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 Γ_{1c} $-L_{1c}$ ($\Gamma_{1c}-X_{1c}$)

3 274.964 356.2585545573880Tm934 1 Tf 0.767 0 TD (L)Tj626F12 1 Tf 6.985 0 0 6.985 67.02 330.897 2Tm 1/F1803/F(1)1 Tf 0.58 0 TD (c)T

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