

Ab initio study of structural, elastic, electronic and optical properties of spinel SnMg_2O_4

M. Reffas, A. Bouhemadou, R. Khenata T. Ouahrani, S. Bin-Omran

Abstract :

Ab initio study of structural, elastic, electronic and optical properties of the cubic spinel oxide SnMg_2O_4 has been reported using the pseudo-potential plane-wave method within the local density approximation and the gradient generalized approximation for the exchange and correlation potential. Computed lattice constant and internal free parameters are in good agreement with the available experimental results. The elastic constants and their pressure dependence are predicted using the static finite strain technique. A linear pressure dependence of the elastic stiffnesses is found. A set of isotropic elastic parameters and related properties, namely bulk and shear moduli, Young's modulus, Poisson's ratio, Lamé's coefficients, average sound velocity and Debye temperature are numerically estimated in the frame-work of the Voigt–Reuss–Hill approximation for SnMg_2O_4 polycrystalline. Band structure shows that SnMg_2O_4 has a direct band gap (Γ – Γ), which increases with increase in pressure. Density of states and Mulliken population analysis show that the Mg–O bond is typically covalent due to the O-2p and Mg-2p states hybridizations. In order to understand the optical properties of SnMg_2O_4 , the dielectric function, optical reflectivity, refractive index, extinction coefficient and electron energy loss function are calculated for radiation up to 40 eV. The pressure dependence of the zero-frequency limit of the real part of the dielectric function $\epsilon_1(0)$ and of the refractive index $n(0)$ has been investigated. This is the first quantitative theoretical prediction of the elastic, electronic and optical properties of the SnMg_2O_4 compound, and it still awaits experimental confirmation.

Keywords : Semiconductor; Ab initio; Elastic constants; Electronic properties; Optical properties; Chemical bonding.

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