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Research Article

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Computational study of structural and electronic property of the predicted compound-Os2TiBi

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ABSTRACT

The nature of chemical bonding between the atoms in the compound Os2TiBi is studied by applying the Wien2k code – A Full Potential Linear Augmented Plane Wave Method. The electron density plots, Density of States histograms and band structure are plotted for the compound Os2TiBi. From this study we report that Os2TiBi exhibits metallic nature and there exists bonding between Os and Bi. It is of nonmagnetic type.

Key words: Heusler alloys, Electronic structure, electron density,

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INTRODUCTION

During last century, Heusler alloys (1) have attracted many researchers (2, 3, 4) due to its diverse electronic properties. Many researchers have been working on Heusler alloys to look for the spintronic (5, 6) topological insulators and also for thermoelectric materials (7,8). Many Heusler compounds have been synthesized and many have been predicted. To the best of our knowledge, band structure study of the compound Os2TiBi has not yet been reported earlier in the literature. Heusler compounds take L21 structure and are of two types full Heusler and half Heusler. The full Heusler type has space group of 225, four inter penetrating FCC lattices with the chemical formula X2YZ. X and Y atoms are transition metals and Z atoms are mainly from III, IV and V group of elements of periodic table. The X atoms occupy (¼, ¼ ,1/4) and (¾,3/4,3/4,), Y atoms at (½, ½,1/2) and Z atoms at (0,0,0).

EXPERIMENTAL SECTION

Computational details:
A computational code wien2k (9) is applied for the present study . An augmented plane wave plus Local orbitals program for calculating crystal property as implemented in the code was used for electron density and band structure calculations of the compound Os_2TiBi. PBE- GGA(Perdew-BurKe-Ernzerhof96) has been used for exchange correlation potential. The lattice constant as predicted by (10) was used. The Muffin tin radius of 2.55a.u, 2.0 a.u, 2.6a.u, was used for Os, Ti and Bi respectively. The number of k point given was 1000 but only 47 irreducible points were generated. The cutoff parameter of Rk_{max}=7,l=10, G_{max} =12a.u $^{-1}$. The crystal structure was given in the figure-1 Xcrysden (11)was used to plot the structure.

RESULTS AND DISCUSSION

The electron density plot of the compound was given in the figure (2) for contour plot was drawn for the grid lines

200, plane323. From the plot we understand that the bonding exits between Bi And Os. Bi atoms have spherical orbitals as its atomic number is high called σ orbitals. We can see many orbits around this element in the contour plot. Bi atom is surrounded by four Os atoms called л orbitals (12). The orbits surrounding Os is also Spherical called * orbitals. Orbitals around Ti is not spherical and is isolated from other two.

Figure 1 structure of Os2TiBi

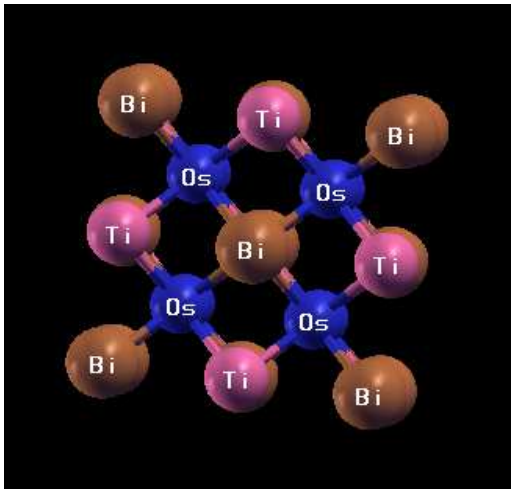
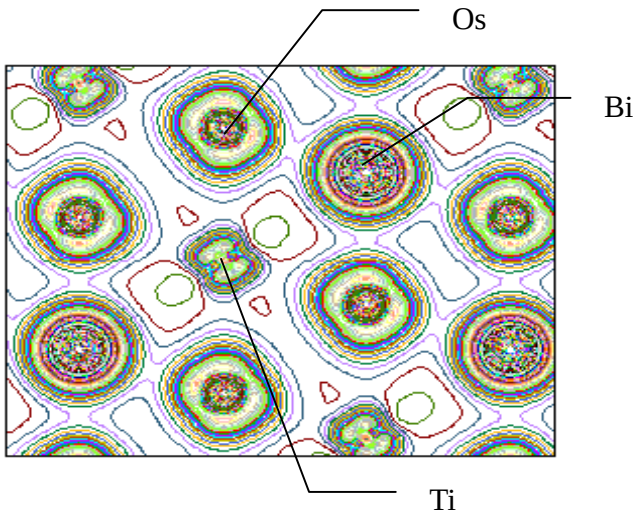


