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Theory of the electronic structure of dilute bismide alloys

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Abstract: We use the tight-binding method to analyse the electronic structure of GaPBi and GaAsBi, where a small proportion of P or As atoms are replaced by bismuth (Bi). Our results confirm that this leads to the formation of resonant defect levels in (above) the valence band for GaAsBi (GaPBi), which have a band-anticrossing (BAC) interaction with the valence band maximum. Our calculations show that the observed reduction in energy gap with increasing Bi composition in GaAsBi includes a contribution from a downward shift of the CBE, which can be described using a conventional virtual crystal approach, and that the effect of this conduction band shift is of similar magnitude to that due to the valence-band BAC interaction. Finally we extend our calculations to the quaternary alloy, GaAsBiN, showing that the effects of Bi and N are to a large extent independent of each other in a random alloy.