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Fermi Surface Study of $ScAu_2$(Al, In) and $ScPd_2$(Sn, Pb) Compounds

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Abstract. A detailed study on the electronic structure and Fermi surface (FS) of superconducting Heusler compounds $ScAu_2$(Al, In) and $ScPd_2$(Sn, Pb) has been carried out using first principles electronic structure calculations. The spin orbit coupling is found to play a major role in understanding the band structure and FS. Analysis of the data shows the importance of spin orbit coupling effect in the above compounds. The bands which cross Fermi level (E_F) are found to be dominated by the Sc d_{t2g}-states. The calculated total density of states are in good agreement with the experimentally reported value for $ScPd_2Sn$. Under compression we find a change in the Fermi surface topology of $ScPd_2Sn$ at V/V_0 = 0.95 (pressure of ≈ 15 *GPa*), which is explained using the band structure calculations.

Keywords: Intermetallic compounds, Superconductivity, Density functional theory, spin-orbit coupling.
PACS: 71.20.Lp, 74, 71.15.Mb, 71.70.Ej.

INTRODUCTION

Heusler compounds crystalize in $L2_1$ structure and have general formula XY_2Z, where X is generally a transition element like Sc, Ti, Y, Zr, Nb, Ta and Hf and Y is a transition metal from the VIIIB or IB period and Z is a IIIrd, IVth or Vth group element like Al, Ga, Ge, In, As, Sn, etc. Among these compounds some are ferromagnetic materials and some are superconductors with superconducting transition temperature (T_c) ranging from 0.74 *K* ($HfNi_2Al$) to 4.76 *K* (YPd_2Pb)[1]. Among these superconducting compounds, $ScAu_2$(Al, In) and $ScPd_2$(Sn, Pb) are having T_c of the order of 2.0 - 4.4 *K*. No further studies are available for these compounds and this provoked us to explore them further. In the present work, we concentrate mainly on the electronic structure properties of these compounds at ambient as well as under compression.

METHODOLOGY

The calculations are carried out by using FP-LAPW method as implemented in the WIEN2k code[2]. For the exchange correlation potential, we have used PBE-GGA (Perdew-Burke-Ernzerhof parameterization of the Generalized Gradient Approximation) approximation[3]. Throughout the calculation, the R_{MT} value for each atom was fixed as 2.1 *a.u.* for Sc, 2.0 *a.u.* for Al, 2.3 *a.u.* for Pd and 2.4 *a.u.* for Au, In, Pb and Sn. $R_{MT} * K_{max}$ = 9 was used for the energy convergence, where K_{max} is the plane wave cutoff. The potential and charge density were Fourier expanded up to G_{max} = 12. All the calculations are performed with total 20000 k-points which gives 560 k-points in the irreducible part of the Brilloun Zone (BZ). Birch-Murnaghan equation of state was used to fit the total energies as a function of primitive unit cell volume to obtain the bulk modulus and the equilibrium lattice parameter of the above compounds. We find all the compounds to be stable with minimum energy with the inclusion of spin orbit coupling. So, all our further calculations are carried out including spin orbit effect.

RESULTS AND DISCUSSION

In this section we present the ground state properties, band structure, density of states (DOS) and FS of the investigated compounds, computed with the inclusion of spin orbit coupling.

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TABLE 1. Ground state properties of $ScAu_2Al$, $ScAu_2In$, $ScPd_2Sn$ and $ScPd_2Pb$ at ambient condition with experimental reports.

Parameters	$ScAu_2Al$	$ScAu_2In$	$ScPd_2Sn$	$ScPd_2Pb$
Experimental lattice constant[1,4-6] a_{exp} (Å)	6.535	6.692	6.503	6.630
Theoretical lattice constant a_{th} (Å)				
LDA	6.443	6.612	6.435	6.522
GGA	6.591	6.791	6.597	6.697
Bulk modulus B (GPa)				
LDA	145	133	153	145
GGA	118	102	122	110
Density of States ($N(E_F)$) (*states/eV/f.u.*)				
Experimental[1]	--	--	1.79	--
Theoretical	1.97	1.84	1.79	1.92

Ground State Properties

The equilibrium lattice constant and bulk modulus are calculated for the present series of compounds by fitting the Birch-Murnaghan equation of state in both Local Density Approximation (LDA) and GGA. It is well known that LDA underestimate the lattice constant and GGA overestimate the same and the calculated values are given in the Table 1. From the calculated bulk modulus values it is seen that $ScPd_2Sn$ have the higher bulk modulus and $ScAu_2In$ possess the lower bulk modus indicating $ScPd_2Sn$ to show more resistance to uniform compression than the other compounds.

