes with bridging arylimidazolidine- N^3, C^2 ligands: Synthetic, structural, reactivity, electrochemical and spectroscopic Studies."
Dalton Trans., 2015, 44, 17030-17044.
- 41.** M.S. Askari, **M. Orio**, X. Ottenwaelder
"Controlled nitrene transfer from a tyrosinase-like arylnitroso-copper complex."
Chem. Comm., 2015, 51, 11206-11209.
- 40.** B. N. Sánchez-Eguía, M. Flores-Alamo, **M. Orio**, Ivan Castillo
"Side-on cupric-superoxo triplet complexes as competent agents for H-abstraction relevant to the active site of PHM."
Chem. Comm., 2015, 51, 11134-11137.
- 39.** C. Esmieu, **M. Orio**, L. Le Pape, J. Pécaut, C. Lebrun, S. Torelli, S. Ménage
" N_2O reduction at a dissymmetric $\{Cu_2S\}$ -containing mixed-valent center."
Chem. Sci., 2014, 5, 4774-4784.
- 38.** S. Cherdo, S. El Ghachtouli, M. Sircoglou, F. Brisset, **M. Orio**, A. Aukauloo
"A nickel dimethyl glyoximato complex to form nickel based nanoparticles for electrocatalytic H_2 production."
Chem. Comm., 2014, 50, 13514-13516.
- 37.** J. Guérin, A. Léaustic, S. Delbaere, J. Berthet, R. Guillot, C. Ruckebusch, R. Métivier, K. Nakatani, **M. Orio***, M. Sliwa, P. Yu
"A multifunctional photoswitch: 6π electrocyclization versus ESIPT and metallation."
Chem. Eur. J., 2014, 20, 12279-12288.
- 36.** J. Jacquet, E. Salanouve, **M. Orio**, H. Vezin, S. Blanchard, E. Derat, M. Desage-El Murr, L. Fensterbank
"Iminosemiquinone radical ligand enables access to well-defined redox-active Cu^{II} -CF₃ complex. "
Chem. Comm., 2014, 50, 10394-10397.
- 35.** M. Gennari, B. Gerey, N. Hall, M.-N. Collomb, J. Pécaut, R. Clerac, **M. Orio**, C. Duboc
"A Bio-Inspired Switch Based on Cobalt(II) Disulfide/Cobalt(III) Thiolate Interconversion."
Angew. Chem. Int. Ed., 2014, 53, 5318-5321.
- 34.** M. Bourrez, **M. Orio***, F. Molton, H. Vezin, C. Duboc, A. Deronzier, S. Chardon-Noblat
"Pulsed-EPR Evidence of a Manganese(II) Hydroxycarbonyl Intermediate in the Electrocatalytic Reduction of Carbon Dioxide by a Manganese Bipyridyl Derivative."
Angew. Chem. Int. Ed., 2014, 53, 240-243.
- 33.** N. Hall, **M. Orio***, A. Jorge-Robin, B. Gennaro, C. Marchi-Delapierre, C. Duboc
"Vanadium Thiolate Complexes for Efficient and Selective Sulfoxidation Catalysis: A Mechanistic Investigation."
Inorg. Chem., 2013, 52, 13424-13431.

