International Journal of Emerging Technology and Advanced Engineering
Website: www.ijetae.com (ISSN 2250-2459, ISO 9001:2008 Certified Journal, Volume 7, Issue 6, June 2017)

Electronic and Optical properties of Zinc Chalcogenides – an Ab-initio Study

Lavanya Kunduru[1], S.C.R.Roshan[2]
[1,2]*Asst.Professor, RGUKT, Basar, Telangana, India*

***Abstract*— Zinc Chalcogenides have attracted a lot of attention in recent past as these have a wide band gap and have optical properties which make these very promising for fabrication in display devices. The Current work presents a study on the optical and electronic properties of Zinc Chalcogenides using density functional theoretical evaluations performed using the local density approximation (LDA) formalism and also the PBE generalized gradient formalism for the exchange-correlation functional. The obtained band structure calculations clearly indicate direct band gap nature of Zinc Chalcogenides. Refractive index for these are evaluated and the importance of these compounds as anti reflection coatings is established from reflectivity calculations.**

***Keywords*—Electronic properties, Structural properties, Material Simulations, Density Functional Theory.**

I. INTRODUCTION

ZnX type of semiconductors have attracted good attention recently due to their wide band gap which makes these material technologically very important in the fabrication of devices such as displays. The optical properties of these materials and in particular of ZnS make it a very good anti reflection coating which can be used in hetero-junction solar cells(1).

The paper is presented as follows. Section I contains the background material that pertains to our study, In Section II, we make a mention of the methodology that we have followed, In Section III, we present and discuss our results.

ZnS crystallizes in Zinc Blende structure with Space group F-43m. The unit cell consists of four formula units.

There are S^{2-} ions at the positions

0,0,0; 1/2,1/2,0; 1/2,0,1/2; and 0,1/2,1/2.

There are Zn^{2+} ions at the positions

1/4,1/4,1/4; 1/4,3/4,3/4; 3/4,1/4,3/4; and 3/4,3/4,1/4.

The Structure of ZnS can be seen from the figure below.

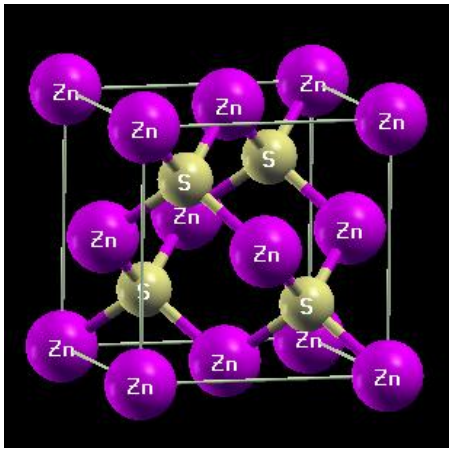

Fig.1 ZnS structure (as seen in XCRYSDEN)

II. METHODOLOGY

We had made use the QUANTUM ESPRESSO (2) which is a computer package for studying the electronic structure and optimization using the molecular dynamics simulation.

The Quantum ESPRESSO contains the packages PWscf (Plane-Wave Self-Consistent Field), for the calculation of electronic-structure properties within the formalism of Density-Functional Theory (DFT), using a Plane-Wave (PW) basis set and pseudopotentials.

We have also used XCrySDen (3) which is a crystalline and molecular-structure visualisation program. The name of the program is an acronym for for Crystalline Structures and Densities and X since this runs under the X-Window environment. It provides a display of iso-surfaces and contours, which can be superposed on crystalline structures interactively rotated and manipulated. The Structure of ZnS can be seen in Fig(1).

International Journal of Emerging Technology and Advanced Engineering
Website: www.ijetae.com (ISSN 2250-2459, ISO 9001:2008 Certified Journal, Volume 7, Issue 6, June 2017)

III. Results And Discussion

We first take an overview of the band structure obtained for ZnS from first principle calculations.

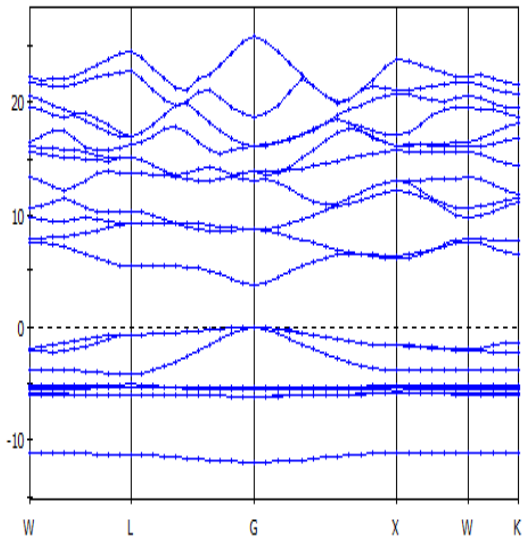

Fig.2 Band Structure of ZnS

Fig.2 shows the obtained Band structure of ZnS, From the Band Structure, since the maximum of the Valence band and the minimum of the conduction band are along the same high symmetrical direction G, The nature of ZnS semiconductor is a Direct band gap semiconductor.

