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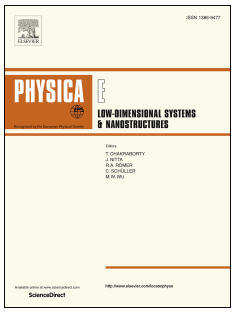

Strain and electric field induced metallization in the GaX (X☐=☐N, P, As, & Sb) monolayer

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Strain and Electric Field Induced Metallization in the GaX (X = N, P, As, & Sb) Monolayer

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Abstract

We investigate the strain and electric field dependent electronic properties of two dimensional Ga-based group III-V monolayer from the first-principles approach within density functional theory. The energy bandgap of GaX monolayer increases upto the certain value of compressive strain and then decreases. On the other hand, the energy bandgap of GaX monolayer is monotonically decreased with increasing tensile strain and become metallic at the higher value. Furthermore, the perpendicular electric field decreases the energy band gap of unstrained GaX monolayer and shows semiconductor to metal transition. These results suggest that the nature of energy bands and value of energy bandgap in GaX monolayer can be tuned by the biaxial mechanical strain or perpendicular electrical field. Additionally, we have also studied the optical response of unstrained GaX monolayer in term of optical conductivity. These findings may provide valuable information to develop the Ga-based optoelectronic devices and further the understanding of the GaX monolayer.

Keywords: Ga-based group III-V monolayer, Electronic Structure, Band Engineering, Optical Properties, Density Functional Theory.

1. Introduction

Gallium based compound such as GaN, GaP, GaAs, and GaSb are widely studied group III-V semiconductors have been of great interest for their fundamental physics and their device applications ranging from light emitting diode (LED), laser diode, detectors to solar cell [1, 2, 3, 4, 5, 6, 7, 8]. The GaN and GaAs are well known direct bandgap semiconductor and used in blue and near-infrared LED respectively [4, 9, 10]. Both the semiconductor are also used in solar cell and laser diodes [11, 12, 13]. Furthermore, the GaP and GaSb semiconductor have indirect bandgap and used in green and infrared LED respectively [3, 2]. It is interesting to understand the structural, electronic and other properties under the dimensional restriction of these Ga-based semiconductors.

Since the successful synthesis of graphene in 2004 [14], has been huge attention in the scientific community toward the search of new two-dimensional (2D) materials [15, 16] and exploring their exotic properties. The search for new 2D materials has been getting intense since last decade because of their unique structure and outstanding electronic, optical and transport properties [17, 18, 19, 20] which have potential for application. In addition, the advantage of 2D materials are that it has high specific surface areas and versatile stacking. Based on the literature reports [19, 21, 22, 23], the 2D materials have various subclasses such as graphene-like materials [22, 23, 24, 25] (graphene, h-BN, BCN, etc.), graphene-like 2D buckled materials [26, 27, 28, 29, 30, 31] (silicene, germanene, arsenene, phosphorene, tinene, antimonene, etc.), transition metal dichalcogenides [32, 33, 34](MoS2, WS2, WSe2, etc.), layered semiconductors [35, 36, 37] (GaSe, GaTe, InSe, etc) and the list goes on. Furthermore, a strong interest in group III-V semiconductor nanosheets has recently emerged and these nanosheets have both graphene-like planner and buckled structure[38, 39, 40, 41, 42, 43, 44, 45, 46]. Based on density functional theory (DFT) calculations,[47, 48] the stability and electronic band structure of monolayer honeycomb structure of group III-V binary compound has been studied. Electronic properties under external stimuli such as strain

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