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First principles study of the electronic and magnetic properties of SnO_2/CrO_2 superlattices

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Abstract – Spin-polarized electronic structure calculations were performed within the spin density functional theory to study the electronic and magnetic properties of SnO_2/CrO_2 superlattices (SLs). The interplay of the SnO_2 and CrO_2 layer thicknesses in the SL, and the resulting magnetic moment per Cr atom is discussed in relation with the potential application of SnO_2/CrO_2 layers in spintronic devices.

In the last years, the dilute magnetic semiconductors (DMS) have attracted great attention from both experimental and theoretical points of view due to their potential application in *spintronic* devices. A key requirement in realizing most devices based on spins is that the host material must be ferromagnetic (FM) above room temperature. In addition, it is necessary to have efficient spin polarized carriers. One approaching to achieve the spin injection is to employ the transition metals doped oxides or semiconductors in a DMS configuration. Another way is to built-up superlattices (SLs) of alternating magnetic and non-magnetic materials, aiming to produce a half-metallic behavior material, since they are 100% spin-polarized at the Fermi level and are, therefore, ideal for the well defined carrier spin injection.

In this work we address the above issue by studying the electronic and magnetic properties of SnO_2/CrO_2 SLs, oriented along the c axis of the rutile structure, which is the stable structure of both SnO_2 and CrO_2. Recently, magnetic tunnel junctions based on CrO_2/SnO_2 epitaxial layers have been demonstrated [1]. Spin-polarized electronic structure calculations were performed within the spin density functional theory by adopting the Projector Augmented Wave method as implemented in the Vienna Ab initio Simulation Package (VASP-PAW). Supercells of sizes 1x1x2, 1x1x5, and 1x1x10, where 2, 5, and 10 are along the tetragonal c-axis and they means, respectively, 1, 2.5, and 5 SnO_2/CrO_2 bilayer. The spin-polarized band structure for the (1x1x5) SnO_2/CrO_2 SL (Fig.1) clearly shows a half-metallic behavior, with the majority-spin (a) being metallic and the minority-spin (b) semiconductor. Our results demonstrate that this feature is already seen for the short period SL (1x1x2), and it remains for the larger period (1x1x10) SL. A FM ground state for the SL is obtained in all cases. The density of states (DOS) presented in (Fig.2) shows the total majority (full line) and minority (dotted line) spins, and the position of the Cr 3d orbital (close to the gap region) and the Sn 4d orbital which appears deep in the valence band region.

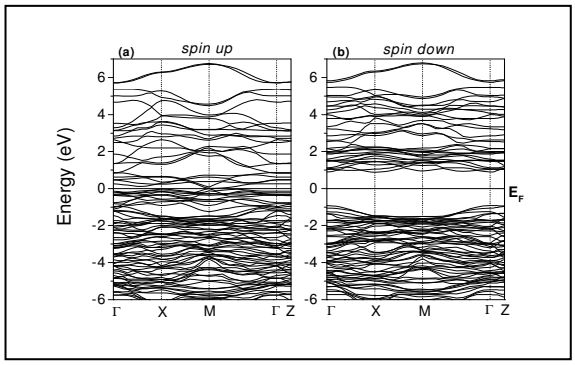

Figure 1: Spin-polarized band structure of a (1x1x5) SnO_2/CrO_2 superlattice, i.e., formed by 2.5 bilayers along the c-axis of the rutile structure.

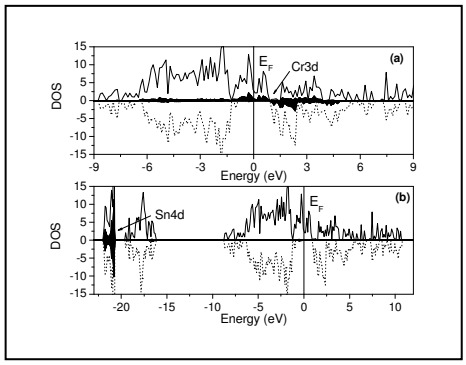

Figure 2: Density of states of a (1x1x5) SnO_2/CrO_2 superlattice, i.e., formed by 2.5 bilayers along the c-axis of the rutile structure. Black shaded DOS corresponds to the Cr3d and Sn4d projected orbitals, respectively.

References

[1] G. X. Miao *et al.*, Appl. Phys. Lett. 89 (2006) 022511.