Diameter dependence of structural and electronically properties of GaAs , GaP and their alloys nanowires.

Dr.Rezek Esteteh
Palestine Technical University – Kadoorie, Tulkarm, Palestine

Abstract

Using ab intio methods, we study the formation energies and the electronic structure of GaAs, GaP and their alloys (GaAsxP1-x) , GaAs and GaP bulk materials has zinc-blende (ZB) structure, but the ground state of nanowires may be either ZB or wurtzite (WZ), depending on energy contribution from their surfaces and edges. The calculated nanowires in this work are cut from the bulk material in the [111] direction and [0001] direction for ZB and WZ structure, respectively. Its found that the WZ formation energy is lower than the ZB formation energy, regardless of the hydrogenation of the surface bonds. In the present work, the energy gap has been calculated with respect to full range of concentration for the alloys.