The value of the Band gap is calculated to be 3.74 eV.

The Refractive index is also plotted for different incident frequencies and the extinction coefficient (k) is observed for different incident energies and studied as shown in Fig (3).

The real (obtained from the imaginary part by using Kramers-Kronig relation) and imaginary parts of dielectric functions are used to calculate refractive index 'n' defined as,

$$n = \frac{\sqrt{\left(\varepsilon_1 + \sqrt{\left(\varepsilon_1^2 + \varepsilon_2^2\right)}\right)}}{\sqrt{2}}$$

and

$$k = \frac{\sqrt{\left(-\varepsilon_1 + \sqrt{\left(\varepsilon_1^2 + \varepsilon_2^2\right)}\right)}}{\sqrt{2}}$$

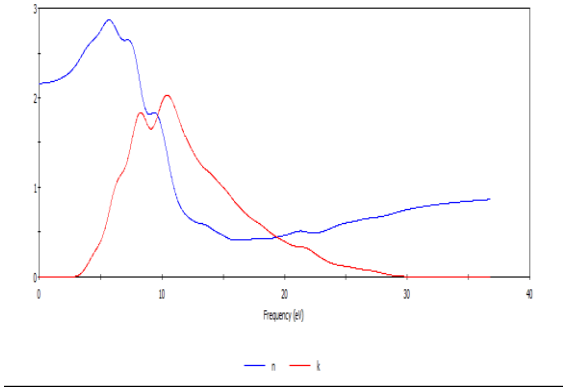

Fig-3 Refractive Index of ZnS

The Blue line shows the variation of refractive index with incident frequencies and the Red line shows variation of extinction coefficient.

For the visible region, the refractive index is measured to be around 2.4.

The Reflectivity of ZnS is measured and shown in Fig-4.

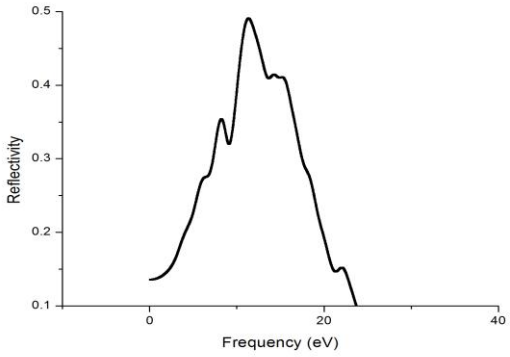

Fig-4 Reflectivity of ZnS

From the reflectivity measurement, we conclude that for the visible region, i.e. around 3-4 eV, the Reflectivity is very low, around 0.15, So, ZnS can be used as a prospective anti-reflection coating for solar cells.

The absorption is plotted in FIG-5 and this shows that the absorption is pretty high in the Ultraviolet region. The relation between absorbance, reflectance and Transmittance, R+T+A =1 holds good all the time.

International Journal of Emerging Technology and Advanced Engineering
Website: www.ijetae.com (ISSN 2250-2459, ISO 9001:2008 Certified Journal, Volume 7, Issue 6, June 2017)

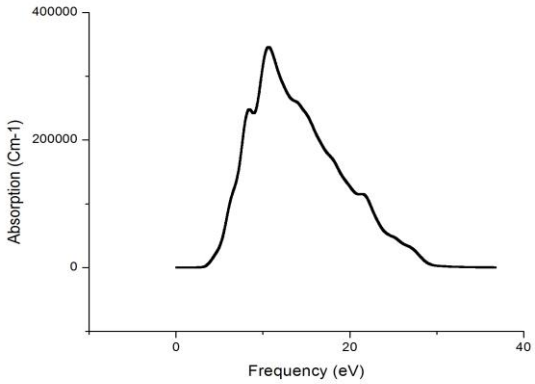

Fig-5 Absorption of ZnS

IV. CONCLUSIONS

We have performed first principle studies of ZnS and we have observed that ZnS is a direct band gap semiconductor with a band gap of 3.74 eV.

From the calculations done for the Optical Properties for ZnS, the Reflectivity is very less in the visible region making ZnS a promising material to be used as an anti reflection coating in hetero-junction solar cells.

Acknowledgements

We would like to thank RGUKT, Basar for the computational Facilities.

REFERENCES

[1] A.S.Verma, Phys.Stat.Sol. B 246, 345-353 (2009).

[2] P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009); URL http://www.quantum-espresso.org.

[3] Kokalj: J. Mol. Graphics Modelling, 1999, Vol. 17, 176--179. Code available from http://www.xcrysden.org.