Structural, mechanical and electronic properties of two-dimensional structure of III-arsenide (1 1 1) binary compounds: An ab-initio study

González García, Alvaro; López Pérez, William; Rivera Julio, Jagger; Peteers, F. M.; Mendoza Estrada, Victor Julio; González Hernández, Rafael J.

Abstract

Structural, mechanical and electronic properties of two-dimensional single-layer hexagonal structures in the (1 1 1) crystal plane of IIIAs-ZnS systems (III = B, Ga and In) are studied by first-principles calculations based on density functional theory (DFT). Elastic and phonon dispersion relation display that 2D h-IIIAs systems (III = B, Ga and In) are both mechanical and dynamically stable. Electronic structures analysis show that the semiconducting nature of the 3D-IIIAs compounds is retained by their 2D single layer counterpart. Furthermore, density of states reveals the influence of σ and π bonding in the most stable geometry (planar or buckled) for 2D h-IIIAs systems. Calculations of elastic constants show that the Young's modulus, bulk modulus and shear modulus decrease for 2D h-IIIAs binary compounds as we move down on the group of elements of the periodic table. In addition, as the bond length between the neighboring cation-anion atoms increases, the 2D h-IIIAs binary compounds display less stiffness and more plasticity. Our findings can be used to understand the contribution of the σ and π bonding in the most stable geometry (planar o buckled) for 2D h-IIIAs systems. Structural and electronic properties of h-IIIAs systems as a function of the number of layers have been also studied. It is shown that h-BAs keeps its planar geometry while both h-GAs and h-InAs retained their buckled ones obtained by their single layers. Bilayer h-IIIAs present the same bandgap nature of their counterpart in 3D. As the number of layers increase from 2 to 4, the bandgap width for layered h-IIIAs decreases until they become semimetal or metal. Interestingly, these results are different to those found for layered h-GaN. The results presented in this study for single and few-layer h-IIIAs structures could give some physical insights for further theoretical and experimental studies of 2D h-IIIV-like systems.

Keywords

Arsenide, Density functional theory, Mechanical properties, Two-dimensional single and few-layer hexagonal structures