World Academy of Science, Engineering and Technology
International Journal of Mechanical and Materials Engineering
Vol:9, No:01, 2015

Ab Initio Calculation of Fundamental Properties of CaxMg1-xA (a = Se and Te) Alloys in the Rock-Salt Structure

Authors : M. A. Ghebouli, H. Choutri, B. Ghebouli , M. Fatmi, L. Louail

Abstract : We employed the density-functional perturbation theory (DFPT) within the generalized gradient approximation (GGA), the local density approximation (LDA) and the virtual-crystal approximation (VCA) to study the effect of composition on the structure, stability, energy gaps, electron effective mass, the dynamic effective charge, optical and acoustical phonon frequencies and static and high dielectric constants of the rock-salt CaxMg1-xSe and CaxMg1-xTe alloys. The computed equilibrium lattice constant and bulk modulus show an important deviation from the linear concentration. From the Voigt-Reuss-Hill approximation, CaxMg1-xSe and CaxMg1-xTe present lower stiffness and lateral expansion. For Ca content ranging between 0.25-0.75, the elastic constants, energy gaps, electron effective mass and dynamic effective charge are predictions. The elastic constants and computed phonon dispersion curves indicate that these alloys are mechanically stable.

Keywords : CaxMg1-xSe, CaxMg1-xTe, band structure, phonon
Conference Title : ICMME 2015 : International Conference on Mechanical and Materials Engineering
Conference Location : Jeddah, Saudi Arabia
Conference Dates : January 26-27, 2015

Open Science Index, Mechanical and Materials Engineering Vol:9, No:01, 2015 publications.waset.org/abstracts/13861.pdf