ELECTRONIC STRUCTURE OF GAN QUANTUM DOTS WITH SUBSTITUTIONAL IMPURITIES

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We present results on the electronic structure of spherical GaN quantum dots with a substitutional impurity, either acceptor or donor, obtained within the sp^3s^* tight-binding model. The binding energy of an impurity placed at the centre of a dot tends toward its experimental bulk value as its size increases [1]. The impurity is modelled by the Coulomb potential, □ $e^2/\varepsilon r$, that equals U_0 for $r = 0$. In order to estimate the value of this parameter, we calculate the binding energy for a starting U_0 and increasing size ($4.53 \leq R \leq 81.57$ □); we fit it by means of a scaling law; and we repeat the calculations for other values of U_0. In the limit of large radii, the experimental bulk binding energies of the acceptor and donor, ~230 meV and ~30 meV respectively, are provided by $U_0^{acceptor}$ = 7 eV and U_0^{donor} = -3.5 eV. The size-dependent average radii of the ground-state hole and electron orbits are also obtained. When the impurity is placed off-centre, the calculated binding energy decreases with increasing radial distance.

Reference:

[1] J. Perez-Conde, A.K. Bhattacharjee, Solid State Communications, **135** (2005) 496-499.