Band Structure

The calculated band structure for all the compounds including the spin orbit effect is shown in the Fig 1.

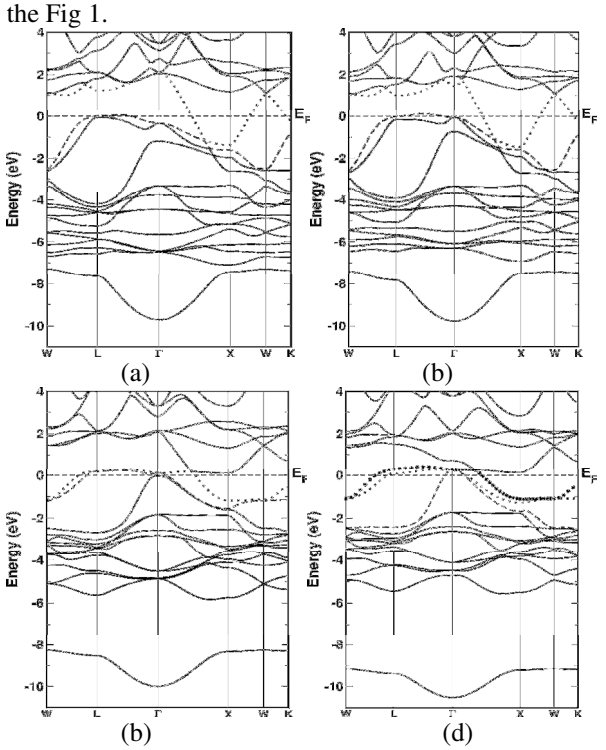

FIGURE 1. Band structure for (a) $ScAu_2Al$, (b) $ScAu_2In$, (c) $ScPd_2Sn$ and (d) $ScPd_2Pb$.

The overall band structure scenario is similar for all the compounds except the number of bands crossing the E_F. The number of bands to cross the E_F is three in the case of $ScPd_2Pb$ and two in the case of remaining compounds. As we move from Au containing compounds to Pd containing compounds, the gap in the valence region from the lowest valence band to second lowest valence band increases. In all the compounds the lowest valence band is due to the Z (Z = Al, In, Sn and Pb) element *s*-states in the respective compound. It is found that the bands crossing the E_F is dominated by Sc d_{t2g}-states with the admixture of (Au, Pd) d_{eg}-states for all the above mentioned compounds.

Density of States

To explore further, we have calculated the DOS and the same is plotted in the Fig 2 and the values of total DOS is given in the Table 1. From the table, it is evident that the calculated total DOS value is in good agreement with the experimental value for $ScPd_2Sn$. For the remaining compounds, we don't find any experimental comparison to our results.

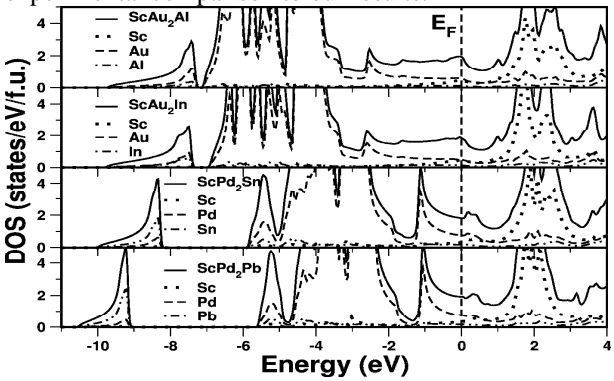

FIGURE 2. The total and partial density of states for all the compounds.

