FIRST PRINCIPLE CALCULATIONS OF ISOLATED BANDS IN HALF METALLIC INTERMEDIATE BAND MATERIALS.

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The field of nanostructure physics has been growing rapidly in recent years and much theoretical and experimental insight has been gained giving access to a more efficient device oriented applications. In the nanotechnology area one of the main objectives is the production of materials with specific characteristics from the bulk materials. In this context we present here the study of a quantum design of a novel material with semiconductor characteristics that presents an intermediate half-filled band between the valence and the conduction bands of the host semiconductor.

We have studied band structures of diluted semiconductor compounds of the Ga_4As_3X and Ga_4P_3X type, X being a transition metal, at different dilutions using accurate ab-initio codes based on the density functional theory (Fig.1). Recent discovery of ferromagnetism behaviour in half-filled diluted magnetic III-V semiconductors have attracted much attention recently as ideal materials for spin injection into semiconductors in spintronic technology. Moreover, in solar cells devices, using as high efficient photovoltaic material the intermediate band (IB) could be created in order to enforce light absorption of low energy photons. This IB must be energetically isolated from the two other bands to avoid heat dissipation from non-radiative recombination. This behavior it is also shown in Fig.2.

In the same line, we have carried out ab-initio spin polarized calculations like the semiconductor materials $CuInSe_2$ thin-films that have been used widely in photovoltaic device applications. This system appears to have a big structural tolerance to large range of anion-to-cation off stoichiometry and can be doped n and p type by introduction of native defects, without extrinsic impurities. In this manner this systems vary its electronic properties with concentration in a nontrivial way. Using these properties we have study different doppings for several similar systems including defects and vacancies in a substitutional and intersticial way, in order to produce the half metal Intermediate Band. Moreover, first results of DFT spin polarized DOS for the spinel structure of $TiIn_2S_4$ half metallic material is shown in Fig.3. The spinel structure for In_2S_3–like structure with vacant in cationic tetrahedral positions is also shown in the same figure.

Our goal in this work for these different systems is to present accurate calculations of band diagrams and density of states (DOS) showing half metallic intermediate band. We use different ab-initio self-consistent computed codes as ABINIT, SIESTA, CASTEP and VASP within the DFT method, using in all cases both the local density (LDA) and the generalized gradient correction (GGA) approximations for the exchange and correlation potential.

References:

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Figures:

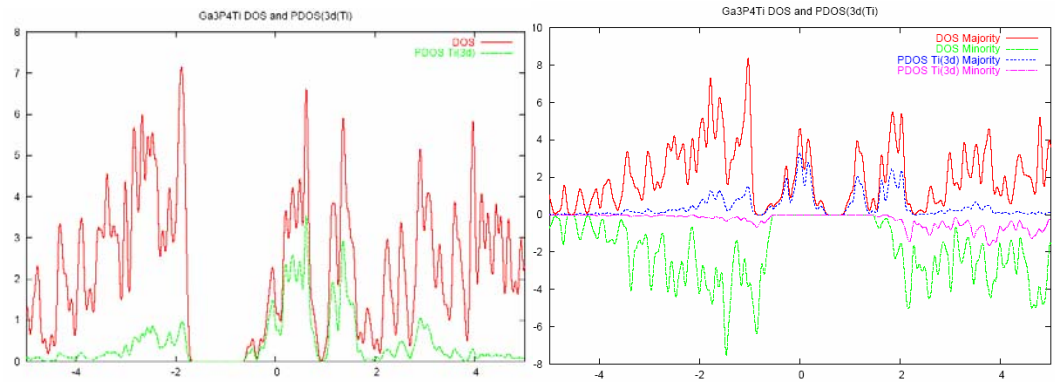

Fig.1. DFT-GGA Total density of states (DOS) and projected contribution of Ti states calculated for the $TiGa_3P_4$, represented for the non polarized spin (right) and spin polarized up and down (left).

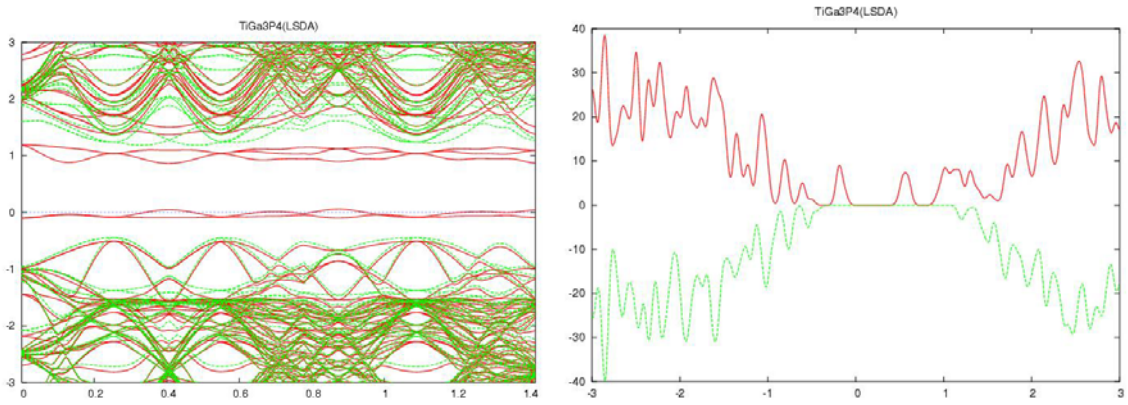

Fig.2. DFT Spin polarized up and down band structure calculations for diluted $TiGa_{31}P_{32}$ showing an isolated intermediate band at the Fermi level (left) and the total density of states (DOS) of this structure (right).

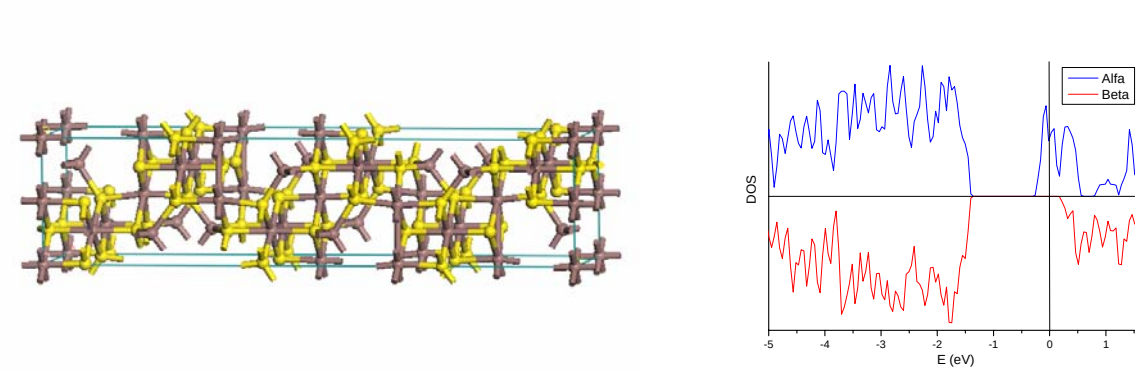

Fig.3. Spinel-type structure for In_2S_3 with vacant in cationic tetrahedral positions (right). First results of first principle spin polarized DOS for the spinel structure of $TiIn_2S_4$ half metallic material.