

Transport properties and electronic structure of intercalated compounds MTiS₂ (M = Cr, Mn and Fe)

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ABSTRACT

New material systems of intercalated compounds MTiS₂ (M= Cr, Mn, Fe) have been systematically studied by *ab-initio* method. In order to investigate the effect of charge transfer from guest 3d transition metal atoms to host TiS₂, the electronic and transport properties have been calculated using full potential linearized augmented plane wave (LAPW) + local orbitals (lo) scheme, in the framework of density functional theory (DFT) with generalized gradient approximation (GGA) for the purpose of exchange correlation energy functional. From the energy bands and density of states it is observed that the 3d-states of M atoms contribute mainly to the conduction band, which results in increase in electrical and thermal conductivity of highly intercalated TiS₂. The calculated electronic component γ which is derived from specific heats of intercalated TiS₂ is quite high (2-50 mJ/mol K²) and increases substantially on intercalation. The 3d-states of transition metal M and Ti atoms which split due to the exchange interaction imparts magnetic properties to the MTiS₂ systems. The calculated transport properties have been analysed on the basis of the density of states and correctly explain the origin of different magnetic ordered phases. Copyright © 2015 VBRI press.

Keywords: Ab initio calculations; chalcogenides; electronic structure; transport properties.

Introduction

Titanium sulphide is a semiconductor with a very small indirect bandgap or semi-metallic ground state. Yan-Bin et al. [1] reported that in self- intercalated TiS₂, coulomb interaction with Ti atom decreases the overlapping/mixing of orbital and shows metal like behavior. Strong covalent bonding in TiS₂ exists due to strong hybridization of Ti 3d and S 3p states, however there exist very weak interlayer Van der Waals attraction (vdW), hence guest species can be easily intercalated into the pure material. On intercalation with transition metals, strong hybridization occurs among M (Cr, Mn, Fe) 3d, Ti 3d and S 3p states. This has been supported by X-ray photoemission spectroscopy (XPS), angle resolved resonant photoemission spectroscopy (ARPES), angle resolved inverse photoemission spectroscopy (ARIPES) and high field magnetization measurements [2, 3]. Studies of the electronic structure were also carried out by various methods based on 1st principles. The molecular-orbital method was applied to analyse the nature of chemical

bonding in intercalated TiS₂ [4]. Similarly, from the calculations by self consistent APW method, it was concluded that d-orbitals of intercalant M-atoms hybridize strongly with S p-orbitals such that the Ti-S bonds become weaker than the M-S bonds [5-7]. From these studies it was concluded that the properties of MTiS₂ was dependent on the guest atom and showed unusual transport properties such as magnetic ordered phases e.g. spin-glass, cluster-glass and ferromagnetic ordering [8-12].

Intercalated transition metal chalcogenides thus exhibit exotic behavior due to their layered and two dimensional symmetric structures. Since transition elements exhibit more than one oxidation state, investigation of role of transition elements in electronic and transport properties of intercalated TiS₂ is of great interest. However, literature survey showed that transport properties have not been investigated using band calculation methods. In this work, the temperature dependence of various transport properties have been studied using full potential linearized augmented plane wave (FPLAPW) scheme, in the framework of DFT. The calculated transport properties such as electrical

resistivity, specific heats etc. have been analysed on the basis of the extent of band overlap and density of states.

Theoretical methodology

Electronic properties

The full potential linearized augmented plane wave (FPLAPW) scheme as incorporated in Wien2k code is amongst one of the most accurate methods for calculation of electronic structure [13]. It is based on the density functional theory (DFT) for the treatment of exchange and correlation and provides a relatively efficient and accurate method to evaluate ground state energy states of condensed materials. The latest generalized gradient approximation (GGA) proposed by Wu and Cohen for the exchange and correlation potential is used. We have performed the spin polarized calculations for highly intercalated $M_x\text{TiS}_2$ ($x=0.25$). The convergence of this basis set is controlled by a cut-off parameter $R_{\text{MT}}K_{\text{max}}=7$, where K_{max} is the magnitude of the largest $\mathbf{k}$ -vectors. The maximum radial expansion l_{max} is set to be 10. The iteration is halted when the difference charge density and energy was less than $0.0001 \text{ e}^- \text{ a}_0^{-3}$ and 0.001 Ry respectively, between steps taken as convergence criterion. The energy cut-off between the core and valence states was set at -6.0 Ry . Here R_{MT} for Ti = 2.42 and S = 2.43 Å. A mesh with 100 $\mathbf{k}$ -points in the irreducible Brillouin zone (IBZ) were used for TiS_2 and MTiS_2 .

