

# Electronic structure and x-ray magnetic circular dichroism in hybrid heterostructure $\text{Sr}_2\text{CrReO}_6/\text{BaTiO}_3$

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The integration of ferromagnetic and ferroelectric materials into hybrid heterostructures yields multifunctional systems with improved or novel functionality. We here report on the electronic structure and magnetic properties of hybrid heterostructure combined the ferromagnetic double perovskite  $\text{Sr}_2\text{CrReO}_6$  and ferroelectric  $\text{BaTiO}_3$  calculated in the local spin density approximation (LSDA) as well as the LSDA+ $U$  approach using the fully relativistic spin-polarized Dirac LMTO method. The x-ray absorption spectra (XAS) and x-ray magnetic circular dichroism at the Re and Cr  $L_{2,3}$  edges were investigated from first principles. A qualitative explanation of the XMCD spectra shape is provided by the analysis of the corresponding selection rules, orbital character and occupation numbers of individual orbitals. The complex fine structure of the Cr  $L_{2,3}$  XAS in  $\text{Sr}_2\text{CrReO}_6$  was found to be not compatible with a pure  $\text{Cr}^{3+}$  valency state. The interpretation demands mixed valent states. We found that possible oxygen vacancies lead to a mixed valency at the Cr site.