PhD 2023-2026 Ecole Doctorale de Chimie de Lyon

Magnetic metal-organic frameworks

Aimants à charpente métal-organique

Laboratoire des **M**ultimatériaux et **I**nterfaces (LMI UMR 5615)

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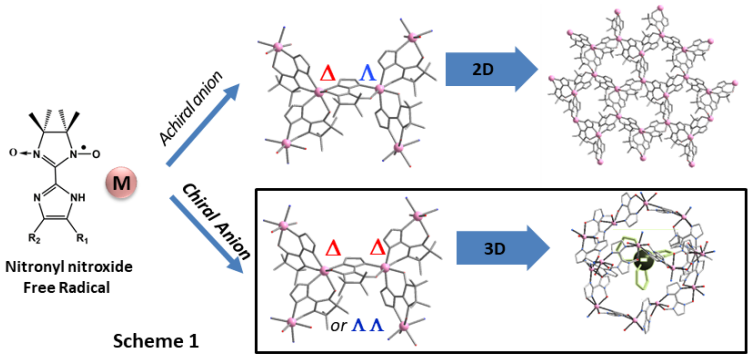
Keywords: Coordination chemistry; magnetism; crystallography, computational modeling

Contexte: Our team build **molecule-based magnets** by coordination of magnetic metal ions with nitronyl nitroxide free radicals as magnetic bridging ligands. Along this approach, we synthesized 2D metal-radical frameworks that are magnets with Curie temperatures (Tc) near liquid nitrogen [1-3].

Objective of the PhD is to build 3D metal-radical frameworks with high Tc.

PhD project: In our metal-radical frameworks, three chelating radicals are around each metal ion (D3 symmetry). This induces chiral topologies Δ or Λ (Scheme 1). In 2D coordination polymers, there is alternation of Δ and Λ chiralities but 3D frameworks requires homo-chirality of the metal sites to be either Δ or Λ [4].



Scheme 1

The PhD work is first concerned with synthesis of nitronyl nitroxide free radicals and chiral counter-ions to build the 3D metal-radical frameworks in a host-guest supramolecular game. Next will be the determination of their crystal structure mainly by electron diffraction in relation with the study of their magnetic properties to understand the magneto-structural relationships to be supported by molecular DFT calculations. Molecular modeling is to be used for the rational design of radicals and counter anions.

Situation: This is an **interdisciplinary** basic research project that aims **smart materials** with **multifunctional** applications (Chemistry/Physics/Artificial Intelligence) and involves partners in Grenoble (AI, electron diffraction) and Poitiers (prediction of 2D and 3D crystal structures) to be visited all along the PhD work as the PhD candidate will be involved in all aspect of the project with shared supervisions.

Requested abilities: Solid curriculum in chemistry with ability to apprehend physical phenomena. Strong motivation for inorganic synthesis; computational modeling; crystallography and magnetic studies. Basic knowledge in computer science. Ability to work independently

Skills to be developed: Synthesis in organic and coordination chemistry; crystal structure determination from X-ray and electron diffraction; magnetic studies; Molecular DFT calculations.

Candidates are invited to send a CV and two recommendation letters

References: [1] O. Kahn Acc. Chem. Res., **2000**, 33, 647-657 (link) ; [2] D. Luneau, A. Borta et al. Inorg. Chim. Acta, **2008**, 361, 3669-3676 (link) ; [3] A. Lannes, D. Luneau Inorg. Chem., **2015**, 54, 6736-6743 (link) ; [4] D. Luneau Eur. J. Inorg. Chem., **2020**, 2020, 597-604 (link) ; [5] C. Lecourt, Y. Izumi et al. Dalton Trans., **2020**, 49, 15646-15662 (link) ; [6] S. Decurtins, H. Schmalle et al. New. J. Chem., **1998**, 22, 117-121 (link)