Institut des Sciences Chimiques de Rennes

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Team: Organométallics: Materials & Catalysis
http://iscr.univ-rennes1.fr/omc/

Doctoral School Matter, Molecules and Materials (ED-3M 596)

Université Bretagne Loire - Université de Rennes 1

Ph.D. Proposal (2018-2021)

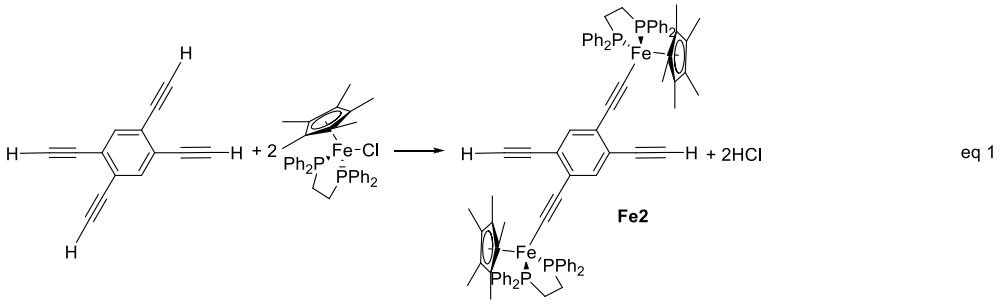
Funding: This Ph.D. will benefit from 3-year financial support from the Ministry of Higher Education, Research and Innovation (MESRI)

Title: **Organométallics 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.[1] 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.[3] The project will consist in the design and synthesis of a novel tetranuclear complex **Fe4** following a two-step reaction sequence, alowing a selective access to the binuclear **Fe2** intermediate (Scheme 1).



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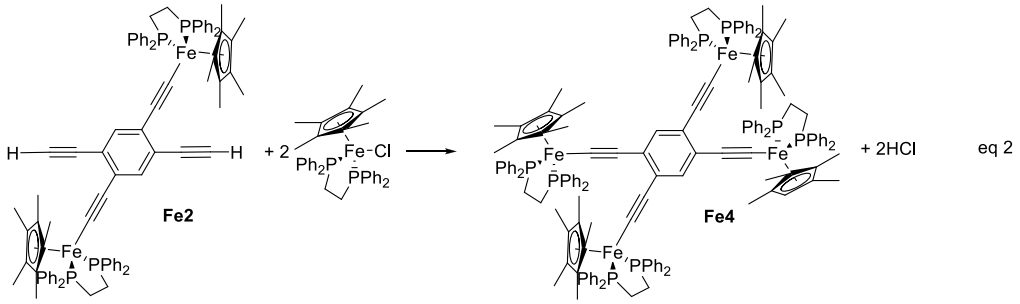

Scheme 1: proposed synthetic procedure of complexes **Fe2** and **Fe4**

Compound **Fe2** is also expected to serve as starting material for the construction of heterotetranuclear Fe2M2 species and of small oligomers **[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 **[Fe4]$^{2+}$** and **[Fe2M2]$^{2+}$** entities where two positive charges are delocalized over four metal centers, viz the required situation for a QCA.

***References*:**

1. C. Lent *Science* **2000**, *288*, 1597.
2. http://iopscience.iop.org/article/10.1088/0957-4484/4/1/004/pdf
3. R. Makhoul, H. Sahnoune, V. Dorcet, J.-F. Halet, J.-R. Hamon, C. Lapinte *Organometallics* **2015**, *34*, 3314-3326.

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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