- 32.** A. Kochem, G. Gellon, N. Leconte, B. Baptiste, C. Philouze, O. Jarjayes, **M. Orio**, F. Thomas
"Stable anilinyll radicals coordinated to nickel: X-Ray crystal structure and characterization."
Chem. Eur. J., 2013, 19, 16707-16721.
- 31.** M. Eckshtain-Levi, **M. Orio**, R. Lavi, L. Benisvy
"Nickel(III) complexes of di-amidato-di-phenolato ligands: Effect of H-bonding."
Dalton. Trans., 2013, 42, 13323-13326.
- 30.** S. Delbaere, **M. Orio**, J. Berthet, M. Sliwa, S. Hatano, J. Abe
"Insights into the recombination of radical pair in hexaarylbiimidazoles."
Chem. Comm., 2013, 49, 5841-5843.
- 29.** J.-L. Mathias, H. Arora, R. Lavi, D. Yufit, **M. Orio**, N. Aliaga, L. Benisvy
"Redox-switchable tetra-copper assembly of N,N-, N,O-phenolate-phenanthroimidazolate bridging ligands."
Dalton. Trans., 2013, 42, 2358-2361.
- 28.** D. de Bellefeuille, M.S. Askari, B. Lasalle-Kaiser, Y. Journaux, A. Aukauloo, **M. Orio**, F. Thomas, X. Ottenwaelder
"Reversible double oxidation of the non-Innocent bridge in a nickel(II)-salophen complex."
Inorg. Chem., 2012, 51, 12796–12804.
- 27.** L. Chiang, A. Kochem, O. Jarjayes, T.J. Dunn, H. Vezin, M. Sakaguchi, T. Ogura, **M. Orio**, Y. Shimazaki, F. Thomas, T. Storr
"Radical localization in a series of symmetric nickel(II) complexes with oxidized salen ligands."
Chem. Eur. J., 2012, 18, 14117–14127.
- 26.** A. Kochem, H. Kanso, B. Baptiste, H. Arora, C. Philouze, O. Jarjayes, H. Vezin, D. Luneau, **M. Orio**, F. Thomas
"Ligand contributions to the electronic structures of the oxidized cobalt(II) salen complexes."
Inorg. Chem., 2012, 51, 10557–10571.
- 25.** M. Gennari, B. Gerey, N. Hall, J. Pécaut, H. Vezin, M.-N. Collomb, **M. Orio**, C. Duboc
"Structural, spectroscopic and redox properties of a mononuclear Co^{II} thiolate complex - the reactivity toward S-alkylation: an experimental and theoretical study."
Dalton. Trans., 2012, 41, 12586-12594.
- 24.** M. Eckshtain-Levi, H. Arora, R. Lavi, D. Yufit, **M. Orio**, R. Wanke, L. Benisvy
"A novel di-compartmental *bis*-(2-hydroxyisophthalamide) macrocyclic ligand and its mononuclear Cu(II) and Ni(II) complexes."
Dalton. Trans., 2012, 41, 12457-12467.
- 23.** **M. Orio**, O. Jarjayes, B. Baptiste, C. Philouze, C. Duboc, J.-L. Mathias, L. Benisvy, F. Thomas
"Geometric and Electronic Structures of Phenoxy Radicals Hydrogen Bonded to Neutral and Cationic Partners."
Chem. Eur. J., 2012, 18, 5416-5429.

- 22.** J. Jacq, S. Tsekhanovich, **M. Orio***, C. Einhorn, J. Einhorn, B. Bessières, D. Jouvenot, F. Loiseau
"Structure and Dynamics of the Excited States of 1,3-Diarylisobenzofurans: An Experimental and Theoretical Study."
Photochem. Photobiol., 2012, 88, 633-638.
- 21.** C. Dubois, R. Haudecoeur, **M. Orio**, C. Belle, C. Bochot, A. Boumendjel, R. Hardré, H. Jamet, M. Réglie
"Versatile effects of aurone structure on the mushroom Tyrosinase activity."
Chem. Bio. Chem., 2012, 13, 559–565.
- 20.** M. Hureau, A. Moissette, H. Vezin, C. Brémard, **M. Orio**
"Influence of confinement effect on electron transfers induced by t-stilbene sorption in medium pore acidic zeolites."
J. Phys. Chem. C., 2012, 116, 1812–1825.
- 19.** A. Kochem, O. Jarjayes, B. Baptiste, C. Philouze, H. Vezin, K. Tsukidate, F. Tani, **M. Orio***, Y. Shimazaki, F. Thomas
"One-electron oxidized copper(II) salphen complexes: phenoxyl versus diiminobenzene radical species."
Chem. Eur. J., 2012, 18, 1068 – 1072.
- 18.** **M. Orio**, C. Bochot, C. Dubois, G. Gellon, R. Hardré, H. Jamet, D. Luneau, C. Philouze, M. Réglie, G. Serratrice, C. Belle
" The Versatile Binding Mode of Transition-State Analogue Inhibitors of Tyrosinase towards Dicopper(II) Model Complexes: Experimental and Theoretical Investigations."
Chem. Eur. J., 2011, 17, 13482–13494.
- 17.** M. Gennari, **M. Orio**, J. Pécaut, E. Bothe, F. Neese, M.-N. Collomb, C. Duboc
"Influence of mixed thiolate/thioether *versus* dithiolate coordination in the accessibility of the uncommon +I and +III oxidation states for the nickel ion: An experimental and computational study."
Inorg. Chem., 2011, 50, 3707-3716.
- 16.** A. Kochem, **M. Orio**, C. Philouze, H. Jamet, A. D'Hardemare, F. Thomas
"Radicals of free and zinc(II) coordinated ν -diazophenols."
EurJIC, 2011, 1, 45-48.
- 15.** S. Torelli, **M. Orio**, J. Pécaut, H. Jamet, L. Le Pape, S. Ménage
"A $\{Cu_2S\}^{2+}$ Mixed-Valent Core Featuring a Cu-Cu Bond."
Angew. Chem. Int. Ed., 2010, 49, 8249 –8252.
- 14.** S. Durot, L. H. Hossain, S. Hamman, H. Jamet, **M. Orio**, I. Gautier-Luneau, C. Philouze, J.-L. Pierre, C. Belle
"Separation of Geometric Isomers of a Dicopper Complex by Using a F-19-Labeled Ligand: Dynamics, Structures, and DFT Calculations."
Inorg. Chem., 2010, 49, 7832-7840.