Transport properties

The calculation for the transport properties is carried out using the BoltzTrap code which is interfaced with Wien2k [14]. The Fourier expansion of band energies is carried out to determine the gradient along the energy bands to obtain the group velocities. For Fourier expansion of the band energies, the BoltzTrap code uses star functions for maintaining the space group symmetry. The bulk semi classical properties such as electrical and thermal conductivities etc., can be obtained from the Boltzmann theory. In the presence of electric and magnetic fields and thermal gradient, the current density $\mathbf{j}$ can be written as-

$$J_i = \sigma_{ij} E_j + \sigma_{ijk} E_j B_k + v_{ij} \Gamma_j T \quad (1)$$

where, σ_{ij} is the conductivity tensor given in terms of group velocity and inverse mass tensor. Transport tensors can then be calculated from the conductivity distribution. To calculate the temperature dependent properties, we have taken an energy grid of 0.0005 Ry , with energy span of $\pm 0.4 \text{ Ry}$ around Fermi level. The range around the Fermi energy in which energy bands are included is 0.15 Ry . Transport properties are computed in a temperature grid of 1 K and in a temperature range of 0 to 500 K .

Results and discussion

Energy bands and density of states

TiS_2 has a CdI_2 type hexagonal crystal structure with space group $P\bar{3}m1(164)$. The Wyckoff positions for Ti is $1a$

(origin); the two S atoms are placed at $2d (1/3, 2/3, 0.2501)$ and $(2/3, 1/3, -0.2501)$; with lattice parameters $a = 3.407$ and $c = 5.695 \text{ Å}$ [15]. TiS_2 exhibits octahedral prismatic structure in which there is strong covalent bonding between Ti and S atoms and weak Van der Waals attraction between the layers. The structure of TiS_2 and the Brillouin zone (IBZ) for CdI_2 type hexagonal structure are shown in Fig. 1. Due to weak attractive vdW contacts between the slabs, TiS_2 can be easily cleaved along inter sandwich planes and hence can be easily intercalated by guest species. The guest atom M (Cr, Mn, Fe) occupies the $1b (0, 0, 0.5)$ position, the structure of M intercalated in TiS_2 is shown in Fig. 2 [15].

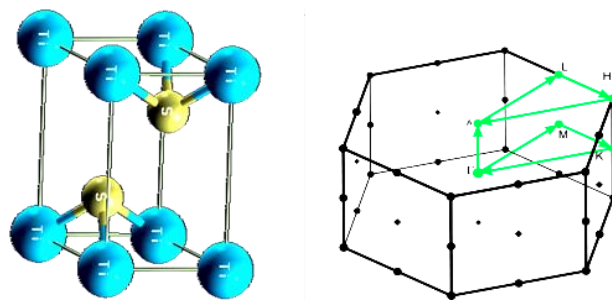


Fig. 1. (a) Crystal structure of TiS_2 (b) irreducible brillouin zone (IBZ) of CdI_2 type crystal with high symmetry points Γ -M-K- Γ -A-L-H.

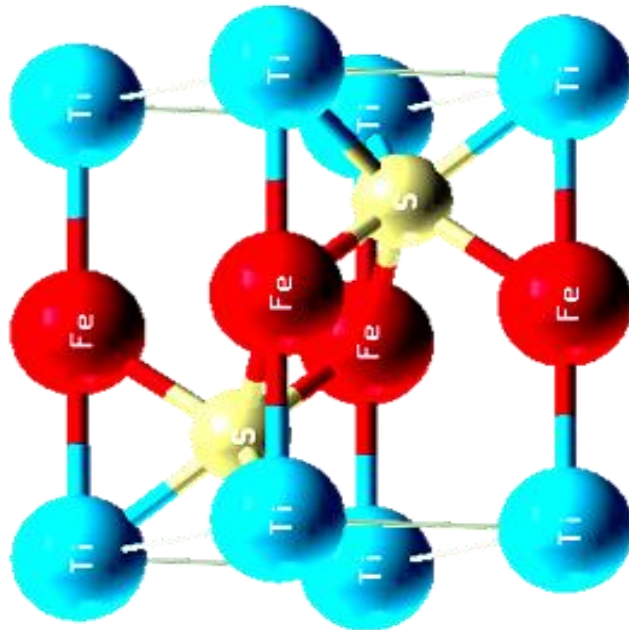


Fig. 2. Crystal structure of FeTiS_2 .

