

First and second harmonic generation of the XAl_2Se_4 ($X=Zn,Cd,Hg$) defect chalcopyrite compounds

Abstract

The chemical bonding of the $ZnAl_2Se_4$, $CdAl_2Se_4$ and $HgAl_2Se_4$ defect chalcopyrites has been studied in the framework of the quantum theory of atoms in molecules (AIM). The GW quasi-particle approximation is used to correct the DFT-underestimation of energy gap, and as a consequence the linear and nonlinear optical properties are significantly enhanced. The second harmonic generation (SHG) displays certain dependence with the ionicity degree decrease through the dependency of the SHG on the band gap. The occurrence of the AIM saddle point is characterized and some clarifying features in relationship with the density topology are exposed, which enable to understand the relation with the second harmonic generation effect.