Figure 2 contour plot



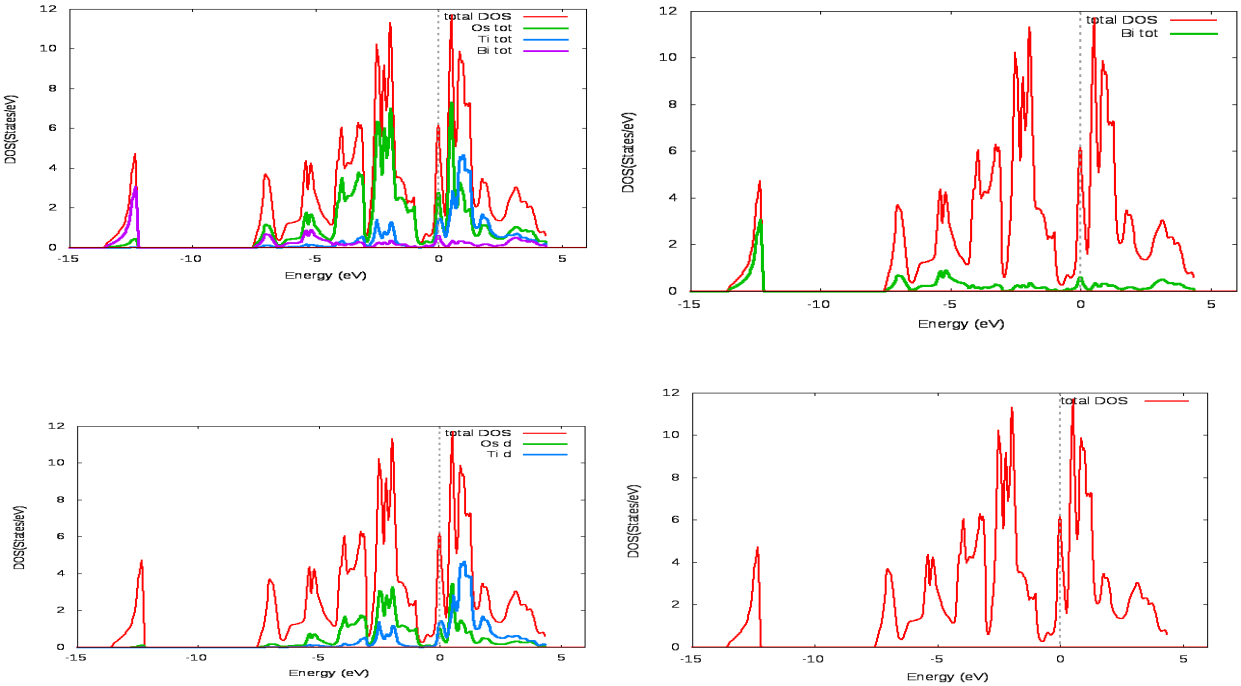


Figure :3 DOS plot for Os2TiBi

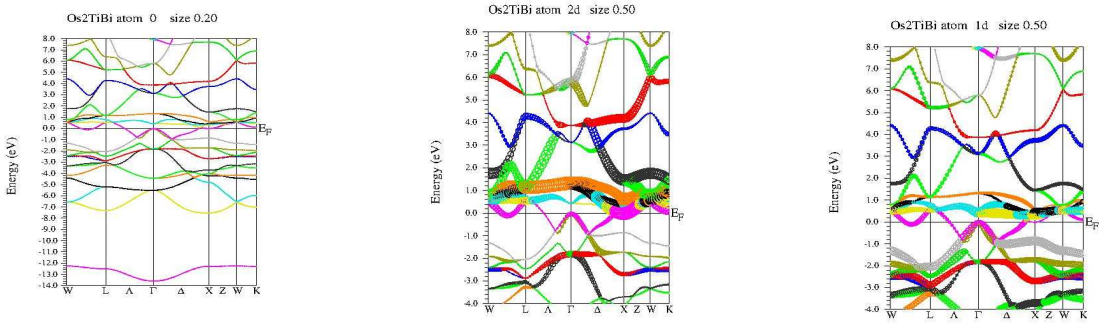


Figure -4 Energy band structure of Os2TiBi

From DOS plot figure 3 we can understand that Os and Ti atoms contribute more at Fermi level . The d states level of Os and Ti interact with each other. There exists an exchange coupling interaction between the d states of these two elements. This is also proved in energy band structure figure 4. The d states cross the Fermi level and make the compound more metallic.

CONCLUSION

The structure properties of Os2TiBi was studied using Wien2k computational code. PBE-GGA interaction potential was used to study the exchange correlation between the elements. Charge density plot reveals that each Bi is surrounded by Os atom. Ti elements lie in between the Bi and Os. The orbitals of Bi is spherical in nature. At Fermi level the d states of Ti and Os cross the Fermi level makes the compound more metallic.

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