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# Band structure and optical properties of ThSe

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## ABSTRACT

*The electronic band structures and optical properties of ThSe are studied by the first principal calculations based on density functional theory (DFT) based linear muffin-tin orbital method (LMTO) within local density approximation (LDA). These studies include the theoretical calculations of electronic dispersion curves, Density of states, band gap, DOS, Fermi energy, frequency dependent imaginary part of the dielectric functions and the optical conductivity etc.. The calculated parameters has been explained and compared with available experimental results. The results are found to be in agreement with earlier available observed results.*

***Keywords: Density functional theory (DFT), linear muffin tin orbital method (LMTO), band structure, density of state, optical conductivity.***

## I. INTRODUCTION

The thorium chalcogenides compounds have been investigated experimentally and theoretically in the last decades because of their interesting electronic, optical and magnetic properties [1-6]. Since recently, we have also carried out theoretical calculations on the series of similar kind of rare earth compounds; it is tempting to take up the whole series from theoretical point of view. And so continuing work on this series, present paper reports ab-initio scalar-relativistic electronic band structures calculations and optical properties for ThSe which have been carried out using density functional theory based linear muffin tin orbital method with in atomic sphere approximation. These calculations of electronic band structures and optical properties for ThSe include band structure, density of state, Fermi energy, frequency dependent imaginary part of the dielectric functions and the optical conductivity etc..

## II. METHOD OF COMPUTATION

For the band structure calculations at ambient & high pressure have been carried out density functional theory based TB-LMTO method with in atomic sphere approximation (ASA). This is the exact transformation of Anderson LMTO method [7] and it combines the desirable features of fixed basis method as well as partial wave method. All the relativistic contributions except spin-orbit couplings are included. The exchange-correlation potential with in local density approximation (LDA) is calculated using formalism of Von-Barth and Hedin [8]. To optimize the calculations, sphere radii are chosen in such a way that the difference in potential at the sphere boundaries is minimum. The self-consistent band calculations are carried out for 512 k-points in the entire Brillouin Zone. Combined correction terms were also included, which account for the non-spherical shape of the atomic cells and the truncation of higher partial wave ($l > 3$) inside the sphere, so that the error in the LMTO method is minimized. The scalar relativistic wave equation is solved in which the most important relativistic corrections namely the Darwin's corrections; mass velocity terms and higher order corrections are included. The eigenvalues are converged up to 10 $^{-5}$ Ryd. The DOS is calculated by using tetrahedron method. For the calculation of the optical properties, the interband contribution to dielectric function is carried out using LMTO-ASA method as detail given in the relevant section.

## III. RESULTS AND DISCUSSIONS

The ThSe compound crystallize in the NaCl type structure at ambient (unlike to ThTe which crystallize in CsCl type crystal structure at ambient). To find the equilibrium lattice parameters, the total energies were computed by changing the cell volume and then these energies are fitted with Birch equation of state to obtain P-V relation. Th and Se atoms occupy the positions (0, 0, 0) and (.5, .5, .5) respectively. Since, at ambient just like ThS, ThSe is also not in close packed structure, we have introduced equivalent empty sphere at positions (.25, .25, .25) and (.75, .75, .75) in such a way that they do not break the symmetry. The valence configurations for Th, and Se are chosen (7s, 6p, 6d, 5f) and (4s, 4p, 4d) respectively to represent the basis set. Using equilibrium lattice parameters, the band structure and total DOS have been calculated and plotted.

