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Electronic and magnetic structure of Ru and Mn in new potential multiferroic materials Ca3Mn2-xRuxO7 (x<=0.5) by X-ray Spectroscopy

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$Ca_3Mn_2O_7$ was proposed as a prototypical multiferroic material in which the ferroelectric and the ferromagnetic ground state arise from the same elastic lattice instability, providing an indirect but high magnetoelectric coupling mechanism.[1] In order to further tune the functional properties of this system towards multiferroicity at room temperature, we have applied chemical doping substituting Mn by Ru.
The electronic and magnetic states states of Mn and Ru atoms in the $Ca_3Mn_{2-x}Ru_xO_7$ (0.05≤x≤0.9) series have been investigated by soft X-ray absorption spectroscopy (soft XAS) and X-ray magnetic circular dichroism (XMCD) at the Mn $L_{2,3}$ and Ru $L_{2,3}$ edges, measured at BL29-BOREAS beamline, and by high-energy resolution fluorescence detection (HERFD) XAS and X-ray Emission spectroscopy measured at ID26 (ESRF) .
The spectral shape of Mn $L_{2,3}$ XAS closely resembles those of the $CaMnO_3$ [2], with a dominant feature at 642.3 eV with a very narrow low-energy shoulder at 640 eV, implying that manganese predominantly exists in a Mn^{4+} oxidation state in the $Ca_3Mn_{2-x}Ru_xO_7$ system, in agreement with HERFD-XAS at Mn K edge measurements. For the higher Ru concentrations, a slight shift to lower energy of the main peak is observed, suggesting an increasing amount of Mn^{3+}. We estimate a ratio of Mn^{3+}/Mn^{4+} of 0.15, which demonstrate that the Ru doping increases the concentration of Mn^{3+}, maybe related to the introduction of oxygen vacancies, similarly to the behavior reported for Ru doped $Ca_3Ti_2O_7$.
According to the sum rules applied to Mn XMCD, the Mn magnetic moment increases with increasing the Ru content for x≥0.3, although the values are substantially lower than expected if the samples were fully ferromagnetic (~3 Bohr magnetons). However, the evolution of the estimated total magnetic moments with the Ru content agree quite well with that of M_S measured at 50 K and an applied magnetic field of 5 T with SQUID. For x≥0.3, the total magnetic moments deduced from the sum rules are slightly higher than the M_S values. Furthermore, the Mn XMCD data measured in remanence provide evidence supporting a canted antiferromagnetic ground state for Ru contents x≥0.7. A very weak Ru $L_{2,3}$ XMCD signal is observed, of opposite sign to the Mn $L_{2,3}$ XMCD, indicating that the direction of the small net Ru 4d magnetic moment is antiferromagnetically coupled to the net Mn 3d magnetic moment. Also, according to the spectral shape, we can conclude that only the $t_{(2g)}$ orbitals contribute to the XMCD signal. This result correlates well with the presence of either Ru4+ low spin ($3d^4$; ${t_{(2g\uparrow)}}^3\ {t_{(2g\uparrow)}}^1$), in agreement with HERFD-XAS measurements at Ru L_3 (detected at the maximum of Ru L-alpha line).

[1] N. A. Benedek and C. J. Fennie, Phys. Rev. Lett. 106, 107204 (2011)
[2] G. Subías et al., Surface Review and Letters, 9(2) 1071-1078 (2002)

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