- 13.** A. Kochem, **M. Orio**, O. Jarjayes, F. Neese, F. Thomas
"Unsymmetrical one-electron oxidized Ni(II)-bis(salicylidene) complexes: A protonation-induced shift of the oxidation site."
Chem. Comm., 2010, 46, 6765-6767.
- 12.** M. Gennari, **M. Orio**, J. Pécaut, F. Neese, M.-N. Collomb, C. Duboc
"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."
Inorg. Chem., 2010, 49, 6399-6401.
- 11.** D.A. Pantazis, V. Krewald, **M. Orio**, F. Neese
"Theoretical magnetochemistry of dinuclear manganese complexes: Broken symmetry density functional theory investigation on the influence of bridging motifs on structure and magnetism."
Dalton Trans., 2010, 39, 4959-4967.
- 10.** **M. Orio**, O. Jarjayes, H. Kanso, C. Philouze, F. Neese, F. Thomas
"X-Ray structures of copper(II) and nickel(II) radical salen complexes: The preference of Galactose Oxidase for copper(II)."
Angew. Chem. Int. Ed., 2010, 49, 4989-4992.
- 9.** C. Gondran, **M. Orio**, D. Rigal, B. Galland, L. Bouffier, T. Gulon, S. Cosnier
"Electropolymerized biotinylated poly (pyrrole-viologen) film as platform for the development of reagentless impedimetric immunosensors."
Electrochem. Commun., 2010, 12, 311-314.
- 8.** **M. Orio**, C. Philouze, O. Jarjayes, F. Neese, F. Thomas
"Spin Interaction in Octahedral Zinc Complexes of Mono- and Diradical Schiff and Mannich Bases."
Inorg. Chem., 2010, 49, 646-658.
- 7.** C. Baffert, **M. Orio**, D.A. Pantazis, C. Duboc, A.G. Blackman, G. Blondin, F. Neese, A. Deronzier, M.-N. Collomb
"Trinuclear terpyridine frustrated spin system with a $Mn^{IV}_3O_4$ core: Synthesis, physical characterization and quantum chemical modeling of its magnetic properties."
Inorg. Chem., 2009, 48, 10281-10288.
- 6.** **M. Orio**, D.A. Pantazis, T. Petrenko, F. Neese
"Magnetic and spectroscopic properties of mixed valence (III,IV) dimers: A systematic study using broken symmetry density functional theory".
Inorg. Chem., 2009, 48, 7251-7260.
- 5.** D.A. Pantazis, **M. Orio**, T. Petrenko, S. Zein, W. Lubitz, J. Messinger, F. Neese
"Structure of the oxygen-evolving complex of photosystem II: information on the S-2 state through quantum chemical calculation of its magnetic properties."
Phys. Chem. Chem. Phys., 2009, 11, 6788-6798.
- 4.** **M. Orio**, D.A. Pantazis, F. Neese
"Basics and applications of biophysical techniques in photosynthesis and related processes: Density Functional Theory."
Photosynth. Res., 2009, 102, 443-453.

3. D.A. Pantazis, **M. Orio**, T. Petrenko, S. Zein, E. Bill, W. Lubitz, J. Messinger, F. Neese
"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."

Chem. Eur. J., 2009, 15, 5108-5123.

2. **M. Orio**, J.-M. Mouesca

"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."

Inorg. Chem., 2008, 47, 5394-5416.

1. O. Horner, J.-M. Mouesca, P.L. Solari, **M. Orio**, J.-L. Oddou, P. Bonville, H.M. Jouve

"Spectroscopic description of an unusual protonated ferryl species in catalase from proteus mirabilis and Density Functionnal calculations on related models. Consequences on the ferryl protonation state in catalase, peroxidase and chloroperoxidase."

J. Biol. Inorg. Chem., 2007, 12, 509-525.

PUBLICATIONS DANS DES OUVRAGES INTERNATIONAUX

1. M. Sundararajan, C. Riplinger, **M. Orio**, F. Wennmohs, F. Neese

"Spectroscopic properties of protein bound cofactors: Calculations by combined Quantum Mechanical/Molecular Mechanical (QM/MM) approaches."

Computational Inorganic and Bioinorganic Chemistry, eds. E.I. Solomon, R.A. Scott and R.B. King, Wiley, 2009, 55-70.