The energy band structures of TiS_2 have been plotted in the energy range -6.0 to 6.0 eV along the high symmetry Γ -M-K- Γ -A directions in the IBZ (Fig. 3). The maximum of valence band is located at the Γ -point, whereas the minimum of conduction band is at L-point, giving a small indirect bandgap of $\sim 0.1 \text{ eV}$. The calculated band structure is in agreement with previous self consistent calculations [1]. (The Fermi energy level coincides with 0 eV in Wien2K). The band structures of TiS_2 intercalated with Cr are plotted in Figs. 4(a and b). The spin polarized fully relativistic calculations yield the spin up and spin down

band structures. The intercalated atom M alters the band structure substantially and there is enhancement in the number of bands in valence and conduction regions. The energy bands also show greater dispersion in the vicinity of the Fermi energy level between -2.5 to 2.5 eV. The band structures of Mn and Fe intercalated TiS_2 are quite similar in nature (not shown here).

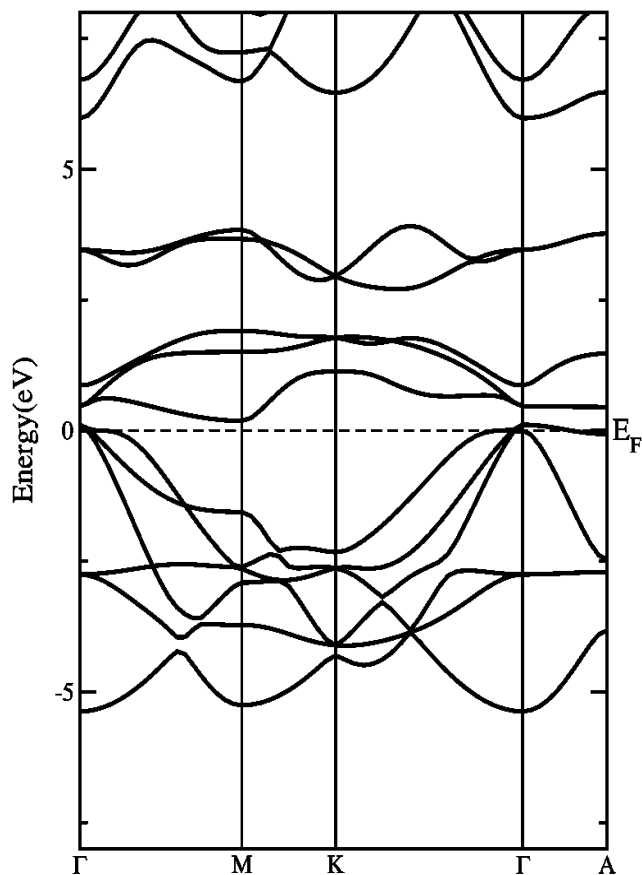


Fig. 3. Energy bands of TiS_2 along Γ -M-K- Γ -A directions.

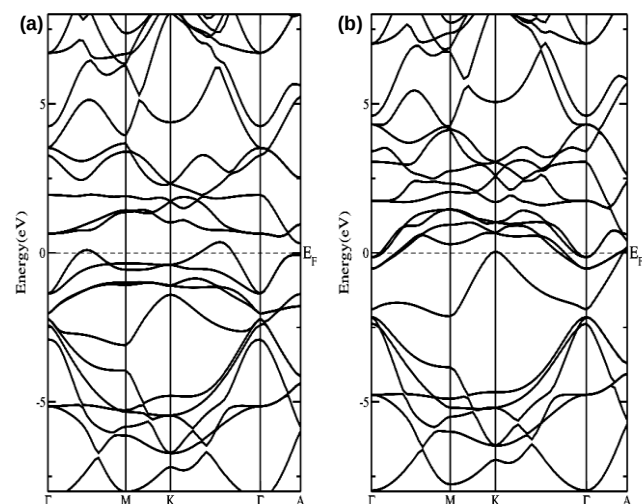


Fig. 4. Energy bands of CrTiS_2 (a) spin up (b) spin down along Γ -M-K- Γ -A direction.

