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Ab initio calculations of exchange interactions, Magnetic and optical properties of (Cu,TM)AlO_2 (TM: Ti, V, Cr, Mn and Fe,): LDA and SIC approximation

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ABSTRACT

In this paper we will use the first-principles calculations to study the electronic structure, magnetic and optical properties of (Cu,TM)AlO_2 (TM: Ti, V, Cr, Mn and Fe) based dilute magnetic semiconductors (DMS), and we will evaluate The energy difference between the ferromagnetic and disorder local moment states. Also, the ferromagnetic stability based on the charge state of magnetic impurities is confirmed by the exchange interactions and the optical absorption spectra obtained by Ab-initio calculations. We prove that when TM introduce simultaneously magnetic moment and intrinsic carriers in (Cu,TM)AlO_2 the ferromagnetic state will be stable.

1. Introduction

In recent years, many studies both experimental and theoretical have focused on diluted magnetic semiconductors DMS with unique properties, paving the way for the new science of spintronics today regarded as one significant technological barrier.

The idea is to manage information using not only the charge of an electron but also the electrons spin properties to create new features and new electronic devices such as diluted magnetic semiconductors (DMS).

There are several types of semiconductors. On one side we have the non-magnetic semiconductors, which do not contain any magnetic member; and other semiconductors having a periodic grating magnetic element. Heating these materials is one way to disrupt the magnetic order and cause the disorder. Thus, for each magnetic material, there is a temperature above which loses its magnetic properties. Beyond this temperature, the material is in a disordered state called paramagnetic. However, these materials are difficult to synthesize and their crystalline structure is quite different from conventional semiconductors such as Si or GaAs. The semiconductors properties are often modified by doping Just introduce impurities within their matrix to obtain a compound N or P. By applying the same principle with a doping of magnetic elements, we obtain new types of DMS which is a mixture between the non-magnetic semiconductor and the DMS based on magnetic elements forming an ordered array.

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Some DMS record the presence of ferromagnetic phase. We can note the results on the Ge doped Mn [1] or Cr [2], or SiC doped Fe, Ni or Mn [3].

Also some semiconductors have high carrier density sufficient for that the ferromagnetic interactions they carry are stronger than the anti-ferromagnetisms. There possibility of controlling the appearance of a ferromagnetic phase by the carrier density is known since 1986 [4]. However, these materials are not compatible with modern electronic component, because their structure crystallographic is too different.

DMS doped manganese are now the subject of several publications. The first test compound thin film was indium arsenide doped with manganese. Munekata et al. postponed the existence of a homogeneous phase in the ferromagnetic $In_{1-x}Mn_x$[5] and they showed that the ferromagnetism was induced by the holes [6]. Both publications have encouraged many groups to study Mn doped semiconductor $Ga_{1-x}Mn_x$ including the compound that is the subject [7] of several experimental and theoretical publications. Also progress growth techniques including better control of the doping of these semiconductors have helped highlight a ferromagnetic phase induced carriers (holes) roaming [8].

Chromium is probably the most used item after Mn. We can refer to the work of Choi et al. [9]. They developed germanium single crystals doped with Cr (1%) and they have reported Curie temperatures in the order of 125 K and Saito et al. [10,11] have reported the presence of a ferromagnetic phase in the ZnTe compound.

2. Computational details

Using the Korringa–Kohn–Rostoker (KKR) method combined with coherent potential approximation (CPA), the relativistic effects have been taken into account by employing the scalar relativistic approximation. The form of the crystal potential has been approximated by a muffin-tin potential, and the wave functions in the respective muffin-tin spheres have been expanded in real harmonics up to l = 2, where "l" is the angular momentum quantum number defined at each site. In the present KKR-CPA calculations, where the package MACHIKANEYAMA2000 coded by Akai [12] is used, 500 K-points in the whole first Brillouin zone were taken into account. In this study, the KKR method within the Local Density Approximation (LDA) has been used for the parameterization of the exchange energy [13].

The delafossite structure can have either P63/mmc (N°194) or R3 m (N°166) space-group The delafossite $CuAlO_2$ is experimentally recognized to be in the rhombohedral group R3 m with the lattice constants are a = 2.84°A and c = 17.02°A [14]. The characteristic physical property of $CuAlO_2$ is its p-type conductivity in as-grown samples [15]. This feature distinguishes $CuAlO_2$ from the other oxides, which normally show n-type conductivity. This makes CuAlO 2 an interesting host material for oxide spintronics. The delafossite $CuAlO_2$ has two cation sites, Cu^{1+} and Al^{3+},and both of them can be substituted by magnetic TM impurities.

Using the KKR-CPA method [16], we could evaluate the effective exchange coupling constants J_{ij} where, as it is described in [17].

The J_{ij} are obtained from

$$J_{ij} = \frac{1}{4\pi}\int_{-\infty}^{\varepsilon_F} dE Im Tr\left[\Delta_i \tau_{\uparrow}^{ij} \Delta_j \tau_{\downarrow}^{ji}\right]$$

where Δ_i is the difference in the inverse single-site scattering t-matrices for spin-up and spin down states, $\Delta_i = t_{i?}^{-1} - t_{i\downarrow}^{-1}$, and τ is the scattering path operator.

As result of the fact of the use of spherical potential and scalar relativistic approximation, the t-matrices are diagonal. Thus, we can decompose the J_{ij} and extract the contribution of L states at the i-th site and L′ states at the j-site as

$$J_{ij}^{L-L'} = \frac{1}{4\pi}\int_{-\infty}^{\varepsilon_F} dE Im Tr\left[\Delta_{iL} \tau_{\uparrow LL'}^{ij} \Delta_{jL'} \tau_{\downarrow L'L}^{ji}\right]$$

This allows calculating element as well as orbital-resolved magnetic coupling constants for disordered.

3. Electronic structure of (Cu,TM)AlO_2 (TM: Ti, V, Cr, Mn, and Fe)

the total and partial density of states (DOS) of (Cu, TM)AlO_2 with (TM: Ti, V, Cr, Mn, and Fe) within LDA and LDA-SIC approximations is calculated in Figs. 1 and 2) The Fermi level is chosen to lie at 0 eV.

As Known in the most of transition metal oxides, the crystal field splitting leads to a separation in d level to t and e part. The same result is observed within LDA approximation, the splitting of the atomic 3d level into five-time degenerate (triply degenerate) t and (doubly degenerate) e subgroups caused by the influence of the crystal field environment; t and e states are less localized in valence band states.

The 3d-state are localized in the band gap, the position of the Fermi level in t and e states depend on the occupancy of the d band, and define how the compound behave in term of the half metallicity.

According to the electronic structure calculations, a good half-metallic behavior was predicted for Ti, V, Fe and Co doped **$CuAlO_2$**, near half metallic behavior was observed for Cr and Mn doped **$CuAlO_2$**, and no half-metallic behavior in V doped **$CuAlO_2$**.