

## XAS Studies of the Double Perovskite $\text{Sr}_2\text{Cr}_{1.2}\text{Mo}_{0.8}\text{O}_{6-\delta}$

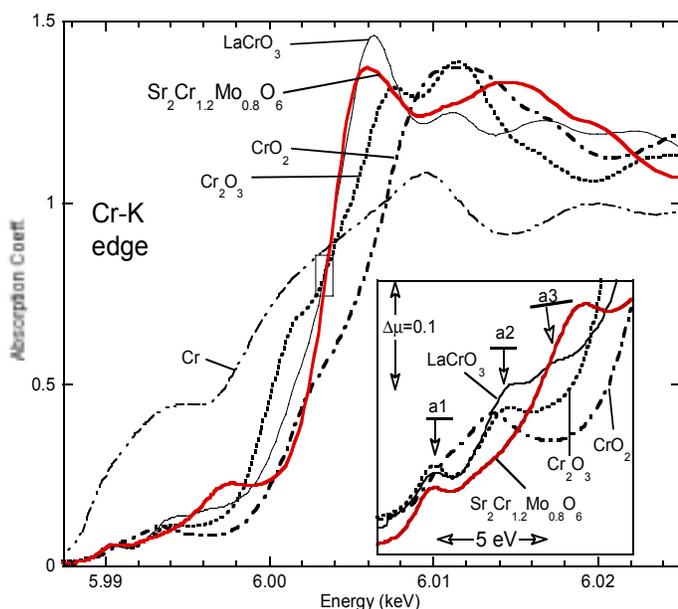
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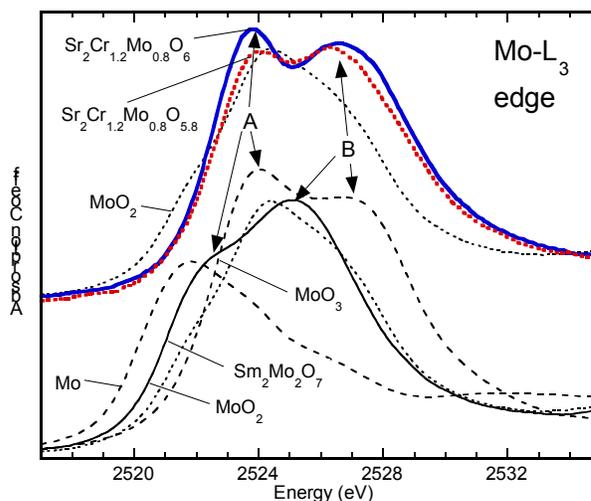
Beamline(s): X19A

$\text{Sr}_2\text{Cr}_{1.2}\text{Mo}_{0.8}\text{O}_{6-\delta}$  ( $\delta=0, 0.2$ ) is of interest as a large low-field magnetoresistance material. In view of the importance of the transition metal valences in the magnetic properties of such materials, we have investigated the Cr-K and Mo-L<sub>3</sub> edges of these compounds. The rising part of the  $\text{Sr}_2\text{Cr}_{1.2}\text{Mo}_{0.8}\text{O}_6$ , Cr-K main edge (Figure 1) can be seen to have a chemical shift identical to that of the  $\text{Cr}^{3+}$  standards (see the box in the Figure) and well separated from that of the  $\text{Cr}^{4+}$  standard. The pre-edge features of the Cr-K edge spectra are shown in the inset of Figure 1. The  $\text{Sr}_2\text{Cr}_{1.2}\text{Mo}_{0.8}\text{O}_{6-\delta}$  pre-edge manifests a three feature (a1/a2/a3) structure similar to the  $\text{Cr}^{3+}$  standards whereas the  $\text{Cr}^{4+}$  standard has a quite distinct bimodal feature structure. Among the  $\text{Cr}^{3+}$  materials the sharp-low-energy a1-feature is particularly distinctive with the intensities and positions of the a2 and a3 features varying between compounds. Thus structure of the pre-edge also supports the assignment of a  $\text{Cr}^{3+}$  state for these  $\text{Sr}_2\text{Cr}_{1.2}\text{Mo}_{0.8}\text{O}_{6-\delta}$  materials.

The two strong white line features (A & B in Figure 2) at the Mo L<sub>3</sub>-edge in the  $\text{Mo}^{6+}\text{O}_3$  and in the pyrochlore- $\text{Sm}_2\text{Mo}_2\text{O}_7$  standards should be noted. The low (high) energy peak, A (B) is due to  $4d-t_{2g}$  ( $4d-e_g$ ) final states. Although a number of solid state and atomic effects are involved, the A/B intensity ratio can be used to probe the Mo-valence. The ratio of the A to B spectral weight shows a dramatic decrease between the  $\text{MoO}_3$  (with a formal 6:4 ratio of  $t_{2g}$  to  $e_g$  available final states) and the pyrochlore- $\text{Sm}_2\text{Mo}_2\text{O}_7$  (with a formal 4:4 final state ratio). The A/B feature ratio of the  $\text{Sr}_2\text{Cr}_{1.2}\text{Mo}_{0.8}\text{O}_{6-\delta}$ ;  $\delta = 0$  and 0.2 spectra (in Figure 2-top) indicates a Mo-valence much greater than 4 and less than 6 for both  $\delta = 0$  and 0.2 materials. Moreover, a clear decrease in the relative A-feature strength between the  $\delta = 0$  to 0.2 spectra strongly supports a direct Mo-valence reduction in response to the decreasing O-content. Thus it appears that the formal Mo-valence assignments of 5.5+ and 5+ for the  $\delta = 0$  and 0.2 materials are qualitatively quite consistent with the Mo XAS results.



**Figure 1.** Cr K-edge x-ray absorption spectra of  $\text{Sr}_2\text{Cr}_{1.2}\text{Mo}_{0.8}\text{O}_6$ ,  $\text{CrO}_2$ ,  $\text{LaCrO}_3$ ,  $\text{Cr}_2\text{O}_3$ , and Cr-metal. In the Inset the pre edge features of the oxide spectra are compared (with the  $\text{Sr}_2\text{Cr}_{1.2}\text{Mo}_{0.8}\text{O}_6$  spectrum displaced downward for clarity).



**Figure 2.** The Mo L-edge x-ray absorption spectra of Mo-metal,  $\text{MoO}_2$ ,  $\text{Sm}_2\text{Mo}_2\text{O}_7$ , and  $\text{MoO}_3$  standard materials. (top) The Mo L-edge spectra of  $\text{Sr}_2\text{Cr}_{1.2}\text{Mo}_{0.8}\text{O}_{6-\delta}$  ( $\delta=0, 0.2$ ) along with the  $\text{MoO}_2$  standard.