Minicolloque n° MMPS26 ⊟ **Oral** ☐ **Poster**

Transition metal K-edge XMCD and Prussian Blue Analogs : Towards quantitative magnetic information

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For the last 30 years, X-ray Magnetic Circular Dichroism has become a widely used tool to investigate fundamental properties of matter. At the $L_{2,3}$-edges of 3d transition metals (TM), where the magnetic 3d orbitals are directly probed, the signals are well understood and quantitative information can be directly extracted thanks to sum rules. Measurements at the TM K-edges offer the advantages to be bulk sensitive and compatible with extreme conditions measurements, but at these edges, the delocalized p orbitals are probed and the interpretation of the signals remain controversial.

To better understand the physical effects at the origin of these TM K-edge XMCD signals and be able to extract quantitative information, we are engaged in their fundamental investigation using Prussian Blue analogs (PBAs) as models compounds. The versatile chemistry of PBAs indeed enables to work with a completely new experimental approach. In a first study [1], we could establish the effect of external parameters (temperature, magnetic field) on the XMCD intensity and thus determine the optimized experimental conditions for our whole project. We then concentrated on two series of bimetallic PBAs, $A_4[Fe(CN)_6]_{2.7}$ (A=Mn,Co,Ni,Cu) and $B_4[Cr(CN)_6]_{2.7}$ (B=Mn,Fe,Co,Ni) (Fig. 1). They were systematically investigated by a laboratory (powder XRD, SQUID magnetometry, IR spectroscopy) and synchrotron (TM K-edge X-ray absorption spectroscopy and XMCD) coupled approach to get the full macroscopic and local pictures; in addition, XAS and XMCD are element-selective, which allows to individually study each side of the cyanide bridge (i.e. the A or B ion, and the Fe or Cr one). The detailed analyses of the XMCD signals of these two series at the A/B K-edges enabled to show that the parameters of the main 1s→4p contribution (shape, sign, intensity and area) can be related to the magnetic behavior of the probed A^{2+} (B^{2+}) ion [2] (Fig. 2). This is the first time that the magnetic information contained in TM K-edge XMCD are identified and related to a spectral feature of the signal.

[1] A. N'Diaye et al., J. Sync. Rad. 28 (2021) https://doi.org/10.1107/S1600577521004884
[2] A. N'Diayeet al., Submitted. *Towards quantitative magnetic information from transition metal K-edge XMCD of Prussian Blue analogs*

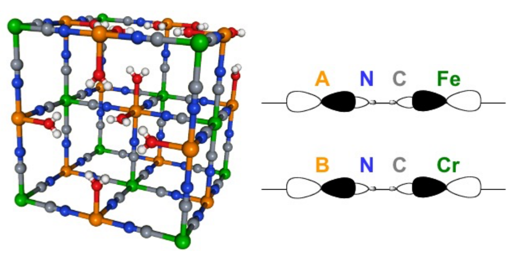

Figure 1 : Unit cell of the AFe and BCr PBAs series

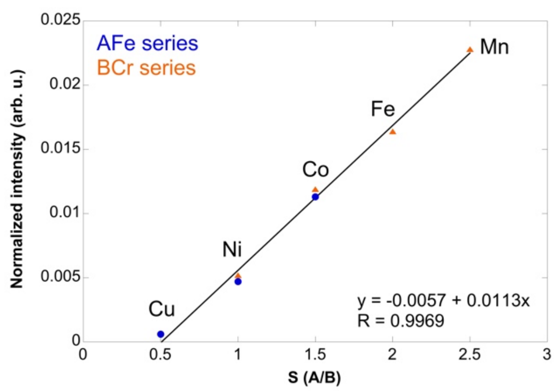

Figure 2 : Evolution of the intensity of the main 1s→4p contribution of the A/B K-edge XMCD signal as a function of the spin of the A/B ion.