

Energy levels of isoelectronic impurities by large scale LDA calculations

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Abstract

Isoelectronic impurity states are localized states induced by stoichiometric single atom substitution in bulk semiconductor. Photoluminescence spectra indicate deep impurity levels of 0.5 to 0.9 eV above the top of valence band for systems like: GaN:As, GaN:P, CdS:Te, ZnS:Te. Previous calculations based on small supercells seemingly confirmed these experimental results. However, the current ab initio calculations based on thousand atom supercells indicate that the impurity levels of the above systems are actually much shallower (0.04 to 0.23 eV), and these impurity levels should be compared with photoluminescence excitation spectra, not photoluminescence spectra.

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