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Soft X-ray Emission Studies of Lanthanum and Calcium Manganates

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Beamline(s): X1B

Introduction: Lanthanum manganate $LaMnO_3$ and calcium manganate $CaMnO_3$ are at either end of the widely studied $La_xCa_{1-x}MnO_3$ series which exhibits many interesting phases. The techniques of soft x-ray emission (SXE) and soft x-ray absorption (SXA) spectroscopy are applied to the study of these two materials, $LaMnO_3$ and $CaMnO_3$.

Methods and Materials: Single crystals of $LaMnO_3$ and $CaMnO_3$ were grown and mounted in vacuum in our experimental chamber. These crystals were then studied using soft x-ray emission and soft x-ray absorption spectroscopies at beamline X1B with a high resolution x-ray emission spectrometer.

Results: SXE and SXA spectra were recorded for both materials at the O *K*-edge, the Mn *L*-edge, and also the Ca *L*-edge in the case of $CaMnO_3$. Fig.1 compares the O *K*-edge SXA and SXE spectra which represent the oxygen local partial density of states (LPDOS), of $LaMnO_3$ and $CaMnO_3$.
The electronic structure of both of these manganates is influenced by the extensively hybridized Mn *3d*/O *2p* orbitals. Recording the SXE spectrum at different photon energies allows for the observation of resonant inelastic x-ray scattering (RIXS) features. Shown in Fig. 2 and in Fig. 3 are a series of Mn *L*-edge SXE spectra obtained from the threshold of the Mn SXA spectrum upwards. The elastically scattered photon peak can be seen progressing to higher energies with each successive spectrum. In each instance the first spectrum shown primarily consists of the elastic peak and a loss spectrum which is a result of both charge-transfer excitations and *d-d* excitations within the material. This allows an estimate to be made for the on-site *d-d* Coulomb interaction U_{dd} and the hybridization strength *V* in comparison to detailed calculations.

Conclusions: The Mn RIXS spectra of both lanthanum and calcium manganate provide detailed information on excitation processes and the electronic structure of these materials

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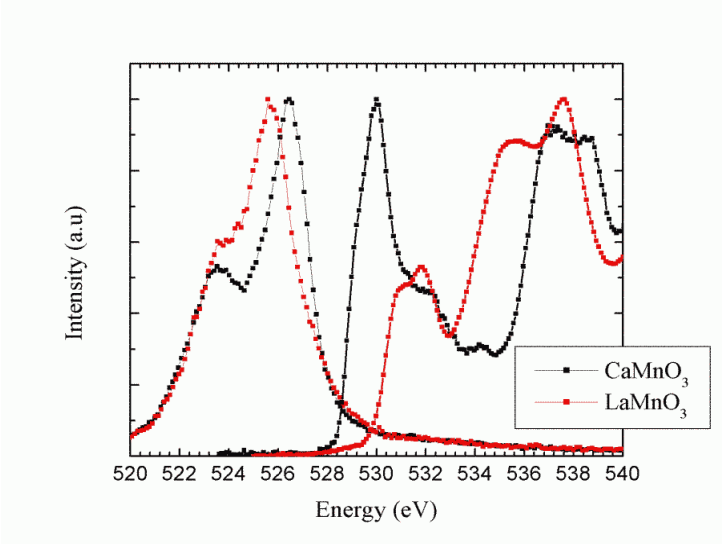

Figure 1 O *K*-edge SXA and SXE of $CaMnO_3$ (black) and $LaMnO_3$ (red).

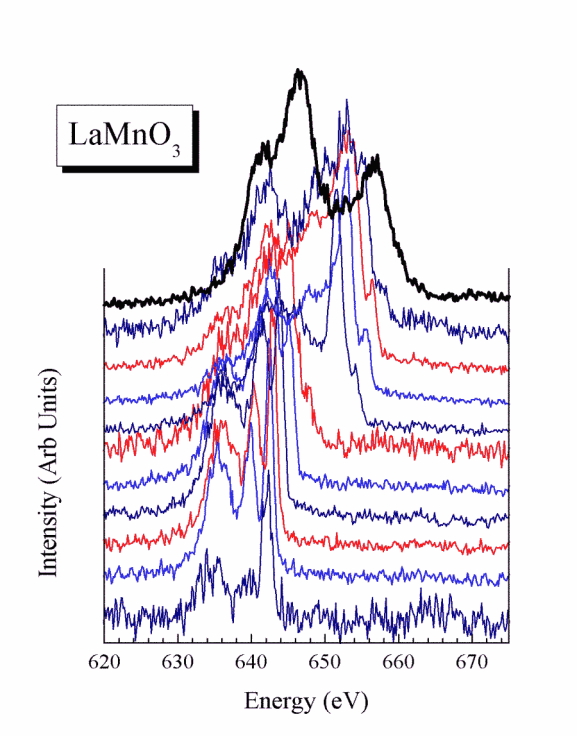

Figure 2 A series of Mn *L*-edge SXE spectra obtained from $LaMnO_3$. Each successive spectrum is due to a higher incident excitation energy.

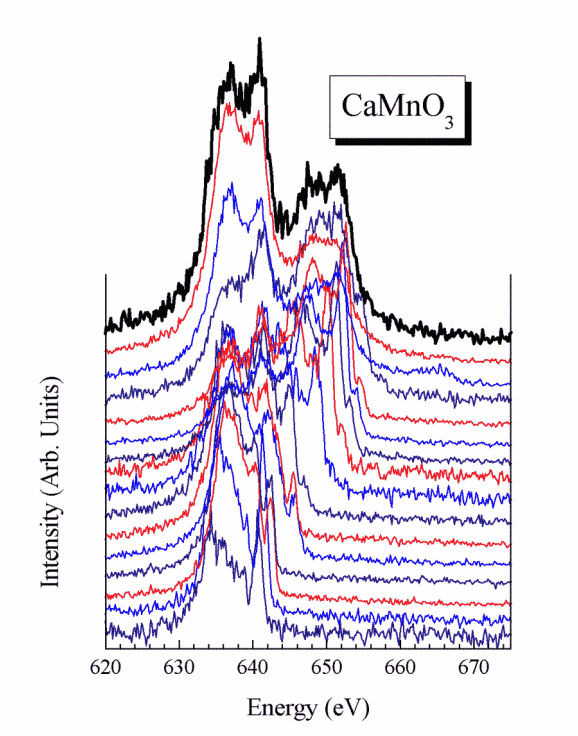

Figure 3 A series of Mn *L*-edge SXE spectra obtained from $CaMnO_3$.