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Abstract

Calculations of structural, electronic and optical properties of (ZnSe)n/(ZnTe)n superlattices

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Abstract:
An investigation into the structural, electronic and optical properties of superlattices (SLs) (ZnSe)n/(ZnTe)n was conducted using first principles calculations based on density functional theory (DFT). The total energies were calculated within the full-potential linear muffin-tin orbital (FP-LMTO) method augmented by a plane-wave basis (PLW), implemented in LmtART 7.0 code. The effects of the approximations to the exchange-correlation energy were treated by the local density approximation (LDA). The ground state properties of binary compounds are determined and compared with the available data. We have seen more carefully and accurately that the different superlattices configurations have no effect on the electronic properties; in particular, we did not observe any dependence between the band gap behavior and the used layers. The optical constants, including the dielectric function □(□), the refractive index n(□) and the reflectivity R(□), are calculated for radiation energies up to 35eV.

Biography:
He is a professor in Université Djillali Liabès de Sidi Bel-Abbès, Algeria

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