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Short-term mobility program: Spectroscopic properties of Sr_2RuO_4 and $Sr_3Ru_2O_7$ systems (Prof. E. Pavarini)

Report

During the short-term mobility program at the CNR-INFM SuperMat laboratory, Prof. Eva Pavarini has been interacting and discussing with Dr. M. Cuoco, Prof. C. Noce and other collaborators of them about the physics of perovskite ruthenates both based on Sr- and Ca- alkaline elements. The focus of the program has been on the analysis of the X-ray absorption spectra at the oxygen K-edge for the Sr_2RuO_4 and $Sr_3Ru_2O_7$ within local density functional (LDA) approaches and other related computational schemes that make use of the information and parameters derived from LDA to build up a “realistic” tight-binding model Hamiltonian for the systems upon examination.

Still, part of the program has been devoted to the discussion of the electronic structure of eutectic ruthenate materials of the type Sr_2RuO_4-$Sr_3Ru_2O_7$, and about the mechanisms behind the origin of spin and orbital order in the Ca_2RuO_4 and $Ca_3Ru_2O_7$ both driven by temperature or by an applied magnetic field.

Concerning the analysis of the XAS for the Sr_2RuO_4 and $Sr_3Ru_2O_7$ systems, a basic discussion of the available experimental data has been done focusing on the spectral features as a function of the electric polarization in the range of energies where the transition to the oxygen O 2p bands refer to the unoccupied states that are formed by the hybridization between the Ru 4d and the O 2p orbitals.

One of the problem that has been considered deals with the estimate of the crystal field splitting for the t_{2g} and the e_g bands as well as its connection/identification within the XAS spectra. Previous analyses have based the interpretation of the K-edge XAS spectral features by using a “pure” Ru 4d multiplet picture by indirectly weighting the oxygen contributions. From the LDA preliminary study it has been concluded that such approach is questionable and can lead to a quantitative misunderstanding of the absorption spectra especially because the Ru-O hybridization is quite large and contribute to yield wide O 2p bands in the range of energy of interest.

Another problem that has been considered refers to the polarization dependence of the spectra and the possible identification of the orbitals that contribute to the absorption. Due to the 1s energy difference between the apical and planar oxygen it has been possible to indicate the terms that have in-plane or out-of-plane polarization dependence. This feature together with the symmetry properties of the Ru t_{2g} bands in forming bands with the neighbour O 2p allow to deduce some general observations on the nature of the XAS spectra in the ruthenates.

A plan to study of the orbital dependent density of states at the oxygen site has started during the short-term program and the outcome of the analysis is in progress.

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