From the DOS plots, it is seen that the maximum contribution at E_F is due to the (Au, Pd) atom with the admixture of Sc atom in all the compounds. At an energy around 2 *eV*, the contribution to the total DOS

is dominated by the Sc atom in all the compounds. As we move from Au to Pd containing compounds, the contribution of Pd atom at the E_F is more than the Au atom. We have also observed a sharp peak in the bonding region below the E_F in the Pd containing compounds.

Fermi Surface Topology

To understand further, we have plotted the FS for all the compounds in the Fig 3. In all the compounds, the first FS is due to band with broken line, second one due to the dotted line band and the third one is due to the thick dotted line band (in the case of $ScPd_2Pb$). The band structure and FS topology is same for the Au containing compounds. In that first FS is having the hole character due to the band crossing E_F from valence to conduction band along L-Γ direction and the second FS is having both hole and electron character due to the band crossing the E_F at X point from conduction band to valence band and again from valence band to conduction band at W point.

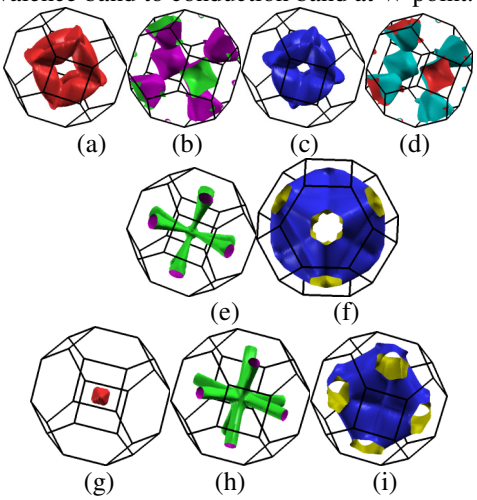

FIGURE 3. Fermi surface for $ScAu_2Al$ (a,b), $ScAu_2In$ (c, d), $ScPd_2Sn$ (e, f) and $ScPd_2Pb$ (g, h, i).

In the case of $ScPd_2Sn$ we have two FS, in that first FS have tube like structure from L to Γ point having hole character, and the remaining one is the electron sheet. In the case of $ScPd_2Pb$ we have three bands to cross the E_F and we have three FS as shown in Fig 3(g, h, i). In that the first FS correspond to the band crossing at Γ point from valence to conduction band indicating the hole nature. In the same way the next FS also has the same hole nature. The third FS in this compound is electron sheet due to the band crossing from conduction to valence band through both X and W points.

Under Compression

To study the pressure effect on the electronic structure and FS of the present compounds, we have performed the calculations under uniform compression with V/V_0 = 1, 0.95, 0.90 0.85, 0.80 for all the compounds. We did not find any change in the band structure and FS topology for $ScAu_2$(Al, In) and $ScPd_2Pb$ compounds. In the case of $ScPd_2Sn$ we observed the change in the FS topology starting from V/V_0 = 0.95 (at the pressure of ≈ 15 *GPa*). At this compression the topology of the first FS starts changing due to the band shifting downwards towards E_F. At V/V_0 = 0.85 where the FS are given in Fig 4, we find the change in the second FS also which has addition an pocket at the Γ point of the FS as shown in Fig 4(b).

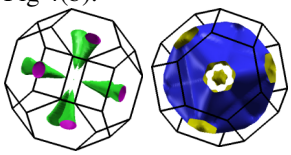

FIGURE 4. Fermi surface for $ScPd_2Sn$ (a, b) at V/V_0 = 0.85.

CONCLUSSIONS

We have investigated the electronic structure properties of the present compounds. The calculated ground state properties are in good agreement with the experiments. The calculated band structure indicates the metallic nature of these compounds. From the calculated DOS, we observed that the maximum contribution is from the (Au, Pd) atoms with the admixture of Sc atom in all the compounds. For $ScPd_2Sn$ the calculated total DOS value agree quite well with the experiment. From the calculated FS we observed that the $ScAu_2$(Al, In) compounds have one hole pocket and one mixed character FS. In $ScPd_2Sn$ compound, we have one hole and one electron sheet. For $ScPd_2Pb$ we have two hole pockets and one electron sheet. Under compression we have observed changes in the FS for the $ScPd_2Sn$ compound, which might further induce a non-monotonic variation in T_c which might be taken up as a future work.

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