Band structural, structural properties and stability of $Sr_xCa_{1-x}Te$ ternary alloy.

M. Labidi[1,2], S. Labidi[1], K. Klaa[1], and R. Bensalem[1]

1Ecole Préparatoire aux Sciences et Techniques, B.P.218 Annaba 23000 Cité safsaf

2Laboratoire des Nanomatériaux, Corrosion et Traitements de Surfaces, Département de Physique, Faculté des Sciences, Université Badji Mokhtar, B.P 12, 23000 Annaba, Algerie

Email: labidimalika4@yahoo.fr

ab initio calculations were carried out for the structural, electronic, and thermodynamic properties of $Sr_xCa_{1-x}Te$ ternary alloy. The full potential linearized augmented plane wave (FP-LAPW) method was employed within density functional theory (DFT). For the electronic properties**,** in addition to the GGA correction, Engel-Vosko's (EV-GGA) formalism was also applied. The effect of composition on lattice constant, bulk modulus and band gap was investigated. Deviations of the lattice constant from Vegard's law and the bulk modulus from linear concentration dependence (LCD) were observed for the alloy. The microscopic origins of the gap bowing were explained by using the approach of Zunger and co-workers. Moreover, the thermodynamic stability of this alloy was investigated by calculating the excess enthalpy of mixing. ΔH_m as well as the phase diagram.

References

[1] S. labidi, M. Boudjendlia, M. labidi and R. Bensalem, Chin. J. Phys. **52**, 1081 (2014)