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Energy gaps and refractive indices of $Pb_{1-x}Ca_xS$

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Abstract

The composition dependence of energy gaps and refractive indices in the $Pb_{1-x}Ca_xS$ alloy system in the rock salt structure are reported within the density functional theory (DFT) by using the full potential linearized augmented plane wave (FP-LAPW) method and the different models in which the effect of composition disorder is involved.

The calculated energy gaps and refractive indices are in good agreement with experiments for the parent compounds. The band structure was calculated by GGA correction. In addition, the EVGGA scheme has been used to obtain more accuracy. The bowing is found to originate from charge-transfer effects, while the volume deformation and the structural relaxation contribute to the bowing parameter with a smaller magnitude. The refractive index exhibits nonlinearity, however, showing different bowing parameters, which arise from the effects of compositional alloy disorder. The same trend is observed for the dielectric constant.

Keywords: FP-LAPW, Electronic structure; Refractive index; $Pb_{1-x}Ca_xS$ alloy