**Title:** Organometallics as models of Quantum Cellular Automata (QCA)

**Project description:**

Quantum-dot cellular automata (QCA) is a paradigm for nanoelectronics, in which binary information is encoded in charge configuration of a QCA cell and transferred via Coulomb interactions between neighboring cells. At the molecular level, the simplest molecular QCA cell is a symmetric mixed-valence complex in which the binary states 0 or 1 are represented by the location of a mobile electron (or a hole) at one metal center or at the other. However, square arrays with four redox sites are generally considered more versatile and efficient cell designs for use in logic applications. A detailed description of QCA can be found in reference 2.

In this context, the preparation of a binuclear iron complex in which the two organometallic moieties are located at the 1,2-position of a benzene ring has recently been described. The project will consist in the design and synthesis of a novel tetranuclear complex Fe4 following a two-step reaction sequence, allowing a selective access to the binuclear Fe2 intermediate (Scheme 1).

![Scheme 1](image-url)
Compound Fe2 is also expected to serve as starting material for the construction of heterotetranuclear Fe2M2 species and of small oligomers \([\text{Fe2}]_n\) that could be viewed as models of quantum wires in their partially oxidized state. A challenging aspect of the work would be the characterization of the oxidized forms of Fe4 and Fe2M2 complexes, and especially the \([\text{Fe4}]^{2+}\) and \([\text{Fe2M2}]^{2+}\) entities where two positive charges are delocalized over four metal centers, viz the required situation for a QCA.

**References:**

**Profile of the applicants:**

The applicants must be recently graduated from a Master degree in Chemistry, and possess a good background in molecular chemistry. Skills in organometallic and/or coordination chemistry will be appreciated but not discriminative. We are looking for an autonomous, motivated and enthusiastic young scientist with a team working ability. Parts of the work will be collaboratively carried out with other research groups on local, national and international scale.

**Application:**

CV + motivation Letter + master transcripts + 2 names / contacts of former advisor/professor for possible recommendation.

**To apply to this position, please contact:**

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