ELECTRONIC STRUCTURE AND OPTICAL PROPERTIES OF DILUTED MAGNETIC PHOTOVOLTAIC MATERIALS

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The aim of this work is to study the properties of a new type of materials like TiGaX, with X= As or P, to improve solar cell devices using quantum mechanical calculations. The promising properties of such materials that present a half metallic intermediate band inside the semiconductor band-gap[1], encourage developing a more sophisticated scheme in order to verify the properties already found. In this work we present first, a study of the properties of such materials using the recently implemented very precise Exact Exchange (EXX) frameworks. Results obtained confirm previous calculations done using local and semi-local Density Functional (DFT) calculations.

In order to obtain optical transitions to characterize optical properties of this kind of materials, we have also performed accurate calculations of phonons dispersion diagrams and electron-photon couplings of the alloys using also first principle computed codes. The material may absorb photons of low energies to promote electrons from the valence band to the half-filled intermediate band, and from this one to the conduction one, presenting both direct and indirect band gaps in their structures (fig.1).

Beside that, recent spin polarized calculations of these kinds of materials present in some of them large spin-polarization at Fermi energy and could be considered as ideal materials for spin injection into semiconductors. Results will be presented at the Conference.

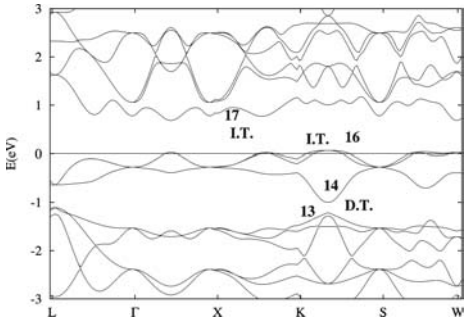

Fig.1. Ab initio band diagram structure characterization of TiGaP

1) P. Wahnón and C. Tablero, Phys. Rev. B. **65** 165115 (2002).

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