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Pressure induced metallization in cadmium telluride

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Abstract
The metallization of the group II-VI compound Cadmium telluride (CdTe) is investigated through its band structure obtained using the full potential linear muffin-tin orbital (FP-LMTO) method. The ground state properties and band gap values are compared with the experimental results. The values of pressure under reduced volume are calculated using Birch-Murnaghan's equation of state. The metallization pressure P_M is 47.58 GPA. The results of metallization pressure in *CdTe* is compared with that of Cadmium Selenide (CdSe). Its metallization pressure P_M is 66.28 GPA. It is found, that the charge transfer from *s* and *p* states to the *d* state will cause metallization and the metallization pressure increases with a decrease of the lattice constant.

Keywords: Metallization, cadmium telluride, cadmium selenide

1. Introduction
The physical properties of materials undergo a variety of changes when they are subjected to high pressure [1]. The increase of pressure means the significant decrease in volume, which results in the change of electronic states and crystal structure. With the development of high pressure experimental techniques, investigations on pressure-induced structural phase transition, semiconductor-metal transition and superconducting transition are getting the attention of all. In particular, there is a great interest in the pressure induced structural phase transition and metallization of the group II-VI compound Cadmium Telluride (CdTe). Group II-VI compound CdTe is a wide band gap semiconductor with a range of technological applications including electronic and electro-optic devices, catalysis, chemical sensors and conductive solar cell window layers [2, 3]. Hence, to gain a fundamental understanding of the structural phase transition and metallization of CdTe, the electronic band structure studies of this material is essential and this motivated the present investigation. The electronic configuration of Cd and Te are [Kr] $4d^{10} 5s^2$ (Z = 48) and [Kr] $4d^{10} 5s^2 5p^4$ (Z = 52) respectively. The valence electronic configurations chosen in our calculation are $4d^{10} 5s^2$ for Cd and $5s^2 5p^4$ for Te. The band structures of CdTe corresponding to various pressures are obtained using the full potential linear muffin-tin orbital (FP-LMTO) method [4]. The calculated total energies were fitted to the Murnaghan's equation of state (EOS) [1], to determine the phase transition pressure and other ground state properties.

2. Results and Discussion
The ground state properties of CdTe are studied from their total energies obtained from our calculation. The total energy is calculated as a function of reduced volume for both B3 and B1 phases of CdTe (*V/Vo*= 1.0 to 0.3 insteps of 0.1). Here *Vo* is the experimental equilibrium volume corresponding to experimental equilibrium lattice constant. The calculated total energies were fitted to Murnaghan's equation of state [1] to obtain the equilibrium lattice constant and find other ground state properties (Table.1)

$$P=1.5B_0 [(Vo/V)^{7/3}-(V/Vo)^{5/3}] [1+0.75(Bo^1-4)\{(Vo/V)^{2/3}-1\}]$$

The values of pressure under reduced volume are calculated and given in Table.2. In CdTe, at normal pressure ZnS structure has minimum energy and at high pressure NaCl structure has minimum energy [3].

At normal pressure, CdTe is a wide gap semiconductor (Fig: 1 and 2) with band gap 1.475 eV. As pressure is increased, there is a charge transfer from s, p to d state, this causes the increase in the width of the valence band and also the empty conduction bands.

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These changes lead to the narrowing of the band gap and at particular pressure, there is a closing of band gap. The band structure and density of state corresponding to metallization of CdTe is shown in Fig: 3 and 4. In CdTe, metallization takes place by the direct closure (Fig: 3) of band gap between valence band and conduction band. The metallization volume of CdTe is *V/Vo=0.62* which corresponds to the pressure P_M *=47.58 GPa* (Table: 3). The metallization occurs because of the closure of band gap between Cd-5p- like valence band and O-5d- like conduction band (Fig: 3). The increase of pressure causes the broadening of bands which results in the decrease of density of states value in most of the energy regions of DOS histograms. Thus in Fig: 4, the heights of the spikes are considerably reduced. When pressure is increased E_F increases whereas no density of states is available at the Fermi level up to metallization pressure [1]. There are appreciable values for DOS at V/Vo=0.62 (Fig: 4) indicating metallization in CdTe.

3. Conclusion

The high pressure band structure, density of states and metallization of CdTe is investigated. The metallization reduced volume is V/V_o=0.62 and the corresponding pressure P_M is 47.58 GPa. The results of metallization pressure in *CdTe* is compared with that of Cadmium selenide (CdSe). Its

metallization pressure P_M is 66.28 Gpa [5]. It is found, that charge transfer from *s* and *p* states to the *d* state will cause metallization and the metallization pressure increases with a decrease of the lattice constant (Table.3).

