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Penetration of dilute nitrogen states deep into the GaPN conduction band*

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We study the electronic structure consequences of perturbations caused by dilute N impurities in GaP by means of large supercell (∼1700 atoms) calculations, using a fully atomistic empirical pseudopotential method. We find that numerous localized states are introduced by a single N atom and N clusters, not only close to the band edge but also throughout the GaP conduction band[1], up to ~ 1 eV above the conduction band edge. Many of these ensuing states have no counterpart in any of the previous simplified models, such as impurity band or band anticrossing models. These high energy N-localized states are essential for understanding of a previously puzzling observation of splitting of PLE intensity at the GaP Γ_{1c} energy into two features, one blue shifting and the other staying pinned in energy with increasing N concentration. Our calculations also explain the observed build up of the featureless spectral intensity between the GaP X_{1c} and Γ_{1c} energies with increasing x, as being due to the $L - L$ like optical transitions from the states *below the VBM*. This work is done in collaboration with Paul Kent and Alex Zunger.

[1] S.V. Dudiy, P.R.C. Kent, and A. Zunger, PRB **70**, 161304 (2004).

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