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First-principles study of GaAs nanowires SEYMUR CAHANGIROV, SALIM CIRACI[1], UNAM-Institute for Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Turkey, CIRACI GROUP TEAM — We present a systematic study of the atomic and electronic structure of GaAs nanowires using first-principles pseudopotential calculations. We consider six different types of nanowires with different diameters all grown along [111] direction and reveal interesting trends between cohesive energy and nanowire type with varying diameters. Generally, the average cohesive energy of nanowires with wurtzite stacking is higher than those with zinc blende stacking for small diameters. We found that most of the bare nanowires considered here are semiconducting and continue to be semiconducting upon the passivation of surface dangling bonds with hydrogen atom. However, the surface states associated with the surface atoms having two dangling bonds in zinc blende stacking occur in the band gap and can decrease the band gap to change the nanowire from semiconducting to metallic state. These nanowires become semiconducting upon hydrogen passivation. Even if the band gap of some nanowires decreases with increasing diameter and hence reveals the quantum confinement effect, generally the band gap variation is rather complex and depends on the type and geometry, diameter, type of relaxation and also whether the dangling bonds of surface atoms are saturated with hydrogen.

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