Table 1: Equilibrium lattice constant (a_o), bulk modulus (B_o) and its pressure derivative ($B_o{}^1$), Energy gap (E_g) of CdTe

Ground State Properties	Present study	Experiment [3]
a_o Å.	12.24	12.56
B_o GPa	44.5	45.5
$B_o{}^1$	5.5	5.97
E_g eV (direct)	1.475	1.5

Table 2: Lattice constant (*a*), Pressure (*P*) and band gap (Eg) for different reduced volumes

V/Vo	a (a.u)	P (Mbar)	Eg (P)
1	12.2495	0	1.475
0.9	11.8267	0.0110	1.4409
0.8	11.3714	0.0653	1.2726
0.6	10.8763	0.2285	0.7667
0.62	10.4451	47.5807	0
0.5	10.3316	0.6734	0
0.4	9.7224	1.9173	0

Table 3: Comparison of CdTe with CdSe

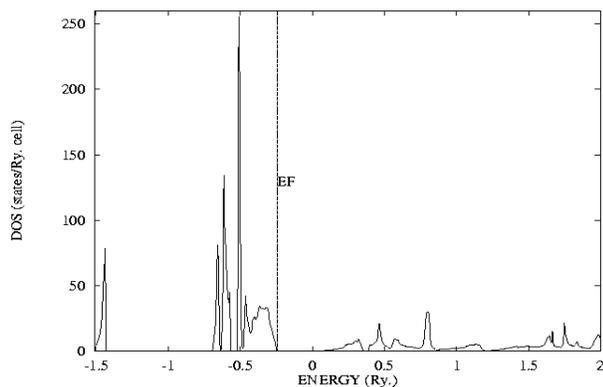| Compound	Lattice constant (au)	Metallization Pressure (Gpa)
CdTe	12.25	47.58
CdSe	11.44	66.28
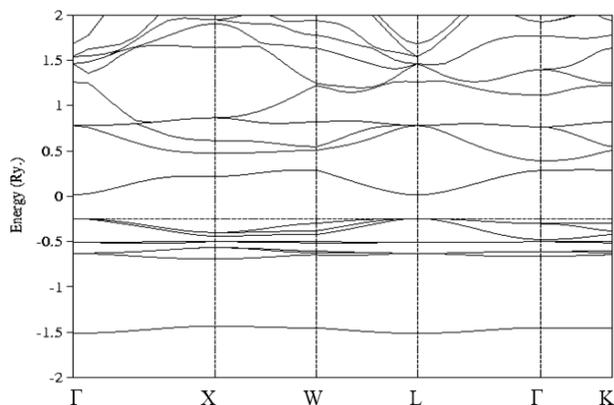
Fig 1: Band structure of CdTe at normal pressure

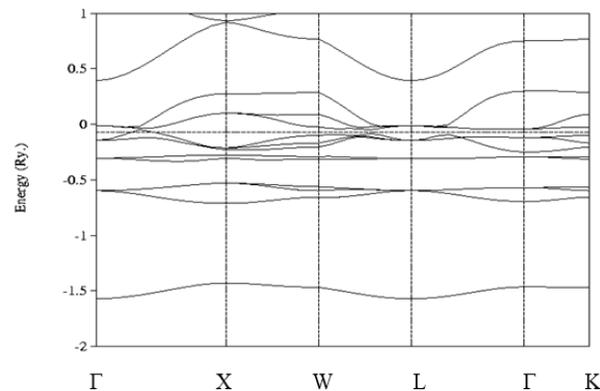**Fig 3:** Band structure of CdTe at metallization pressure

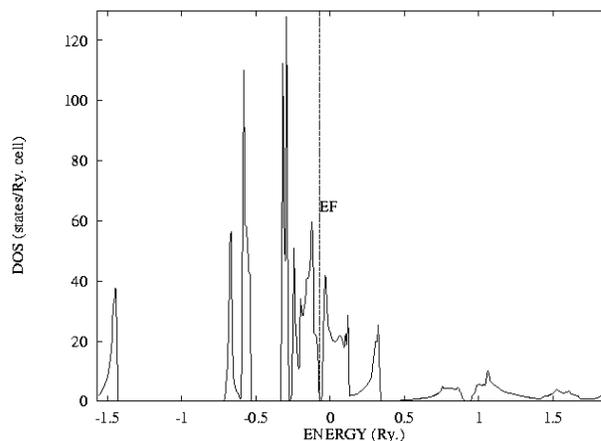**Fig 2:** Density of states of CdTe at normal pressure

Fig 4: Density of states of CdTe at metallization pressure

4. References

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