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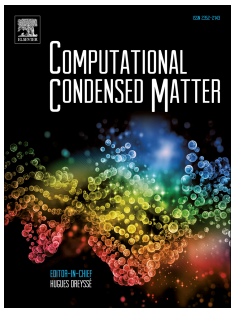

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Results of physical bowing parameters of $ZnSe_xTe_{1-x}$ ternary semiconductor from ab initio study

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Abstract

Based on ab initio calculation, the structural, electronic and optical properties of $ZnSe_xTe_{1-x}$ ternary alloys have been studied using (FP-LAPW) approach. The calculations yielded a lattice parameter and bulk modulus that commonly agree well with experience when they are estimated within the Wu and Cohen-generalized gradient (WC-GGA) scheme. Besides, noticeable improvements in the prediction of electronic and optical properties were found by using the (WC-GGA) plus the modified Becke-Johnson potential parameterization. Strong nonlinear behavior characterizes the evolution of the band gap as a function of the Selenium atomic-composition increment. The positive optical bowing parameter is found in good agreement with the experience. Additionally, the topological analysis of the electronic localization domain indicates a delocalization of charges when the x-concentration to the Se atom is raised. We find that this delocalization is more related to optical properties evolution than to the widening of the energy gap.

Keywords: Bowing parameter, Opto-electronic properties, Structural properties, ternary semiconductor alloys.

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