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Theory of the electronic structure of the dilute bismide alloy GaBiAs

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Dilute bismide alloys, such as GaBiAs, where a small fraction x of the As atoms in GaAs are replaced by bismuth (Bi), are a promising material system for the realisation of highly efficient, temperature stable semiconductor lasers[1]. Experimental and theoretical investigations have shown that with increasing x the band gap (Eg) decreases rapidly, accompanied by a large increase in the spin-orbit-splitting energy (Es), leading to Eg < Es for x > 10%[2]. This condition is of interest for semiconductor laser operation, as the dominant non-radiative Auger recombination pathway is suppressed[3].

We outline our theoretical models of the electronic structure of $GaBi_xAs_{1-x}$ based on a multi-scale approach ranging from atomistic electronic structure models[1] to continuum band structure models[4] suited to device calculations.

We first formulate an atomistic tight-binding (TB) model[1], which accurately describes the main features of the GaBiAs electronic structure and demonstrate how the evolution of the electronic structure with increasing x is influenced by the Bi-related impurity states that are formed as a result of the chemical and size differences between Bi and the As atoms, as well as by alloy disorder.

Based on the TB calculations, we derive a continuum 12-band k.p model for GaBiAs[4] . This describes the band structure in terms of an anti-crossing interaction between the extended states of the GaAs valence band edge and localised Bi-related states. These theoretical models elucidate both the fundamental physics and device properties of dilute bismide alloys.

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