Structural Properties of Scandium Chalcogenides via First Principle Calculations

Pavas, NehaMunjal*, Agnibha Das Majumdar, Uma Kamboj, Ankit Kumar
Department of Physics Lovely Professional University Phagwara
Corresponding Author email:- nehamunjaphy@gmail.com

Abstract. Structural properties of scandium chalcogenides, which used in the production of high-performance magnets, rechargeable batteries, alloys, catalysts, electronics and glasses, have investigated in NaCl (B1) structure using first principle calculations. Exchange correlation scheme of PBE and Becke has been used. The lattice constant and bulk modulus have found using linear combination of atomic orbital method within CRYSTAL06 code. The lattice constant and bulk modulus of ScS, ScSe, and ScTe are reported. The results are found to be compatible with the available experimental and theoretical data of the samples.

Keywords: - Density functional theory, Scandium chalcogenides, LCAO, First principle calculation.

1. Introduction

Over the last decade ab-initio methods that are used to solve the Schrodinger equations and now have the most powerful measurements to investigate enormous numbers of physical and chemical properties for solids. They are also a preferred choice for predicting a new materials and sometime replacing the experiments that are very expensive or even impossible in the laboratory [1-10].

Scandium is a group III element and has rare earth metal properties whereas chalcogenides belong to group VI of the periodic table and known to have excellent properties. Because of the effect of strong correlation in the f-shell electrons in them significant changes in their chemical and physical properties can be induced with the change in pressure [11]. The demand of rare earth metals have been increased over the years due to their use particularly in low carbon technologies. They are also used in the production of high-performance magnets, rechargeable batteries, alloys, catalysts, electronics and glasses[12]. These materials shows phase transition under the high pressure and have good application in non-linear optics. Limited research has been done involving structural properties of rare earth compounds and chalcogenides with experimental as well as theoretical methods.

To best of our knowledge the structural properties of scandium chalcogentides i.e. ScS, ScSe, and ScTe are relatively least studied. Purvee Bhardwaj et.al.[2] have reported electronic and pressure induced structural properties of ScS in phase transition from NaCl to CsCl using first principle calculation and TB-LMTO method has been used to calculate the electronic band structure. A Maachou et.al.[3] has been reported the structural abilities, high pressure structural phase transition from NaCl i.e. B1 to CsCl i.e B2, elastic constant and thermal properties of ScS, and
ScSe using FP-APW+LO method within GGA approximation exchange correlation functional. Electronic States of ScTe Molecule has been determined using ab-initio calculation i.e. Complete active space self-consistant field (CASSCF) and multireference internally contracted configuration interaction (MRCI) methods by Rawad Halabi, Mahmoud Korek[4]. Deepika Shrivastava[5] has been reported the structural phase transition from B1 to B2, electronic and bonding properties, phonon dispersion and superconducting properties with transition temperatures of scandium mono-chalcogenides (ScS, and ScSe) using QUANTUM ESPRESSO code within local density approximation(LDA) scheme of Perdew-Wang.

A A Ahmad et.al.[1] has found the structural parameters, structural phase transition from NaCl-type (B1) to CsCl-type (B2) and ZnS-type (B3) under high pressure, optical parameters, electronic and thermal properties of the scandium chalcogenides i.e. ScX (X=S,Se,Te) using FP-LAPW method in Perdew–Burke–Ernzerh approach of generalized gradient approximation (GGA) within DFT. Jeremy K. Burdett et. al. [6] has been explored the electronic driving force in scandium chalcogenides via first principle linear muffin-tin orbital (LMTO) calculations. LucjanPawlak and MarekDuczmal [7] reported the structural and magnetic properties of scandium chalcogenidesspinels with iron FeSc$_2$ S$_4$, and manganese MnSc$_2$S$_4$,MnSc$_2$Se$_4$ crystalline.

Due to very few research have been done on scandium chalcogenidesScX (X= S,Se,Te). In this paper we present the structural properties of ScX(X=S,Se,Te) in NaCl (B1) rocksalt structure. Here structural properties have studied using the parameters like bulk modulus and lattice constant of the crystals of the compound. The result thus obtain are found to be compatible when compared with the available work on the samples.

