عنوان مقاله:

First-Principles Calculations of Band Offsets in GaAs/AlAs System

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خلاصه مقاله:

The lattice-matched system (GaAs)n/(AlAs)n superlattice is calculated for two different values of n=۳ and ۶ within ab initio pseudopotential density-functional theory using Quantum Espresso package of program exploiting the ultra-soft atomic pseudopotentials. Their band offsets, which is a well-known and inextricable problem at semiconductor interfaces, have been determined in this paper and were compared with experimental results. Discontinuities of valance and conduction bands were obtained as ۰.۴۶ and ۰.۲۵ eV, respectively. The averaged self-consistent potential across the [۰۰۱] interface in GaAs is about ۰.۰۶۱ eV higher than its value in AlAs. The local density of states for both superlattices was also studied. The effect of different factors e.g. orientation, transitivity, and composition dependence is reported in this study. We found that, in the [۱۱۰] direction of GaAs/AlAs superlattice, the dependence of the band offset on the orientation is negligible. The calculated band gap of is linearly dependent on aluminum content.

کلمات کلیدی:

Nanosemiconductors, density functional theory, Band discontinuities, Pseudopotential, Local density of States