In order to interpret the energy bands, the total and partial density of states (TDOS and PDOS) of TiS_2 as well as CrTiS_2 (Figs. 5-6) are plotted in the energy range between -6.0 to 6.0 eV. It is seen that the Ti 3d-states split into t_{2g} and e_g states due to crystal field effect and the S p-states strongly hybridize with Ti 3d states forming bonding and antibonding states. In the vicinity of the Fermi energy level, Ti 3d-states dominate the conduction band, whereas the S 3p-states contribute mainly to the valence band. Since the intercalant M atom occupies the octahedral interstitial sites between sulphur layers, the hybridization between M 3d and S 3p-states becomes stronger than that between Ti 3d and S 3p-states. The hybridized states of Cr/Mn/Fe with host S 3p and Ti 3d-states contribute to states at the Fermi level E_F . It is also observed from the PDOS of Cr, that the spin $\uparrow$ d-states dominate the valence region and spin $\downarrow$ d-states contribute mainly to conduction regions. Intercalation with transition atoms not only induces magnetism in Ti states, the overall contribution of Ti d-states is also suppressed. The states below -2.5 eV are mainly composed of core s- and p-orbitals of M, Ti and S atoms, therefore the DOS below -2.5 eV for intercalated TiS_2 are quite similar in nature.

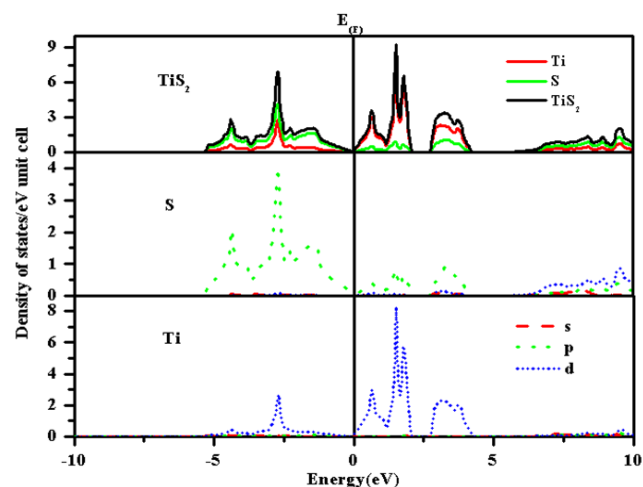


Fig. 5. Density of states of TiS_2 .

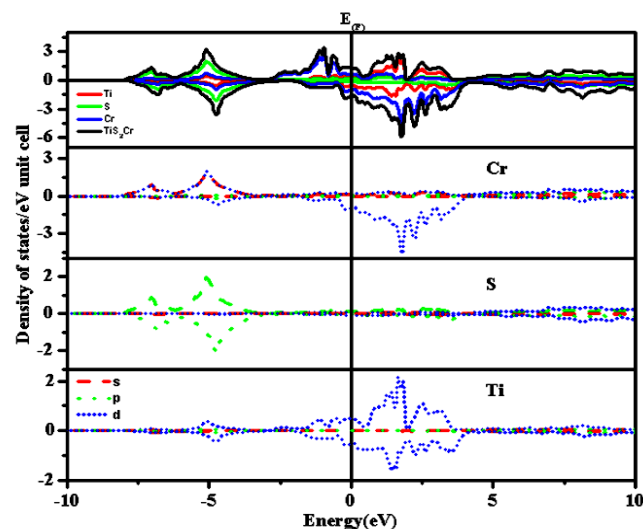


Fig. 6. Density of states of CrTiS_2 .

The bands manifold as seen in TiS_2 is thus substantially shifted due to electron-electron interactions of intercalated atom M with both Ti and S atoms. The position of Fermi energy level is located in the M 3d bands and E_F for TiS_2 at 0.3524 eV, shifts to higher energy value 0.6745, 0.6608 and 0.6370 eV for Cr, Mn and Fe respectively. This implies that additional states are contributed by Cr, Mn and Fe atoms to the host TiS_2 . The unequal 3d spin states of intercalating atom M gives rise to various types of magnetic ordering (depending on the concentration) e.g. CrTiS_2 and MnTiS_2 become paramagnetic whereas FeTiS_2 exhibits cluster-glass ($x=0.25$) ferromagnetism for highly intercalated TiS_2 [3-8].

