ESRF	Magnetic polarization at the non-magnetic ion sites of Mo/W/Re in double perovskites	**Experiment number:** HE-1882
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Report:
We have investigated the Mo, W, and in particular Re $5d$ spin and orbital magnetic moments in ferrimagnetic double perovskite of the type Sr_2CrReO_6 by X-ray magnetic circular dichroism (XMCD) at the $L_{2,3}$ edges. In fair agreement with recent band-structure calculations, at the Re site a large $5d$ spin magnetic moment of $-0.68\,\mu_B$ and a considerable orbital moment of $+0.25\,\mu_B$ are detected. The most important result of our study is that the Curie temperature of the ferrimagnetic double perovskites scales with the spin magnetic moment of the 'non-magnetic' atom.

The spectra were recorded using the total fluorescence yield detection mode. The XMCD spectra were obtained as direct difference between consecutive XANES scans (X-ray Absorption Near Edge Spectrum) recorded with opposite helicities of the incoming X-ray beam. To ensure that the XMCD spectra are free from experimental artefacts the data was collected for both directions of the applied magnetic field of 6 T (parallel and antiparallel to the X-ray beam). The measurements were performed at about 10 K. Since the samples measured in backscattering geometry were very thick, the spectra were corrected for self-absorption effects. The edge jump ratio L_3/L_2 was normalized to 2.20/1. This takes into account the difference in the radial matrix elements of the $2p1/2$ to $5d(L_2)$ and $2p3/2$ to $5d(L_3)$ transitions.

We now discuss the XANES spectra of Sr_2CrReO_6 shown in the left figure. The white lines at the Re $L_{2,3}$ edges have a fine structure which reflects the Re $5d$ density of unoccupied states influenced by the crystal field. The white lines at both edges show a faint shoulder on the high energy side. This can be interpreted as the signature of the crystal field splitting of the $5d$ band into t_{2g} and e_g states (~ 3 eV). More pronounced double peak structures of similar splitting have been already observed at the Mo $L_{2,3}$ and W $L_{2,3}$ edges for the double perovskites Sr_2FeMoO_6 and A_2CrWO_6 ($A =$ Ca, Sr).

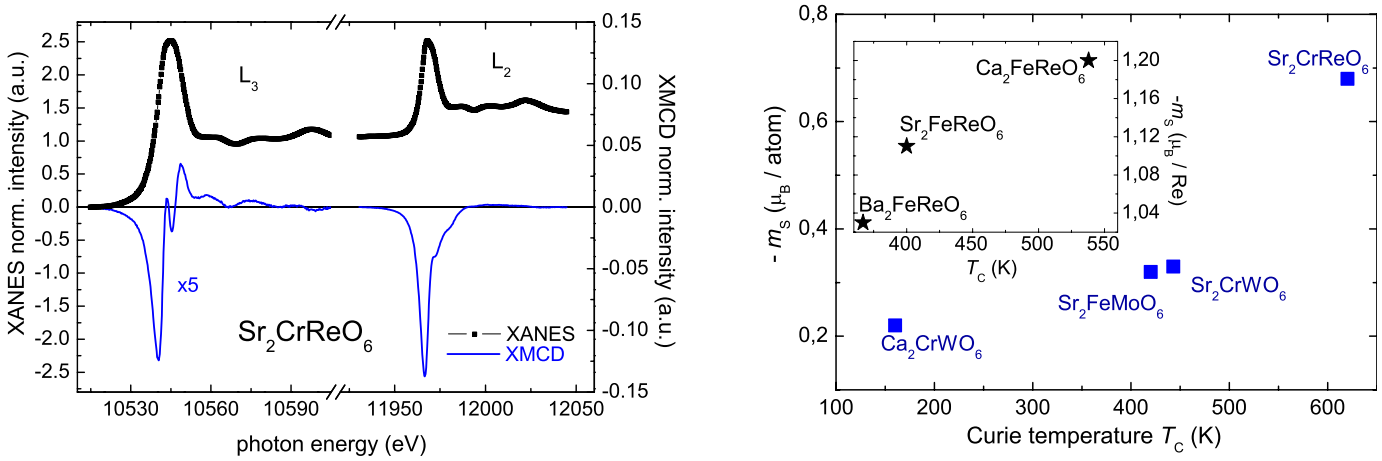

Figure 1: XANES and XMCD spectra for Sr_2CrReO_6 at 10 K (left). Relation between magnetic moment and Curie-temeparture in comparable sets of double perovskites (right).

As shown in the figure (left), for both Re absorption edges we find a rather intense XMCD signal. This is a clear evidence for the existence of a magnetic moment at the Re $5d$ shell. Note that in order to obtain the spin and orbital magnetic moments separately the data must be normalized to the number of $5d$ holes n_h. From band-structure calculations we use $n_\mathrm{h} = 5.3$. This has to be kept in mind when comparing data, as n_h is proportional to the obtained moments. Only the ratio $m_\mathrm{L}/m_\mathrm{S}$ is independent of the estimation of n_h. Both, $m_\mathrm{L}/m_\mathrm{S}$ and m_L, are clearly larger than expected from the calculations including spin-orbit coupling. This underlines the importance of relativistic effects for the heavy Re.

In the figure (right) we summarize currently published data for the spin moment of $B' =$ W, Mo, Re to investigate the relation of Curie temperature T_C and spin magnetic moment m_S at the B' site of the ferrimagnetic double perovskites of the type $A_2BB'O_6$. The data suggests that indeed T_C scales with m_S at the B' site. Of course, we cannot draw final conclusions from this comparison as other factors as structure, hybridization, and site occupation can strongly influence T_C. However, there is a clear trend that a large T_C is accompanied by a large magnetic moment m_S at the B' site. This finding is in good agreement with a simple model of ferrimagnetism in double perovskites mediated by minority spin carriers. In the inset of the right figure we show recent XMCD data on other Re-based double perovskites which show a similar trend. However, the relatively high values of the spin magnetic moment for these samples do not allow a direct comparison with our data. It is of importance to study also these compounds with comparable XMCD set-ups and data extraction.

In summary, based on our XMCD measurements we suggest a new scaling law between the critical temperature of the ferrimagnetic double perovskites and the magnetic moment at the 'non-magnetic' site. This finding may contribute to establish an improved a,d even quantitative model for these half-metallic compounds.

Two publications coming out of this very successful measurement time are already published:
[1] P. Majewski, S. Geprgs, A. boger, M. Opel, A. Erb, R. Gross, G. Vaitheeswaran, V. Kanchana, A. Delin, F. Wilhelm, A. Rogalev, and L. Alff, Phys. Rev. B **72**, 132402 (2005).
[2] P. Majewski, S. Geprgs, O. Sanganas, M. Opel, R. Gross, F. Wilhelm, A. Rogalev, and L. Alff, Appl. Phys. Lett. **87**, 202503 (2005).