Iranian Journal of Physics Research, Vol. 16, No. 1, 2016

Magnetic properties of zigzag (0,9) GaAs nanotube doped with 3d transition metals

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(Received 14 October 2014 ; in final form 24 November 2015)

Abstract

In this work, the electronic and magnetic properties of the pure and doped zigzag (0,9) GaAs nanotube with 11 percents of 3d transition metals (Sc, Ti, Cr, Mn , Fe, Co, Ni) in both far and close situations were studied based on spin polarised density functional theory using the generalized gradient approximation (LDA) with SIESTA code. The electronic structures show that zigzag (0,9) GaAs nanotubes are non-magnetic semiconductors with direct band gap. It was revealed that doping of 11.11 % Fe and Mn concentrations substituted in Ga sites in ferromagnetic phase in far situation and Cr sites in ferromagnetic phase in near situation introduces half metallic behavior with %100 spin polarization. The unique structure of spin polarised energy levels is primarily attributed to strong hybridization of 3d transition metal and its nearest-neighbor As-4p orbitals. The results of this study can be useful for empirical studies on diluted magnetic semiconductors (DMSs) and systemic investigation in 3d transitional metals. We suggest that GaAs nanotubes doped by transition metals would have a potential application as a spin polarised electron source for spintronic devices in the future.

Keywords: DFT, DMS, GaAsn anotube spintronic, transition metals

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