To visualize the nature of charge density in TiS_2 and the changes in the potential fields due to intercalation with transition metal atoms, the contour plots in a specified plane of the crystal were obtained on a two dimensional grid. The valence charge densities for the (011) surface for TiS_2 corresponding to $z=0$, and the spin $\uparrow$ and spin $\downarrow$ charge densities of CrTiS_2 (corresponding to $z=1/4$) are shown in **Figs. 7 (a, b and c)**. The overlapping between electrostatic potential fields of Ti and S atoms are clearly seen, which corresponds to covalent bonding. The layered structure of TiS_2 and the redistribution of the potential fields on intercalation with Cr are also clearly seen. The strong Ti-S interactions are modified and there is formation of bonds of S with Cr atoms.

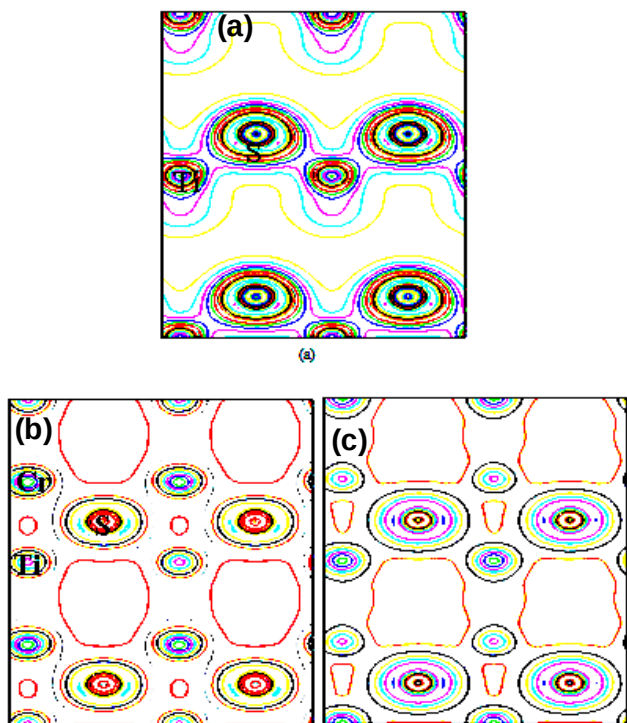


Fig. 7. Electron charge density of (a) TiS_2 (b) CrTiS_2 Spin up and (c) CrTiS_2 Spin down, along (001) plane.

Transport properties

From the band structure and DOS of MTiS_2 , it is seen that the guest atom contribute prominently near E_F , as a result TiS_2 becomes an extrinsic degenerate semimetal. Some experimental measurements of temperature dependent

specific heats, Hall resistivities etc. have been made by some workers, however calculations of transport properties by band structure methods are not available in literature [8-12]. Some of the experimental parameters such as number of charge carriers n , Fermi energy level E_F , number of states at Fermi level $N(E_F)$ etc. can be estimated from the calculated transport data, thereby verifying the accuracy of band calculation method.

The electrical conductivity given in Eqn. 2, can be obtained from the conductivity tensors using:

$$\sigma_{\alpha\beta}(i,k) = e^2 \tau_{i,k} v_{\alpha}(i,k) v_{\beta}(i,k) \quad (2)$$

Here, τ is the relaxation time which depends on the band index i and k vector direction, and $\mathbf{v}$ is the group velocity. The scattering relaxation time of the free carriers in TiS_2 is $\sim 2.6 \times 10^{-14}$ s [16].

One of the most important charge transport property is the electrical conductivity. In **Fig. 8**, the conductivity vs. temperature curves for pure and 3d intercalated TiS_2 are shown. The electrical conductivity of TiS_2 which is $\sim 10^5$ ($\Omega\text{m})^{-1}$ increases in the case of CrTiS_2 and FeTiS_2 (**Table 1**). The conductivity however decreases for TiS_2 intercalated with Mn. In the low temperature regions < 20 K, all the curves show anomalous behavior. Electrical resistivity which can be derived from the calculated electrical conductivity (not shown here), is known to exhibit metallic behavior and decreases with temperature in case of TiS_2 . The calculated room temperature resistivity value of $1.61 \times 10^{-4} \Omega\text{cm}$ for TiS_2 is mainly attributed to electron-electron scattering and compares well with experimental value of $8 \times 10^{-4} \Omega\text{cm}$ [19]. The calculated resistivity values for CrTiS_2 and FeTiS_2 are 0.07×10^{-4} and $0.13 \times 10^{-4} \Omega\text{cm}$ respectively, which is lower than resistivity of TiS_2 . Resistivity of MnTiS_2 ($12.6 \times 10^{-4} \Omega\text{cm}$) is higher than that of TiS_2 and may be attributed to impurity scattering due to high concentration of Mn- atoms. The anomalous decrease of electrical resistivity at low temperatures can be attributed to increase of relaxation time of carrier scattering with decreasing temperature.

