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ChemTech

International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN : 0974-4290
Vol.6, No.3, pp 1736-1738, May-June 2014

ICMCT-2014 [10th – 12th March 2014]
International Conference on Materials and Characterization Techniques

Electronic and thermal properties of metallic CuS_2 Compound with pyrite structure: An *ab-initio* study

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Abstract: A systematic study of thermal properties such as the Debye temperature and electronic specific heat co-efficient have been carried out using the results of *ab-initio* studies of the electronic band structure and related characteristics, for the CuS_2 compound in two different phases, (cubic and orthorhombic phases) under pressure using tight–binding linear muffin-tin orbital method (TB-LMTO) within local density approximation (LDA). Apart from the electronic band structure and structural stability, the density of states (DOS) and Fermi energies (E_F) are also calculated for various pressures. The calculated results are found to be in good agreement with the available results in literature.
Key words: Fermi energy, Density of states, Specific heat capacity and Debye temperature.

Introduction and Computational details

Bither[1] reported for CuS_2 a metallic behavior associated with a temperature independent susceptibility and superconductivity(T_c<2.4K).A lot of experimental work is available for CuS_2, regarding the high-pressure structural phase transition [2].Computations have been carried outto study the structural phase transitions and the ground state properties of CuS_2 using the tight–binding linear muffin-tin orbital method. Space group of CuS_2 is *Pa-3* (205) in cubic structure and *Pnnm* (58) in orthorhombic structure.The band structure calculations for CuS_2 compound in both the structures have been carried out within the atomic sphere approximation [3]. The density of states is calculated by the method of tetrahedron [4]. The ground-state properties were calculated for the lattice parameters that correspond to the minimum of the electronictotal energy.

Result and Discussion

All the electronic properties such as the density of states and energy bands of the cubic and the orthorhombic phases of CuS_2 were computed for the equilibrium lattice parameters. The plots of total energy as a function of cell volume for the cubic and the orthorhombic phases of $CuS_2$are shown in Fig.1. There occurs a structural phase transition from the cubic phase to the orthorhombic phase. We found that in the thermo dynamical condition, thecubic phase is more stable. A comparison of the calculated and experimental [2, 5] lattice parameters of both the phases of CuS_2, presented in Table.1 show a very good agreement between them.

The electronic bandstructure of the cubic phase of CuS_2 along the high symmetry directions of the Brillouin zone is displayed in Fig.2. From the bandstructure clearly evident in the phase of the material that the p- bands dominate in their conduction. The Fermi energies of the cubic and the orthorhombic phases of CuS_2 are 0.6138Ry and 0.5762Ry, respectively.The DOS of the cubic and the orthorhombic phases of CuS_2 are presented in Fig.3. The high DOS around E_F is evidently due to the strong pile up of the p- and d- states in both the phases of CuS_2, and accounts for the structural stability. The calculated and experimental values [6] of Θ_D and γ are presented in Table 1. The Debye temperature (Θ_D) [7] and the electronic specific heat coefficient (γ) [8] are important parameters that are closely related to the thermal properties of materials.

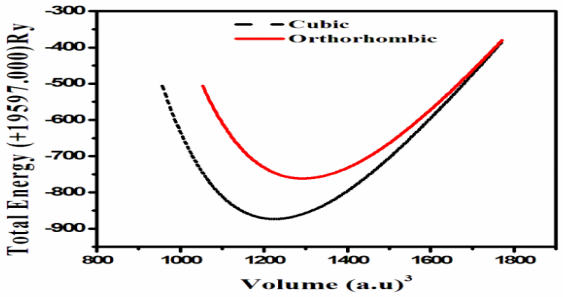

Figure 1. Total energy Vs volume for CuS_2 in various phases.

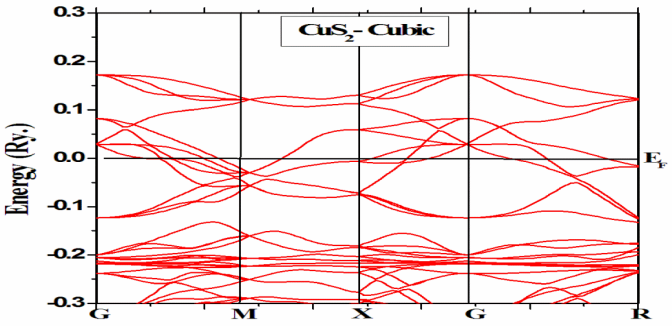

Figure 2. Band structure of CuS_2 along symmetry direction in Cubic phase.

Table 1: Lattice constant (Å), Bulk modulii(B_0), Debye temperature (Θ_D) and Electronic specific heat coefficient (γ) for CuS_2

CuS_2	Lattice constant Å		B_0 (GPa)	Θ_D		γ	
	Present	Expt.		Present	Expt.	Present	Expt.
Cubic	a=5.672	a=5.790 [1,2]	118.36	292	280 [6]	4.60	6.18 [6]
Orthorhombic	a=4.632 b=5.774 c=3.513	a=4.651[5] b=5.793 c=3.532	115.38	308	-	4.75	-

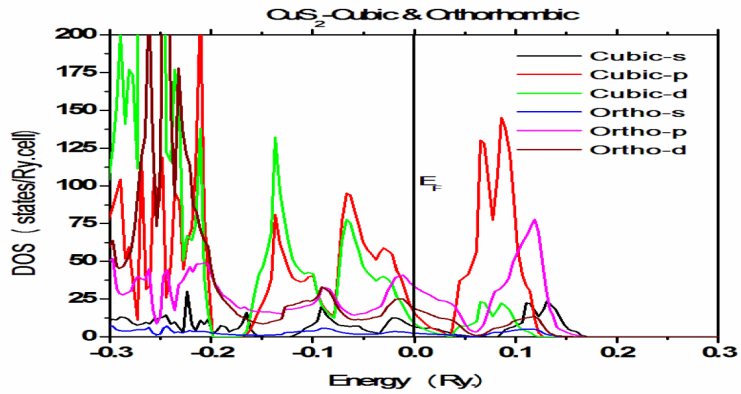

Figure 3. Density of states at Fermi level for CuS_2 in Cubic and Orthorhombic phases

Conclusions

The electronic bandstructure studies of CuS_2compound in the cubic and the orthorhombic phases are carried out using the self-consistent tight binding linear muffin-tin orbital method. From the total energy calculations it can be seen that the cubic phase is more stable phase in the thermo dynamical condition.The density of states at the Fermi energy is found to be strongly influenced by the p- states of sulphur, and, it is also evident in the band structure results. The calculated results are observed to be in good agreement with the available results existing in the literature. Estimation of the Debye temperature (Θ_D) and the electronic specific heat coefficient (γ) have also been made for both thecubic and the orthorhombic phase.

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