

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic transport in dilute GaAs:N GEOFFREY STENUIT, STEPHEN FAHY, Tyndall National Institute, Cork, Ireland — Plane-wave pseudopotential-based DFT (density functional theory) are used to determine the electronic properties (band structure, effective mass and energy gap) of dilute GaAs:N with substitutional nitrogen concentration $x = 1 - 3\%$. Calculations are performed using LDA (local density approximation) for the exchange-correlation functional and applied to large supercells (more than 64 atoms) to achieve the dilute limit. Scattering cross-section, as well as the mobility are derived from the nitrogen concentration dependence of the band gap in GaAsN. The effects of an N₂ split interstitial substitution on the electronic properties are also discussed. Finally, the presence of a localized nitrogen state in such material is also studied within this ab initio framework.

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Date submitted: 26 Nov 2005

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