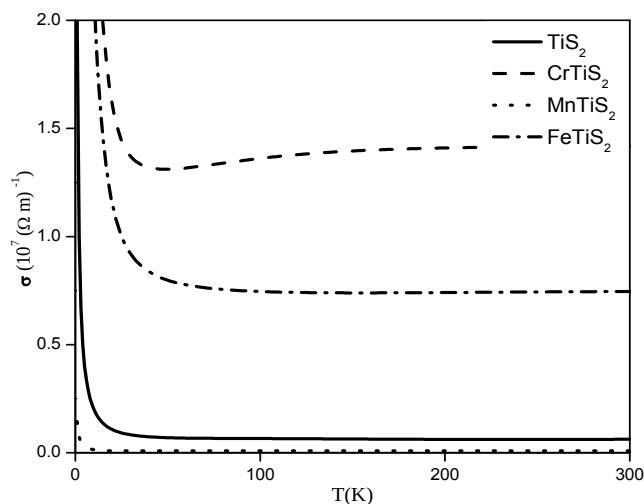


Fig. 8. Variation of electrical conductivity (σ) with temperature (T).

Thermal conductivities can also be derived from the electrical conductivity tensor. The plots for thermal

conductivity vs. temperature are shown in **Fig. 9**. It is seen that on applying a polynomial fit, the thermal conductivity curves show a T^2 dependence. Thermal conductivity of TiS_2 increases upto a value of 15 W/mK with increasing temperature. The calculated room temperature conductivity of TiS_2 is 5.96, which is comparable to experimental values for 6.8 $\text{Wm}^{-1}\text{K}^{-1}$ [17].

Table 1. Transport properties of intercalated TiS_2 compounds at ambient temperature.

Compound	$\sigma (\Omega\text{m})^{-1}$ (10^6)	k (W/mK)	c_p (J/mol-K)	χ (m^3/mol) (10^{-9})
TiS_2	0.62	5.96	0.35	0.2
CrTiS_2	14.17	104.08	3.98	2.27
MnTiS_2	0.08	60.15	3.37	1.91
FeTiS_2	7.45	55.01	5.01	2.72

For MTiS_2 , $\kappa(T)$ values at ambient temperatures is 104.08, 68.15 and 55.01 $\text{Wm}^{-1}\text{K}^{-1}$ for Cr, Mn, Fe respectively, which are substantially higher than thermal conductivity of TiS_2 . All the $\kappa(T)$ curves follow both the T^2 and Wiedemann-Franz law and are in agreement with experimental measurements of the basal thermal conductivity. It is observed that at low temperatures all the curves deviate from T^2 behaviour. Since, heat transport in titanium dichalcogenides is known to be essentially due to lattice contribution κ_l , the increase in the slope on intercalating may be due to increase in the electronic component κ_e . The transition elements M (Cr, Mn, Fe) contribute the additional electrons in the vicinity of Fermi level.

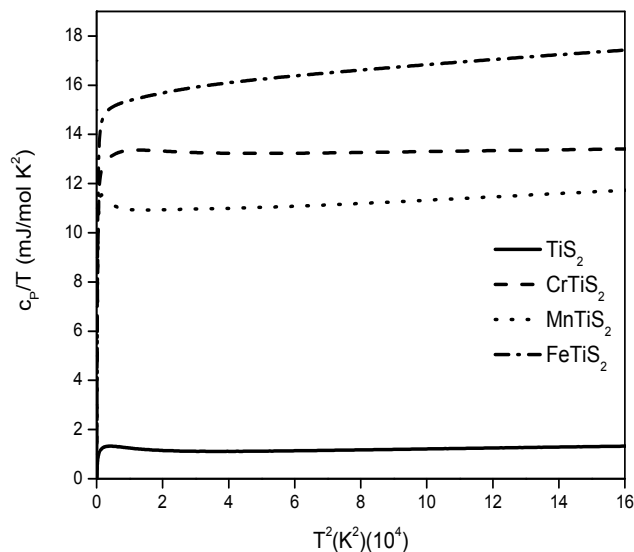


Fig. 9. Variation of thermal conductivity (κ) with temperature (T).

