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## Spin Dependent Near Edge X-Ray Absorption Measurements: Determination of the Local Magnetic Ordering in $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$

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Beamline(s): X21

**Introduction:** Based on LSDA+ U calculations of  $\text{LaMnO}_3$ , Elfimov *et al.*[1] suggested that the pre-edge structure in the x-ray absorption spectrum is caused by the hybridization of the Mn 4p orbitals with the ordered Mn 3d orbitals on neighboring Mn ions either directly or via the intervening O orbitals. The main edge is therefore very sensitive to the local Jahn-Teller distortion but at most weakly affected by the occupation of the Mn 3d states. Although Bridges *et al* [2] and our previous work [3] gave some insight on the temperature dependence of the pre-edge Mn K-edge x-ray absorption spectra of  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ , neither of them provide a detail explanations of the observed changes in the spectra and did not relate these changes with the changes in the electronic and magnetic ordering which occurred on crossing a phase boundary. We utilized spin polarized x-ray absorption to extract the spin polarized density of states and local magnetic order in manganites.

**Methods and Materials:** Samples of  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$  series were synthesized and characterized as described in Ref. [4]. Measurement samples were prepared by finely grinding the materials and brushing the powder onto adhesive tape.

The Mn spin polarized XANES measurements were performed at the National Synchrotron Light Source's (NSLS) 27 pole wiggler Beamline X21A. The experimental details were described elsewhere [3].

**Results and Conclusions:** A systematic study of spin dependent Mn K-edge x-ray absorption spectra was performed on  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ . By examining the changes in the pre-edge spectra which occur on magnetic ordering at low temperature, we are able to extract the spin dependent density of Mn 3d states. The energy separation between the d states were also determined. Comparisons with local spin density calculations were made. The approach is of general applicability to cubic and layered perovskite systems. In its simplest case it can be used to determine the change in the local magnetic order (ferromagnetic vs. antiferromagnetic) about a transition metal site on going through a transition or as the result of external perturbations.

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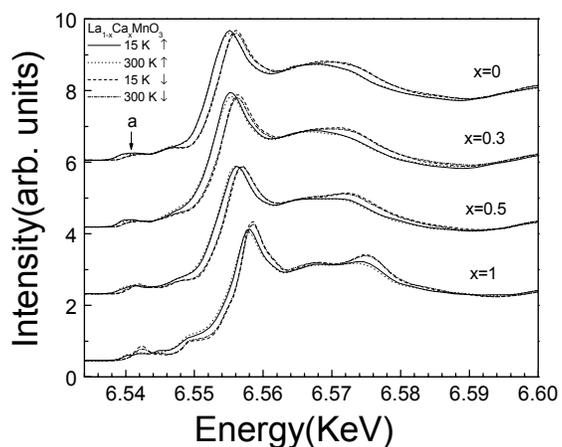
### References:

<sup>1</sup> I.S.Elfimov *et al.*, Phys. Rev. Let. 82, 4264 (1999).

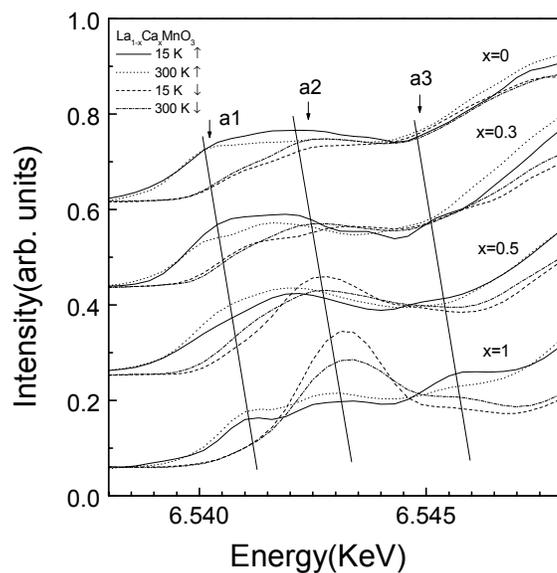
<sup>2</sup> F. Bridges *et al.*, Phys. Rev. B61, R9237 (2000).

<sup>3</sup> Q.Qian, *et al.*, Phys. Rev. B **62**, 13472 (2000).

<sup>4</sup> M. Croft, *et al.*, Phys. Rev. B **55**, 8726 (1997).



**Fig. 1.** Spin and temperature dependent XANES spectra of  $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ . The solid line corresponds to spin up electron excited from 1s at 15 K, while dotted line is used for 300 K spin up. The dashed line corresponds to spin down electrons excited from 1s at 15 K, while dashed-dotted line is used for 300 K spin down channel.



**Fig. 2.** The expansion of the pre-edge region feature a of Fig.1. The three straight lines indicate the a1, a2, and a3 features.