Band structure engineering of dilute bismide alloys for photovoltaic applications

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Alloying Bi into a conventional III-V semiconductor brings a number of advantages for device applications. These include in particular (Fig. 1) the ***strong control of the band gap energy*** from near-infrared through to mid-infrared whilst remaining lattice-matched to commercially standard substrates such as GaAs, InP and Ge, as well as the ***extremely high spin-orbit splitting energies*** [1]. It has been predicted that these features can be exploited to produce temperature insensitive lasers, efficient absorption for mid-infrared photodetectors and to develop applications in spintronics. We target here their potential to dramatically improve photovoltaic efficiency.

In this talk we first present an overview of theoretical models to describe the electronic structure of dilute bismide alloys, and then apply those models both to analyze existing materials and devices and also to address the wide design space available using dilute bismide alloys. We present tight-binding (TB) calculations which confirm that the observed variation of the band gap and SO energy with x are well described by a band-anticrossing (BAC) interaction between the extended states of the GaAs valence band (VB) edge and localized Bi impurity states in the VB [2]. Based on the TB calculations, we derive an accurate 12-band **k.p** model for GaBiAs heterostructures [3].

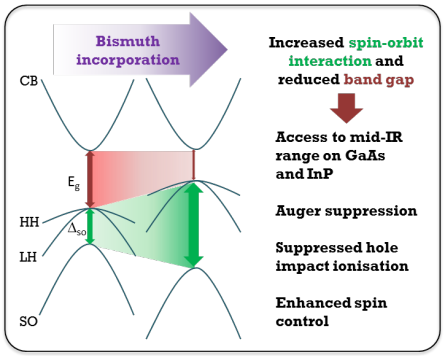

Figure 1 Impact of bismuth on III-V bandstructure and devices

A key challenge in high efficiency multijunction solar cells is the development of a suitable alloy to provide an absorption layer with an energy gap of 1 eV. GaAsBi, BGaAsBi, GaPAsBi and GaNAsBi all have the potential to act as direct gap 1 eV absorption layers, but are highly different in terms of their band structure formation and growth. Using the TB and **k.p** models that we have developed, we present calculations to illustrate the wide flexibility which such alloys offer for the design and implementation of multijunction solar cells, touching also on their wider potential for other types of high efficiency photonic devices.

References:

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