Specific heat measurements are one of the most reliable methods of investigating temperature dependence of materials. To get a better understanding of the anomalous behaviour of electrical resistivity and thermal conductivity at low temperatures, the temperature dependence of heat

capacity is analysed with fitting functions. A least squares fit of the data can be made from the relation:

$$\frac{c_p}{T} = \gamma + \beta T^2 \quad (3)$$

Here γ is the Sommerfeld electronic term which is related to the density of states at E_F and β which represents the lattice contribution to specific heat.

The specific heat vs. temperature curves for MTiS_2 show similar behaviour. It is observed that the variations of c_p with temperature follow the well known Debye form and shows excellent fit at high temperatures. To analyze the low temperature behavior of intercalated TiS_2 , c_p/T vs. T^2 is plotted in **Fig. 10**. From data fitting of the specific heat curves, the value of the electronic specific heat coefficient γ is found to have a value of 1.09 mJ/mol K^2 for TiS_2 , which is in excellent agreement with the value of 2 mJ/mol K^2 obtained from specific heat measurements of Inoue et al. [12]. The slope of specific heat increases for intercalated compounds and the values of coefficient γ are relatively large compared to TiS_2 . The contribution of the nonlinear term β is very small compared to the experimental values [10]. The two parameters obtained from data fitting of TiS_2 and MTiS_2 are given in **Table 2**.

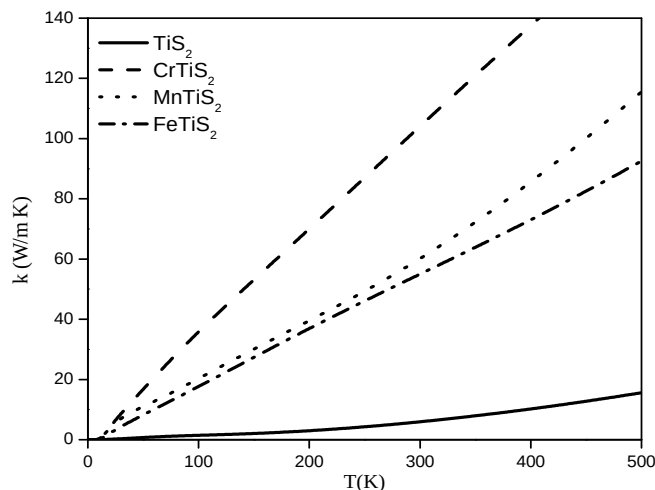


Fig. 10. Variation of specific heat per unit temperature (c_p/T) with temperature (T^2).

The density of states at Fermi energy level $N(E_F)$ can be confirmed from specific heat measurements by using the conventional Sommerfeld theory of a free-electron gas which relates the electronic coefficient γ to $N(E_F)$,

$$\gamma = \frac{\pi^2 k_B^2 N_A}{3n} N(E_F)(1 + \lambda) \quad (4)$$

where N_A is the Avogadro number, k_B is Boltzmann constant, n is the number of atoms.

The variation in the electronic specific heat component γ with transition metal atom M, can be correlated with the change in the density of states at the Fermi level according to the above relation. It is possible to obtain $N(E_F)$ by substituting the value of γ obtained from curve fitting of

c_p/T vs. T^2 into Eqn. 4. The density of states at E_F can also be obtained from the DOS plots (Figs. 5-6). Thus the Sommerfeld electronic term γ which can be extracted experimentally from specific heat measurements can verify the accuracy of our band structure calculations.

Takase et al. have measured the specific heats of intercalated compounds in the temperature range 0.35-5 K using ac calorimetric method [19]. For FeTiS_2 , the calculated coefficient γ has a value of $15.17 \text{ mJ mol}^{-1}\text{K}^{-2}$ which agrees well with the experimental value of $13.5 \text{ mJ mol}^{-1}\text{K}^{-2}$, and yields $6.43 \text{ states/eV unit cell}$. For MnTiS_2 , γ is $10.54 \text{ mJ mol}^{-1}\text{K}^{-2}$ which is lower than the experimental value of $48 \text{ mJ mol}^{-1}\text{K}^{-2}$ and yields $4.46 \text{ states/eV unit cell}$. From our calculated specific heats, the value of fitting parameter γ is $1.09 \text{ mJ mol}^{-1}\text{K}^{-2}$ for TiS_2 which yields $0.214 \text{ states/eV unit cell}$.

