Localization and anticrossing of electron levels in $GaAs_{1-x}N_x$ alloys

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The electronic structure in nitrogen-poor $GaAs_{1-x}N_x$ alloys is investigated using a plane-wave pseudopotential method and large supercells. Our calculations give a detailed description of the complex perturbation of

low-nitrogen concentration $GaAs_{1-x}N_x$ alloy relative to GaAs. Crucial for the present application is accuracy in the position and pressure dependence of GaAs Γ_{1c}, L_{1c}, and X_{1c} states: Our method gives 0.32 (0.45) eV for the $\Gamma_{1c}-L_{1c}$ ($\Gamma_{1c}-X_{1c}$) separation, in good agreement with experiment.[20] Table I further shows that the LDA calculated pressure coefficients for the GaAs Γ_{1c}, L_{1c}, and X_{1c} states are well reproduced by the employed pseudopotential, and that the pressure dependence of the band gap is correctly divided into contributions from conduction and valence band edges as compared with LDA calculated values.

Figure 1 shows the behavior of the lowest conduction states as a function of x in $GaAs_{1-x}N_x$ alloy. To analyze the identity of the alloy states ψ_i we expand them in the Bloch states $\{\phi_{n,\mathbf{k}}\}$ of the underlying GaAs, and calculate[17] the spectral projection $\|A_{n,\mathbf{k}}\|^2$ given in Fig. 1 for Γ_{1c}, L_{1c}, and nn

GaAs we find $m_e(\Gamma_{1c}) = 0.08$, $m_e^{\parallel}(L_{1c}) = 0.13$, $m_e^{\perp}(L_{1c}) = 1.51$], we find that nitrogen alloying increases the effective mass of the E_- state, in agreement with experimental observations.[12] This is in contrast with conventional alloys (e.g., InGaAs) where alloying does not promote significant $\Gamma - L$ mixing. The $\Gamma - L$ mixing (delocalization in reciprocal space) indicates localization in real space: Unlike conventional CBM states that are delocalized, the E_- state in $GaAs_{1-x}N_x$ alloy is localized (around the Ga atoms nearest