Electronic, Magnetic, and Optical Properties of Pure GaAs Nanolayer and Doped with Mn and Fe Impurities Located at the [001] Surface

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ABSTRACT

The GaAs nanolayer has received much attention due to its wide application. Due to the importance of the GaAs nanolayer, in this paper, using two Mn and Fe impurities, the probability of the metallic to the semiconductor phase transition and vice versa, as well as the displacements of the optical coefficients' peaks of this nanolayer are investigated. For this purpose, the structural, electronic, and magnetic properties of pure GaAs nanolayer and this nanolayer with Mn (GaAs + Mn) and Fe (GaAs + Fe) impurities located at the nanolayer surface are investigated using the density functional theory. The electron density of states, linear coefficients of electronic specific heat, band structures, and the total and local magnetic moments at the impurity atomic position of these nanolayers are calculated and compared. The real and imaginary parts of the dielectric function, static dielectric functional, uniaxial anisotropy, reflectivity, absorption, electron energy loss function, and the optical conductivity of pure GaAs, GaAs + Mn, and GaAs + Fe nanolayers for electric field parallel and perpendicular to the nanolayer surface within GGA and GGA_EV approaches are investigated and compared.

Keywords: density functional theory, GaAs nanolayer with impurity, magnetic moment, band structure, optical properties

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