S. Ouendadji, Int J Mater Sci Res. 2017
http://dx.doi.org/10.18689/2638-1559.a1.004

Theoretical Analysis of the Effective Masses, Bonding and Optical Properties of Zinc-Blende Cadmium Chalcogenides

S. Ouendadji
Laboratoire de Physique des Rayonnements, Departement de Physique, Faculty des Sciences, University de Annaba, Algeria

We present the results of density functional calculations to study the electronic structures and the effective masses for II-VI zinc-blende wide band gap semiconductor compounds by computing the curvature of the principal band extrema at the Γ point. We also calculated the optical properties of the technologically important,using the full potential linearized augmented plane wave method within the (GGA) approximation .Our calculations were performed to evaluate the dielectric function (realand imaginary parts),and the loss function of the II–VI semiconductors. Also the refractive index and the extinction coefficient are all studied. Detailed comparisions are made with published experimental and theoretical data and show generally good agreement. The present results regarding the studied quantities are predictions and may serve as reference for experimental work.

Keywords: FP-LAPW, DFT, cadmium chalcogenides, effective masses, optical properties