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Effect of doping Si on the structural, electronic and optical properties of GaAs nanostructures

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Abstract
In the recent years, with advances in material growth, there has been a considerable interest in the compound semiconductors of group III-V, in particular GaAs. Silicon (Si) is the most suitable substance for the n-gallium arsenide type [1]. In this study, the structural and electron properties of $Ga_6As_4H_{10}$ and $Ga_6As_3SiH_{10}$ nanocrystals are investigated using the quasi-potential and density functional formulation (DFT) method and with the approximation of LDA in the quantum espresso package. The results of the calculations show that the larger the size of the nanocrystal, the more the decrease of band gap. By replacing the Si atomic impurity by the As atom in the $Ga_6As_4H_{10}$ nanocrystal, the energy gap becomes smaller than the non-degenerate state, and the fermi level approaches the edge of the conduction band, in which the $Ga_6As_3SiH_{10}$ nanocrystal is a n-type semiconductor. The charge density of the charge around the atoms shows an ion-covalent bond between Si and Ga atoms. In this study, the optical properties of gallium arsenide nanocrystals have been investigated; calculations are performed with single-particle approximation. Gusin software is also used to obtain the optical spectrum of the nanocrystal. The optical spectrometry for gallium arsenide nanocrystals shows the transition to blue.

Keywords: n-type impurity, gallium arsenide nanocrystal, density functional theory, electron properties

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