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Band structure engineering and transport properties of aluminium phosphide nanoribbon – A first-principles study

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ABSTRACT

The band structure and transport properties of pristine, boron, gallium and arsenic substituted AlP nanoribbon are studied using density functional theory. The band structure of pristine, boron, gallium and arsenic substituted AlP nanoribbon exhibits semiconducting behavior. The substitution of boron decreases the band gap of AlP nanoribbon. The substitution of group-III semiconductor has much influence in density of states. The major contribution is observed in *p* and *d* orbitals. The electron density increases with boron substitution and there is a slight decrease in electron density for gallium substitution. The transmission of AlP nanoribbon molecular device is analyzed with two probe method. The substitution impurity and bias voltage influence the transmission across AlP nanoribbon. From the results, it is inferred that the band structure and electronic transport properties can be fine-tuned with substitution impurity along AlP nanoribbon.

1. Introduction

Nanoscience and technology opened a new era in fundamental research in nanoscale, the economic nanoscale manufacturing of devices leads to more coherent science and engineering applications. The recent advancement in the group-III and V compound semiconductor attracted the scientific

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community due to their applications in semiconductor industries. This motivates scientific community for numerous theoretical and experimental studies in the group III–V compound semiconductors such as gallium arsenide, indium phosphide, aluminium phosphide and gallium phosphide, etc. Among these compound semiconductors aluminium phosphide (AlP) receive a considerable attention due to lower mass, which leads to higher vibrational frequencies [1]. Aluminium phosphide (AlP) is a wide-band compound semiconductor with a band gap of around 2.5 eV. Usually, AlP is alloyed with binary materials for applications in optoelectronic devices [2].

To this time, even though numerous experimental and theoretical studies are reported in AlP and their counter parts group III–V semiconductors [3–5]; to the best of our knowledge; the band structure engineering and transport properties of aluminium phosphide nanoribbon with substitution impurities have not been investigated. The systematic computational study could be a pioneer step for the experimental characterization of nanostructures. Ling Guo studied carbon monoxide adsorption on cationic, neutral, and anionic aluminium phosphide clusters [6] and also reported the electronic structure and properties of neutral and charged aluminium phosphide clusters [7]. Mirzaei et al., reported boron doped and carbon doped AlP nanotubes [8,9]. Rezaei-Sameti reported SiC-doped aluminium phosphide nanotubes [10]. Density functional theory (DFT) is an effective method to study the structural and electronic transport properties of nanostructures [11–13]. The motivation of the present work is to tailor the band structure and electronic transport properties of AlP nanostructures with improved performance in optoelectronic devices with the incorporation of substitution impurities. Moreover, controlling the transport phenomena along nanoelectronic devices is a challenging task. To date, there are numerous reports in molecular electronic devices, which are used for rectification, switching, optoelectronics and spintronics applications [14–23]. The novel aspect of the work is to design AlP nanoribbon with substitution impurities and AlP nanoribbon is used as a molecular device. The molecular electronic device may have a single molecule between the electrodes which acts as source and drain. The state-of-the-art of the present work is to construct AlP nanoribbon and to fine-tune the band structure and electronic properties with substitution impurity and the designed AlP nanoribbon are used as a molecular device between the electrodes. In the present work an attempt has been made to fine-tune, the properties of AlP with substitution impurities such as boron, gallium and arsenic and the results are reported.

2. Computational details

The present investigation on AlP nanoribbon is carried out by DFT method utilizing TranSIESTA module in SIESTA package [24]. DFT method explores the band structure, density of states and transmission coefficient for the present system. In the reported work, generalized gradient approximation (GGA) with Perdew–Burke–Ernzerhof (PBE) exchange correlation functional, (GGA–PBE) functional is employed throughout the work [25,26]. The sampling of Brillouin zone is carried out by $1 \times 1 \times 1$ k points. By reducing the atomic forces of atoms as small as 0.05 eV/Å, the molecular geometry is optimized. The real-space grid for electrostatic potentials is considered in the mesh cut-off energy of 10^{-5} eV that realizes the balance between the efficiency and accuracy in calculation. The electronic properties of AlP nanoribbon are determined with vacuum padding of 10 Å modeled along x and y directions to remove the interaction of AlP nanoribbon with its periodic images. The atoms along the nanoribbon are free to move in their position till the convergence with a force less than 0.05 eV/Å on each individual atom in AlP nanoribbon is achieved. The complete optimization of AlP nanoribbon is supported by double zeta polarization (DZP) basis set [27,28].

3. Results and discussion

3.1. Structures of AlP nanoribbon

Initially, AlP nanoribbon is designed from International Centre for Diffraction Data (ICDD) card number 79-2500. For pristine AlP nanoribbon, there are twenty-four aluminium atoms and twenty-four phosphorus atoms forming a hexagonal structured AlP nanoribbon and both ends of AlP nanorib-