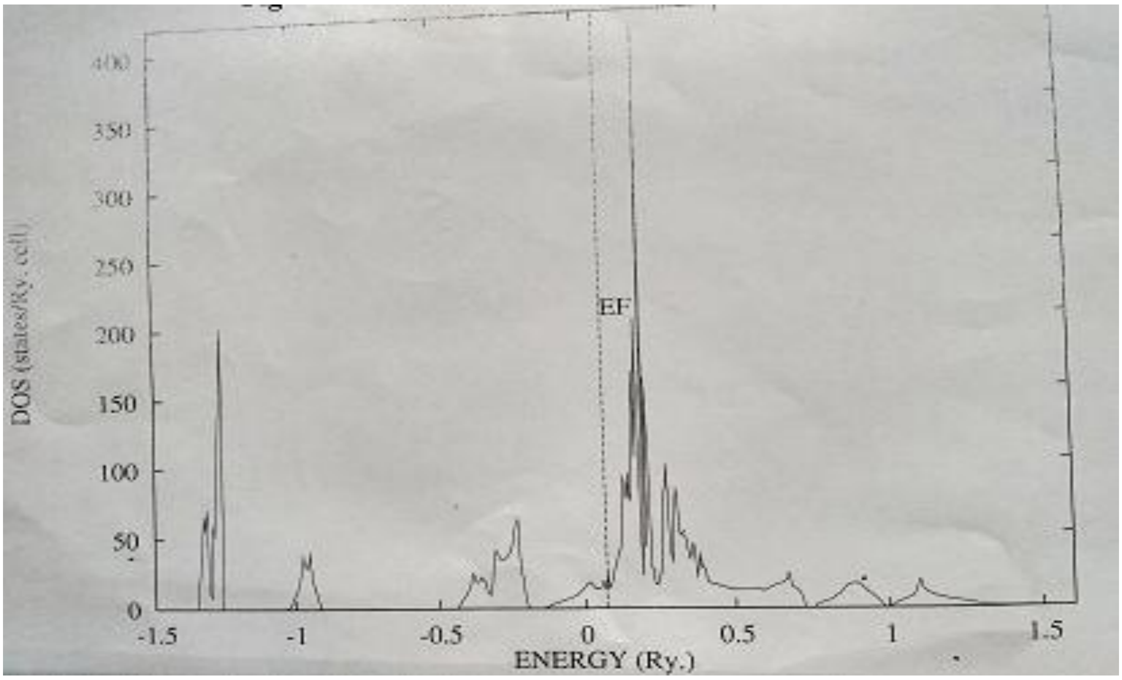

**Fig. 1: The total density of state (DOS) for ThSe in NaCl phase**

The overall profiles of bands structure and DOS are found to be similar to those of other binary rare earth compounds. Fermi energy is shown by the dotted line. The contributions of different bands/states indicated in plots as may be seen in Fig.1 which shows that the peaks in lowest energy region are due to 6p states of thorium and the peaks in next higher energy region arises from 4s states of Se in ThSe case. While the subsequent higher energy peaks in valence region just below $E_F$ are predominantly due to 7s states of thorium and 4p states of Se in ThSe case. The DOS at fermi energy shows the metallic nature of compound. The DOS at higher energy region in conduction band (just above $E_F$) is mainly due to 6d states of Th and 4d states of Se in ThSe case.

Further, to calculate optical properties, the interband contribution to dielectric function is calculated by well-known LMTO-ASA methods. The optical matrix elements are explicitly calculated and included in frequency dependent imaginary part of the dielectric function. We have calculated dielectric function by expanding the wave function to include the s, p, d and f states because this will make a better representation of the wave function and hence more accurate result. Thus, the calculations of frequency dependent imaginary part of the dielectric functions for this material have been calculated summing all possible transitions from occupied to unoccupied states, taking the appropriate transit in matrix element in account. Finally, the complex optical conductivity Re[σ(ω)] is calculated using

$$\sigma(\omega) = -i\omega\varepsilon(\omega)/4\pi$$

where Im [(ω)] is dielectric function. Using this definition, the real part of the optical conductivity is essentially the imaginary part of the dielectric function scaled with the transition energy. The difference in the spectral behavior of the optical conductivity and the dielectric function are due to multiplication with photon energy. The calculated optical conductivity of B1 phase of ThSe is plotted in Fig. 2 which shows that the major peaks at 0.04, .1, 0.30, 0.64, 0.75, 0.86, and 0.92 Ry. After going through a peak it can be seen that calculated optical conductivity increases with increase in energy.

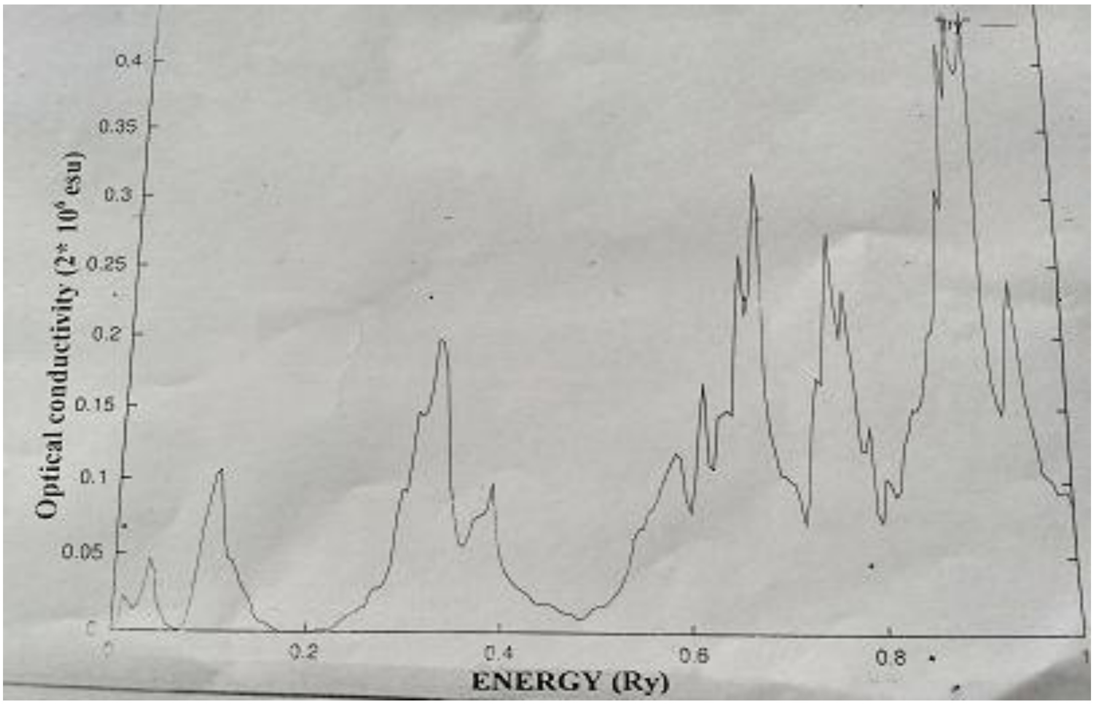

**Fig. 2: The calculated optical conductivity of B2 phase of ThSe**

## IV. CONCLUSIONS

The detailed theoretical electronic band structure properties of ThSe has been reported. These studies have been carried out using density function theory (DFT), band methods namely tight binding linear muffin tin orbital method TB (LMTO) within LDA. Further, optical properties of ThSe have been calculated using the LMTO-ASA method. The optical matrix elements are explicitly calculated and included in frequency dependent imaginary part of the dielectric function. We have calculated dielectric function by expanding the wave function to include the s, p, d and f states because this will make a better representation of the wave function and hence more accurate result which further used to calculate the optical conductivity. The calculated optical conductivity has been plotted and discussed in detail to find the origin of the peaks in optical conductivity profile.

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