

Substitutional Nitrogen Impurity in Carbon Nanotubes

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The effect of substitutional nitrogen impurity on the electronic structure of carbon nanotubes is investigated using *ab-initio* density functional theory. We study the localization of the impurity state and the density of states of semiconducting zigzag and metallic armchair carbon nanotubes as a function of nitrogen concentration. Comparison is made with the N-doped graphene sheet and the fullerene $C_{59}N$.

For an isolated impurity, analysis of the spin density shows that the impurity state in the semiconducting nanotube is localized around nitrogen and falls off exponentially with typical extent of about 20 Angstrom. In case of a metallic nanotube, the impurity state is delocalized. Interestingly, in both cases we observe the oscillations of the spin density with the period equal to the primitive cell vector of graphite sheet, which arises from an RKKY-type polarization by the impurity. An important difference in the character of these oscillations between armchair and zigzag cases appears as the presence or absence respectively of the mirror left-right symmetry along the axis of the nanotube.

In order to understand the effect of the impurity on the electronic properties of carbon nanotubes we performed a detailed analysis of the band structure and the density of states. In the case of the semiconducting zigzag nanotube it appears that nitrogen forms an impurity level lying in the band gap of the pristine nanotube. This singly occupied level is likely to be electronically and chemically active. The corresponding peak in the density of states moves towards the bottom of conduction band and broadens simultaneously as the nitrogen concentration increases. The impurity concentration also has a significant effect on the size of the band gap.