2. Computational Method

In this present work, the structural properties of scandium chalcogenides have studied in rocksalt structure via Linear combination of atomic orbitals first principle technique using exchange correlation scheme of PBE and Becke within CRYSTAL06 code. The basis set for Sc, S, Se and Te have taken from CRYSTAL coding [8]. To calculate the structural properties of scandium chalcogenides the information from the basis set have optimized for each component for their minimum energy with respect to the volume. A mesh of 165 special k-points of Brillouin zone that are irreducible with sufficient tolerances was taken for binary compounds. This self-consistency was achieved within 10 cycles and 55% mixture of successive cycles is taken into account. The lattice constant and bulk modulus found for ScS, ScSe, and ScTe within NaCl (B1) structure.

3. Result and Discussion

The structural properties calculated by total energy with respect to volume of permite cell of crystal. Fig.1 and Fig.2.Show the energy versus volume curve for binary compounds i.e. ScX(X=S,Se) in NaCl(B1) structure. The lattice constant and bulk modulus were calculated as a function of volume and fitted in BrichMrughman equation of state.The doted curve in these figures represents the calculated energies by DFT and line curve represent the fitted energy to
universal Mrughman’s equation of state. The results are expressed in Table 1. and the results which we obtained are good agreement with available experimental and theoretical data.

| Compound | Lattice constant | Bulk modulus |
|----------|------------------|--------------|
| Present  | Exp. other work  | Present Exp. Other work |
| ScS      | 5.19 5.199[9]5.21[3] | 113 103.11[10] 115.33[3] |
| ScSe     | 5.4 5.398[9]5.385[3] | 93.25 --- 95.92[3] |
| ScTe     | 5.815 --- --- | 60 --- 69.62[1] |

Table 1: Present and previously calculated lattice constant (a) and bulk modulus (B0) of binary compounds

4. Conclusion

We have investigated the structural properties of scandium chalcogenides in rocksalt structure by using linear combination of atomic orbitals under the density functional theory. The reported calculation provides the results as bulk modulus and lattice constant via first principle. The obtained values for the bulk modulus and lattice constant of ScS, ScSe, ScTe are in the good agreement with the available experimental and theoretical data.

5. References

[1] Tripathi, S.N., Srivastava, V., Pawar, H. et al. First-principles investigation of structural, electronic and mechanical properties of some Dysprosium chalcogenides, DyX (X = S, Se and Te). Indian J Phys (2019). https://doi.org/10.1007/s12648-019-01564-x
[2] Tripathi, S.N., Srivastava, V. & Sanyal, S.P. First Principle Mechanical and Thermodynamic Properties of Some TbX (X = S, Se) Compounds. J Supercond Nov Magn 32, 2931–2938 (2019). https://doi.org/10.1007/s10948-019-5052-1

[3] A. Maachou, H. Aboura, B. Amrani, R. Khenata, S. Bin Omran, Dinesh Varshney, “Structural stabilities, elastic and thermodynamic properties of scandium chalcogenides via first principles calculation”, Computational Materials Science 50 (2011) 3123-3130.

[4] R. Halabi, M. Korek “Ab Initio Calculation of the Electronic States of ScTe Molecule below 19,500 cm−1” Journal of Modern Physics, 2016, 7, 106-113.

[5] D. Shrivastava, S.P. Sanyal “Structural Stability of scandium monochalcogenidesScS and ScSe under pressure and superconductivity: A first principles study” Computational Condensed Matter 21(2019) e00418.

[6] Jeremy K. Burdett, and Slavi C. Sevov “Origin of Nonstoichiometry in ScS and Other Early Transition Metal Chalcogenides” J. Phys. Chem. 1995, 99, 2696-2700.

[7] L. Pawlak and M.Duczmal “Magnetic and Structural properties of scandium chalcogenidespinels with Iron and Manganese” J. Phys. Chem. 1993.07:1020-1022.

[8] www.tcm.phy.cam.ac.uk. (accessed on 23 april, 2019).

[9] A. Svane, P. Strange, W.M. Temmerman, Z. Szotek, H. Winter, L. Petit, Phys. Stat. Solids B 229 (2001) 1459.

[10] Suhithi. M. Peiris, Michael T. Green, Dion L. Heinz, Jeremy K. Burdett, “Experimental and Theoretical Studies of ScS under Pressure” Inorg. Chem. 35 (1996) 6933.

[11] A A Ahmad, S Mahmoud, B Alshafaay, R Halabi and F E Haj Hassan “Fundamental properties of scandium chalcogenides and their alloys: DFT study” Indian J Phys (2019) 93(9):1129–1135.

[12] P.Bhardwaj and S. Singh, “Computational Electronic study of ScS”, Procedia Computer Science 57 (2015), 160 – 167.