Unveiling the structural and electronic interplay in 3d and 4f/5d compounds at high-pressure

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The development of diamond-anvil cells together with the improvement of the characterization techniques in large facilities has led to the expansion of high-pressure (HP) research. The application of HP has given rise to many important breakthroughs during the past decade because it can radically change the physical and chemical properties of materials yielding unexpected modifications. For instance, HP has allowed the discovery of new materials or new phases of known materials with unique properties, such as high T_C superconductors, Mott insulators, half-metals, etc.

Here, we present the study of several striking materials by two complementary techniques: x-ray absorption spectroscopy (XAS) and x-ray diffraction (XRD), both carried out in the European Synchrotron Radiation Facility (ESRF). Firstly, the iridium (Ir) metal has been investigated up to 1.4 Mbar in order to discover experimentally, for the first time, a new electronic transition predicted in the majority of 5*d* transition metals [1]. This new transition is known as Core Level Crossing and it involves the overlap between the 4*f*/5*p* core levels affecting the 5*d* valence orbitals yielding a change in the chemical bonds. The structural stability (Fig.1a) and the electronic properties of Ir metal were studied by XRD at ID15B beamline and XAS at BM23 beamline, respectively. Secondly, we have stablished a physical model to explain the pressure-induced modifications in the electronic structure of europium (Eu) monochalcogenides, Eu*X* (*X* = O, S, Se, Te). All of them exhibit optical, electric and magnetic anomalies around 14 GPa [2] but the reason behind them had never been unveiled so far. We have studied one of these compounds, the EuS, by XAS up to 35 GPa at BM23 beamline (Fig. 1b). Finally, the copper(II) oxide, CuO, itself has seen renewed interest due to the discovery of multiferroicity (MF) at relatively high temperature T_N = 230 K and ambient pressure [3]. However, such a discovery is not free of controversy since different researchers have obtained contradictory results [4]. We have carried out a XAS experiment up to 18 GPa, at BM23 beamline, to analyse the static and dynamics contribution of the local environment around Cu atoms (Fig. 1c) shedding some light on this scientific problem.

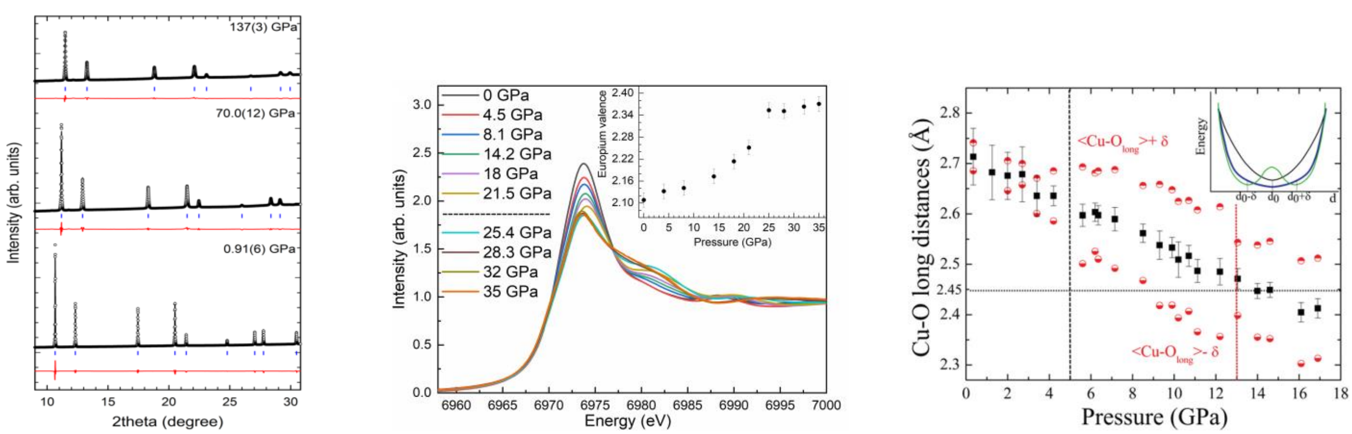

Figure 1. a) XRD diffraction patterns of the Ir metal up to 1.4 Mbar (left graph). b) XAS spectra of EuS, with the Eu valence in the inset, up to 35 GPa (central graph). c) Pressure dependence of Cu-O distance, with its deviation, up to 18 GPa (right graph).

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