PUBLICATIONS DANS DES ACTES DE CONGRES

15. L Soriano, S Bertaina, M Fourmigué, H Vezin, M Orio

"Electron spin resonance of defects in the organic spin chains compounds (o-DMTTF)₂X."

Bulletin of the American Physical Society, 2021, U71.00187.

14. D. Brazzolotto, L. Wang, M. Gennari, **M. Orio**, F. Meyer, M. Hall, V. Artero, A. Dey, C. Duboc

"Bio-Inspired NiFe Catalysts for H₂ Production."

ECS Meeting Abstracts, 2019, MA2019-04.

13. M. Kafentzi, A. Kochem, A. L. Concia, **M. Orio**, B. Faure, M. Scarpellini, F. Gennarini, N. Le Poul, Y. Le Mest, M. Reglier, A J. Simaan

J. Biol. Inorg. Chem., 2017, 22, S207.

12. D. Brazzolotto, L. Wang, M. Gennari, F. Meyer, **M. Orio**, V. Artero, C. Duboc

"Bio-inspired heterodinuclear NiFe catalysts for H₂ production."

Abstracts of papers of the American Chemical Society, 2017, 253.

- 11.** Ivan Castillo, B. N. Sánchez-Eguía, **M. Orio**,
"Reactive copper-oxygen species with mixed benzimidazole/thio- and selenoether platforms relevant to the active site of PHM."
Abstracts of papers of the American Chemical Society, 2016, 251.
- 10.** D. Brazzolotto, M. Gennari, N. Queyriaux, F. Meyer, **M. Orio**, V. Artero, C. Duboc
"Structural and functional mimic of the NiFe hydrogenase with unprecedented Ni-centered chemistry."
Abstracts of papers of the American Chemical Society, 2016, 251.
- 9.** Ivan Castillo, B. N. Sánchez-Eguía, **M. Orio**,
"Bis(benzimidazole)thioether-copper complexes inspired on the active site of PHM and their reactivity with O₂."
Abstracts of papers of the American Chemical Society, 2014, 248.
- 8.** N. Leconte, J. Ciccione, C. Philouze, F. Thomas, **M. Orio**
"Geometric and Electronic Structures of Ni(II) Complexes of Non-Innocent Tetradentate Phenylenediamine Ligands."
J. Biol. Inorg. Chem., 2014, 19, S509.
- 7.** C. Esmieu, S. Torelli, C. Lebrun, L. Le Pape, S. Ménage, **M. Orio**, J. Pécaut
"Bio-inspired copper complexes catalysts for N₂O activation."
J. Biol. Inorg. Chem., 2014, 19, S508.
- 6.** N. Hall, C. Duboc, A. Jorge-Robin, C. Marchi-Delapierre, **M. Orio**
"A unique dioxovanadium(V) thiolate complex: an efficient and selective catalyst for sulfoxidation. Comparison with an oxovanadium(IV) thiolate complex."
J. Biol. Inorg. Chem., 2014, 19, S558.
- 5.** M. Gennari, D. Brazzolotto, **M. Orio**, F. Neese, M. Van Gastel, S. DeBeer, J. Pécaut, C. Duboc
"Bio-inspired thiolate metal complexes structural, spectroscopic and redox properties, reactivity."
J. Biol. Inorg. Chem., 2014, 19, S731.
- 4.** **M. Orio**, H. Vezin, M. Bourrez, F. Molton, C. Duboc, S. Chardon-Noblat, A. Deronzier
"Innovative molecular electrocatalyst for carbon dioxide reduction: Experimental and theoretical characterization of a key-intermediate."
J. Biol. Inorg. Chem., 2014, 19, S530.
- 3.** F. Neese, D. A. Pantazis, **M. Orio**, M. Römel, S. DeBeer-George, C. Duboc, W. Lubitz
"Quantum chemical studies of the spectroscopic properties of mono- to oligonuclear manganese clusters: zero-field splitting, exchange coupling, X-ray absorption and magnetic circular dichroism."
J. Biol. Inorg. Chem., 2009, 14, S133.
- 2.** F. Neese, D. A. Pantazis, **M. Orio**, D. Liakos, D. Ganyushin
"Spin dependent properties of open-shell transition metals: Experiment and quantum chemistry."
Abstracts of papers of the American Chemical Society, 2008, 236.

1. M. Orio, J.-M. Mouesca

"DFT study of g_{av} (average g value) among [2Fe-2S] clusters. Impact of localization (trapping forces) and delocalization (double-exchange) factors on the $\{g_{av}\}$ values of (i) plant-type Ferredoxins and Rieske centers (and related Cys / His / Ser mutants), (ii) Xanthine oxidase clusters I and II, and (iii) various [2Fe-2S] model complexes."

J. Biol. Inorg. Chem., 2007, 12 (Suppl 1), S258.