ESRF

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Report:

Structure of double-perovskites of the type $A_2BB'O_6$ (A being an alkaline-earth element and B and B' transition-metal ones) was studied in the past but new interest has been focused on them since they have become candidates to work in spin electronics. In this sense, recently, magnetoresistance has been observed for Sr_2FeMoO_6 at room temperature and Curie Temperatures T_C= 300-420 K and ferrimagnetism have been reported for the whole series A_2FeMoO_6 (A= Sr, Ba, Ca).

The perovskite structure nominally consists of BO_6 and $B'O_6$ octahedra alternately ordered in a simple cubic lattice. In order to understand the electronic properties of the series we have studied the local structure around the Fe and Mo atoms by means of X Ray absorption spectroscopy at their K edges. Experiments were performed at 30 K and at room temperature. The Mo-O distances show very small variations along the series and reasonably

agree with previous results obtained from neutron powder diffraction. This indicates a similar local electronic structure. There are still marked differences in the Fe-O bond lengths. A chemical shift is observed in the XANES spectra (see figure1) of the series that can be attributable to different oxidation states of the Fe atoms in the compounds. More quantitatively, EXAFS analysis point out a mixed valence state between +2 and +3 for the Barium and Calcium samples while for the Strontium one results quite agree with an expected Fe^{3+} valence state.

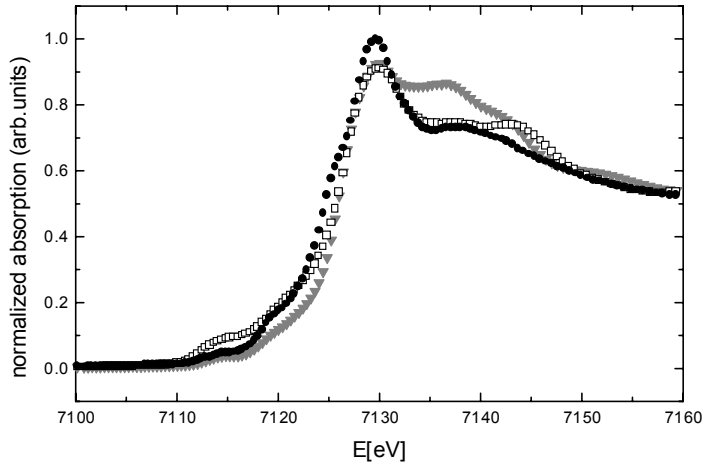

Fig.1. Comparison between XANES spectra of the Sr (triangles), Ba (squares) and Ca (circles) double perovskites at 30 K.

In the case of the $Sr_2Fe_{1-x}Cr_xMoO_6$ series, the XANES spectra show almost no difference for the cases x= ¼, ½, ¾, 1 in the K edges of molybdenum, iron (see figure 2) or chromium. The EXAFS analysis also suggest an homogeneous oxidation state of the Fe and Cr ions that shall be +3 in this case following the previous conclusions.

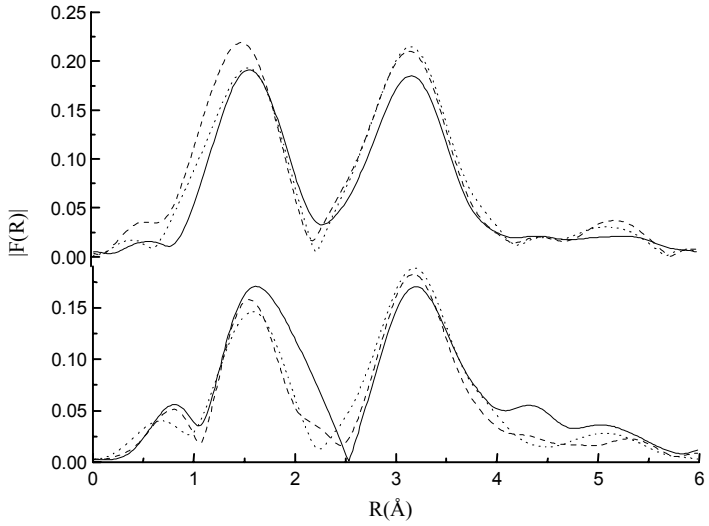

Fig.2. Fourier filtered spectra for the cases x=1/4 (dotted lines), x=1/2 (dashed lines) and x=3/4 (solid lines) at the Cr (up) and Fe (down) edges.