Tight Binding Investigation of the Electronic Structure of Novel Semiconductor Alloys (GaBiP & GaBiAs) for Optical Devices

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In this talk, we are aiming to present a detailed investigation of the electronic properties of a novel class of alloys containing Bismuth (Bi) atoms inside the GaP and GaAs materials. The incorporation of Bi results in band anti-crossing interaction (BAC) effect, much similar to the one widely studied for Nitride based alloys, resulting in large band gap (E_g) bowing. The larger size of Bi atoms gives rise to large spin orbit splitting (Δ_{SO}), which at higher Bi compositions (above 10%) exceeds E_g as indicated by recent photo-reflectance measurements [1]. This opens up possibility to design highly efficient (low loss) and thermally stable optical devices such as lasers. However, despite considerable progress in the experimental growth and characterization of GaBiAs, relatively fewer theoretical studies are available to-date. Previous theoretical studies are limited to low Bi compositions (less than 5-6%) and hence do not provide any analysis of the E_g-Δ_{SO} crossing. Furthermore, the understanding of the large reduction in the E_g is still controversial, while people debating whether it comes from a BAC interaction or as conventional alloy shift.

This work develops and reports a first ten band sp^3s^* tight-binding model for GaBiAs and GaBiP (see for example GaBi bulk band structure in figure 1), with atomic relaxation included using a valence force field energy minimization method. Atomistic modeling allows us to better understand the impact of a single Bi impurity inside a GaAs or GaP matrix. We first develop our understanding of GaBiP alloys where a four-fold degenerate defect level due to Bi incorporation is found just above the valence band edge, and then apply this understanding to GaBiAs. We find that the experimentally measured reduction in E_g includes a contribution both from a BAC interaction that affects the valence band edge and a conventional alloy shift that mainly affects the conduction band edge. We calculate a crossing between the band gap and spin-split-off energies at about 10.5% Bi composition that matches the experimental measurements [1] (see figure 2). Recent x-ray absorption spectroscopy analysis [2] revealed that Bi atoms tend to form pairs and clusters even at ~2% compositions. The impact of a single Bi pair or cluster cannot be studied by continuum modeling approaches and requires a full atomistic approach. By using our model, we firstly provide a detailed analysis of individual Bi pairs and clusters, and then extend the model to analyze their effects in random alloys as a function of increasing Bi composition. Our results indicates that pairs and clusters strongly impact the valence band edge and result in defect states similar to those due to N pairs and clusters in GaAs.

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[1] Muhammad Usman *et al.*, Physical Review B 87, 115104, 2013

[2] Muhammad Usman et al., Physical Review B 84, 245202, 2011

[3] G. Ciatto *et al.*, Phys. Rev B 78, 035325 (2008)

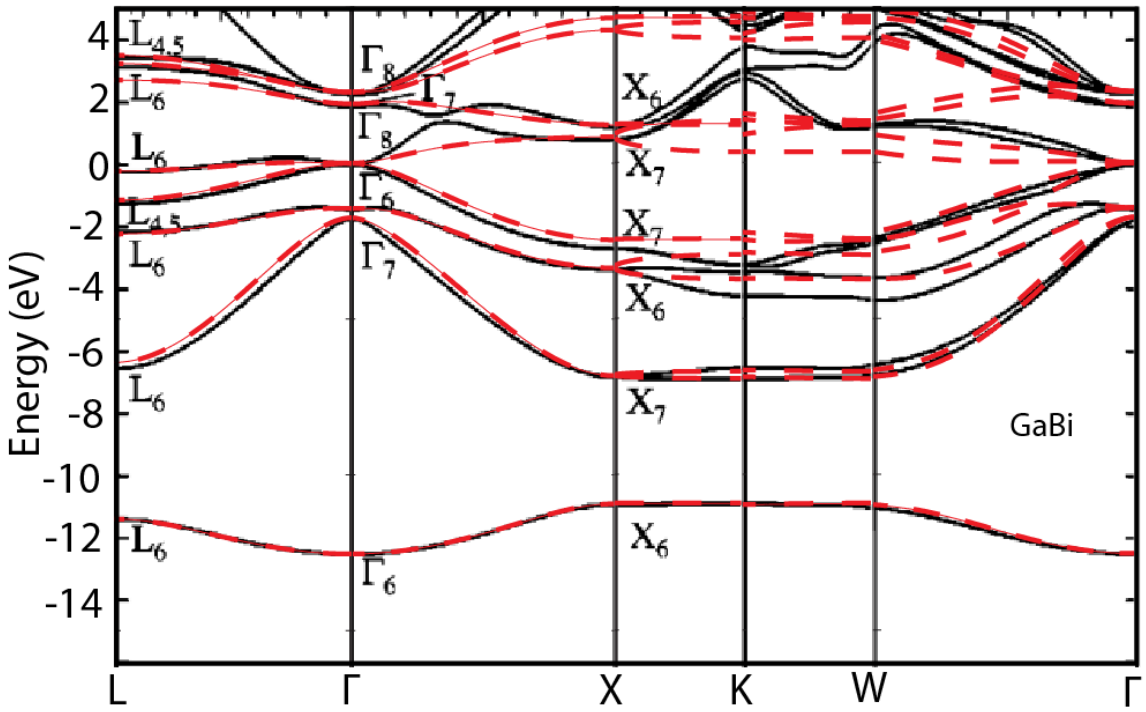

Fig. 1: Bulk band structure of the GaBi. The broken red lines are the bands obtained from our sp^3s^* tight binding parameterization. The solid black lines are the LDA+C bands calculated by A. Janotti et al., Phys. Rev. B 65, 115203 (2002).

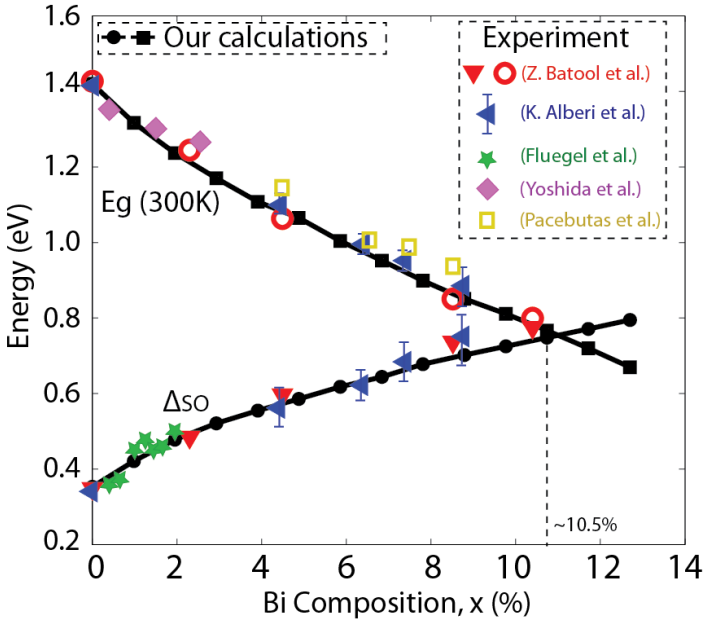

Fig. 2: The band gap E_g and spin-orbit splitting Δ_{SO} are plotted as a function of Bi composition. The solid black lines are data from our model, compared with five experimental sets. Our calculated results demonstrate a close match with the experimental values, exhibiting E_g-Δ_{SO} crossing at about 10.5% Bi composition in agreement with experiment (Z. Batool *et al.*)