Convocatoria de proyectos sinérgicos INMA para realización de tesis doctorales en el marco del Programa de Excelencia Severo Ochoa

LÍNEA DE INVESTIGACIÓN PRIORITARIA SEVERO OCHOA* **Research Priority 3 (RP3). QUANTUM TECHNOLOGIES.** Research Action Line (RAL) 3.2. Hybrid quantum processor

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Quantum properties of two-dimensional arrays of rare earth atoms in contact with superconducting surfaces

BREVE INTRODUCCIÓN Y ESTADO DEL ARTE EN EL PROBLEMA A TRATAR

De-coherence sources and instrumental errors prevent the expression of a true quantum advantage in information processing. Massive efforts are directed towards quantum error correction (QEC). The proposal of RAL 3.2 consists in using quantum states of Lanthanide (Ln) ions with large spin multiplicities (S or J>1/2). In this way, each ion can take more than two different quantum numbers (thus termed ‘qudits’). Ln ions also exhibit large hyperfine coupling. Then both electronic and nuclear spin can be probed by conventional electron spin resonance[1]. This means that quantum information can be encoded in the nuclear spin, which is much more robust against de-coherece sources, and probed through the electronic spin of the f-shell. The rich complete space offers multiple quantum states, enabling the implementation of the so-called embedded QEC[2]. The integration of individual Ln ions with superconducting resonators becomes of crucial relevance. The natural 2D material for this purpose are metal-organic frameworks (MOF) using $Ln^{2+}/^{3+}$ ions as coordinating atoms. Synthesizing the 2D MOF right over a superconducting surface imposes the limitation of requiring ultra-high-vacuum (UHV, pressure $\sim 1\times 10^{-10}$ mbar) conditions. On the other hand, it provides large synthetic flexibility (Ln ion, molecular linker), full reproducibility and, no least, the opportunity to characterize the material with atomic scale precision by means of STM. The research team has proven proficiency in the design, synthesis and characterization of MOFs[3–6]. Our methodology aims at the magnetic and electronic properties of individual candidates to qudit carriers. Furthermore, it is timely to start delving in the issue of the ultimate need of UHV methods for the device fabrication in which single atom sensitivity is a must. The feasibility of MOF synthesis on the surface of superconductors has been shown with transition metal (TM) ions as coordination centres and organic linker **1**[7,8] (Table 1). The emergence of Yu-Shiba-Rusinov (YSR) resonances due to the interaction of the TM atoms with the Cooper pairs[9] allows to track the magnetic interactions among coordinating atoms, and ascertain their spin moment and anisotropy energy[10]. On the other hand, the fabrication of lanthanide coordinated MOFs on normal metals has been shown for Ln=Eu, Gd, Dy, and Er[11], and also for Ho by us (see Fig. 1).

OBJETIVOS DE LA TESIS DOCTORAL

The **main objective** is to grow in-situ MOFs on a perfect surface that simulates that of the superconducting resonator, and to evaluate their functionality as single ion spin qudits.

O1) **Training in advanced Surface Science methods applied to Quantum Technologies**. We expect that upon completion of the PhD, the candidate becomes capable to conduct cutting-edge research in an independent manner using UHV, STM and synchrotron instrumentation.

O2) **Screening of the quality of Ln MOFs on superconductors.** Selection of Ln (Gd, Eu, Ho and Yb), organic linker (compounds **1** and **2** in Table 1) and superconducting surface (Nb(100) and $NbSe_2$(111)) that provides the best long range crystalline order.

O3) **Validation of selected Ln-MOFs as qudits**. Determine the spin moment, valence state, interactions among magnetic centres. Validation: spin moment S>1/2 and smallest possible magnetic anisotropy.

O4) **Determine the impact of realistic device fabrication conditions on the candidates to qudits**. We will study the influence of controlled oxidation of the superconducting surface. After exposing the MOF/superconductor set-up to partial O_2 pressure between 1 atm and 10^{-8} Torr, we will re-examine the validation criteria described for O3.

HIPÓTESIS DE PARTIDA

Ongoing work within the research team in which two different MOFs of relevance for the application have been investigated. In Figure 1, we show a MOF synthesized on Au111 with Ho as coordination centre and DCA (see **1** at Table 1) as organic linker. Fig 2 shows the quality of Fe-DCA MOF on the superconducting surface of $NbSe_2$.

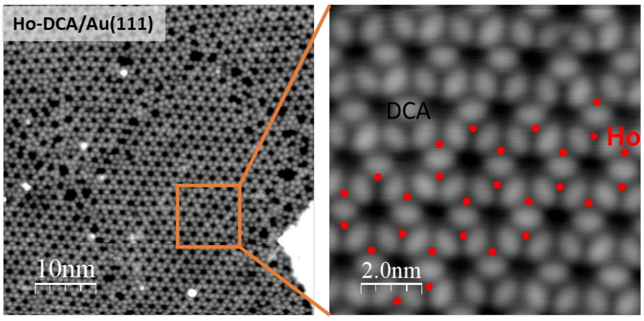

Figure 1.- STM topography image of the Ho-DCA MOF on Au(111). DCA is molecule **1** in Table 1.

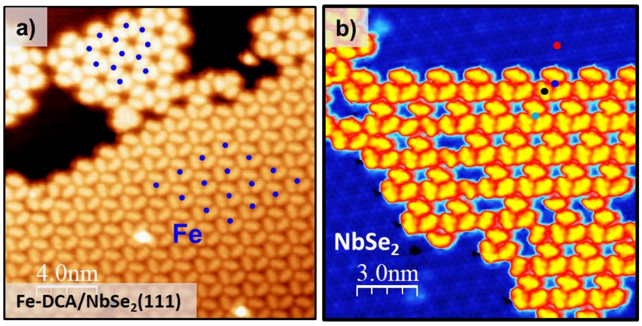

Figure 2.- a) STM topography of the Fe-DCA MOF on $NbSe_2$(111). Two phases with different density of Fe ions appear in this case. b) high density phase together with the charge density wave of superconducting $NbSe_2$.

In view of this preliminary research, starting hypothesis for the PhD project of this application would be:
i. The successful synthesis shown in Figs 1 and 2 can be combined, to obtain Ln coordinated MOFs on superconducting substrates.
ii. After the optimization of the growth process, a combination of STM high resolution spectroscopy (looking for YSR bound states) with XAS and XMCD measurements slots at synchrotron facilities will allow us to pull out reliable figures for the total spin and angular momentum
iii. For the case of strong enough YSR resonances and short Ln-Ln lattice constants to maximize their overlap, we will obtain YSR bands which can be imaged by STM[8].
iv. Placing the Ln-MOFs/Nb(100) under oxidizing conditions will preserve the electronic and magnetic ground state of the MOF.

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