Hyperfine interactions in lanthanide-organic complexes for quantum information processing

Directeur de thèse :
Paul-Antoine HERVIEUX
Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS)
Tel: 03 88 10 72 14 ; e-mail: hervieux@unistra.fr
Co-Directeur de thèse :
Mario RUBEN
Karlsruhe Institute of Technology (KIT)
e-mail: mario.ruben@kit.edu

As an extension of the well-known two-level quantum bits (qubits), multilevel systems, the so-called qu*d*its, where *d* represents the dimension of the Hilbert space, have been predicted to reduce the number of iterations in quantum-computation algorithms. This has been tested experimentally in single-molecule magnets (i.e. metal-organic complex $TbPc_2$) where multilevels are originated from the nuclear spins and the associated dipole and quadrupole hyperfine interactions (HIs) [1].

Controlling or modifying these interactions may open the way to the manipulation of the multilevel systems' properties thus leading to improvements or elaboration of new quantum-computation algorithms. In close collaboration with experimental physicists and materials chemists from KIT we propose to establish a theoretical framework to answer this issue. This project will profit from existing local and external collaborations, both with quantum chemists, nuclear physicists and experimentalists from KIT who synthesize, characterize and manipulate single-molecule magnets.

The project is structured in three main objectives:

- We will explore the possibility to modify the hyperfine interactions by using a static electric field compatible with the experimental limitations;
- The possibility to synthetically upscaling of a molecular Qudit permits to increase significantly the number of accessible nuclear states and therefore the computational power of the quantum device. The role played by the electronic spin making the link between the nuclear spins is under debate. In order to solve this issue we will develop a theoretical model which combines both itinerant (electronic) and localized (nuclear) magnetism and their interplay through various magnetic exchange mechanisms [2].
- For optical read-out purposes, the effect of the nuclear spin on the optical properties of lanthanide complexes will be also explored theoretically.

[1] W. Wernsdorfer and M. Ruben, Adv. Mater. **31**, 1806687 (2019).

[2] J. Hurst, P. –A. Hervieux, and G. Manfredi, Phys. Rev. B **97**, 014424 (2018); Philosophical Transactions A **375**, 2092 (2017).