The increase in the value of the electronic specific heat component of the host TiS_2 indicates the enhancement of density of states at the Fermi level and the itinerant electron nature of intercalated 3d atoms. From our calculations, we also observe that electronic component for MnTiS_2 is smaller compared to CrTiS_2 and FeTiS_2 (Table 2). This anomalous behavior may be attributed to variable oxidation states of Mn, which thereby contribute smaller number of electrons at E_F . The value is highest in Fe intercalated TiS_2 and may be attributed to stronger hybridization between conduction electrons of Ti and Fe atoms, which may lead to more localization of electrons at E_F .

Table 2. Best-fit Parameters for the specific heat of intercalated TiS_2 compounds.

Sample	γ ($\text{mJ/K}^2\text{-mol}$)	β ($\text{mJ/K}^4\text{-mol}$) (10^{-6})	N(E_F)/eV per unit cell)	
			From DOS Curve	Sommerfeld Formula
TiS_2	1.09	1.38	0.214	0.30
CrTiS_2	12.58	2.49	2.91	5.33
MnTiS_2	10.53	5.59	1.69	4.46
FeTiS_2	15.17	8.07	2.82	6.43

The experimental values of electronic specific heat coefficient γ for both TiS_2 and MTiS_2 are quite high and lie between $2\text{-}100 \text{ mJ/mol}^{-1}\text{K}^{-2}$ [12]. Our calculated values are also found to lie within this range. The specific heats for pure 3d transition metals and various pyrites are known to show similar temperature dependence and the corresponding electronic coefficient γ are found in the range of $5\text{-}10$ and $5\text{-}30 \text{ mJ/mol}^{-1}\text{K}^{-2}$ respectively. Thus, the low temperature anomalous behavior of specific heats of intercalated TiS_2 appears to follow the temperature dependence of dilute alloys. The discrepancies between the calculated and experimental values of γ may be because of mass enhancement due to electron-electron or electron-phonon interactions which have not been taken into account.

The transport properties such as electrical and thermal conductivities as well as specific heat coefficient γ are thus seen to strongly depend on the oxidation state i.e. $3d^n$ of the transition metal atom. The band picture also clearly illustrates the variation in hybridization and localization of the states of guest (M) and host atoms (TiS_2) which contribute to density of states at E_F . Experimental

measurements of band structures and $N(E_F)$ for MTiS_2 are required to verify the calculations.

The 3d-states of transition metal M and Ti atoms split due to the exchange interaction. This gives rise to unequal spin-up and spin-down states which imparts magnetic properties to MTiS_2 systems. From plots of density of states it is seen that the $\text{spin}\uparrow$ and $\text{spin}\downarrow$ states of Ti and M are unequal, which implies that the magnetism of M atom is transferred to nonmagnetic Ti atom. From the band structure calculations it is seen that M (Cr, Mn, Fe) atoms add states to the conduction band of TiS_2 which results in shift of the Fermi energy to 0.6745 , 0.6608 and 0.6370 eV for Cr, Mn and Fe respectively. The Fermi level in FeTiS_2 is located close to a sharp peak of the DOS and a large value of $N(E_F)$ is known to be favourable for stabilization of the ferromagnetic state. For CrTiS_2 , the difference between the spin up and spin down states is largest among the chosen transition metal atoms. Magnetism is found to decrease i.e. 3.06 , 3.01 and $2.02 \mu_B$ for Cr, Mn and Fe intercalated TiS_2 respectively. The difference in nature of magnetism is due to the different *spd* hybridization of intercalated transition metal atom with both Ti and S atoms. The magnetic properties of intercalated TiS_2 can thus be correctly understood in terms of itinerant electron model or band picture rather than a localized model. Thus the properties of MTiS_2 are found to be dependent on the guest atom and showed unusual transport properties.

Conclusion

The calculated electronic properties were interpreted in terms of the observed experimental behavior. The temperature dependent transport properties have been understood in terms of band structures and density of states. It is observed that electrical resistivity, magnetic moments and electronic term γ exhibit strong dependence on the number $3d^n$ of M atoms. The magnetic moments as well as the Sommerfeld electronic term γ are found to be in good agreement with experimental values. It is found that the FP-LAPW method is a fairly accurate band calculation method which correctly calculates the transport properties and explains the nature of magnetism of highly intercalated TiS_2 . Further calculations for various levels of doping are suggested for understanding the occurrence of various magnetic ordered phases e.g. spin-glass, cluster-glass and ferromagnetic ordering.

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