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ELECTRONIC STRUCTURE OF A₂FeReO₆ DOUBLE PEROVSKITES PROBED WITH Re 2p RXES

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Ordered double perovskites $A_2BB'O_6$ (A = alkaline earth metals, B = 3d transition metal, and B' =3d, 4d, or 5d transition metal) reveal extraordinary properties in terms of their potential application in magnetoelectronics, namely large spin polarization of the electrical carriers, significant magnetoresistance at room temperature and high Curie temperature [1]. The B = Re double perovskites showstrong magneto-structural coupling as well as an unexpected increase in the Curie temperature with decreasing B-O-B' angle and, thus, a reduction in the effective d-electron hopping integral. Such behavior, that is in contrast to other transition-metal oxides, is attributed to the interplay between structural degrees of freedom with unquenched Re orbital moment [2], giving rise to a competition between the octahedral ligand field and the strong spin-orbit coupling in the 5d orbitals.

Here we show an attempt to verify these assumptions employing high resolution X-ray spectroscopy

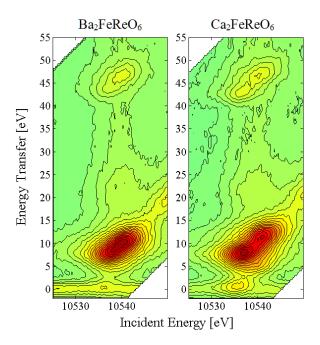


Figure 1: Contour plots of the 2p5d RIXS in Ba_2FeReO_6 (left) and Ca_2FeReO_6 (right) probed at Re L_3 -edge.

to probe the element specific electronic structure of double perovskites and its evolution upon decreasing B-O-B' angle, i.e. going from $A=\mathrm{Ba}$, through Sr to Ca. 2p Resonant X-ray Emission Spectroscopy (RXES) and 2p5d Resonant Inelastic X-ray Scattering (RIXS) have been applied providing us with detailed information on electronic structure of core levels and valence band, respectively, with bulk sensitivity.

We observe that Re-probed electronic structure of core levels, even the shallow ones, is insensitive to local environment. Also the bandwidth of valence band does not show significant differences among the compounds studied. However, the splitting of the features in unoccupied electronic structure as well as intensity and fine structure of the spectral features reveal gradual evolution upon decreasing of B-O-B' angle (Fig. 1). Detailed analysis of the spectral shape of 2p5d RIXS will be performed following the approach of Nikolay Smolentsev et al. [3].

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