JOURNAL OF SCIENCE
SAKARYA UNIVERSITY

Sakarya University Journal of Science

ISSN 1301-4048 | e-ISSN 2147-835X | Period Bimonthly | Founded: 1997 | Publisher Sakarya University |
http://www.saujs.sakarya.edu.tr/

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Recieved: 2020-01-26 17:51:56

Accepted: 2020-02-18 16:21:06

Article Type: Research Article
Volume: 24
Issue: 2
Month: April
Year: 2020
Pages: 406-411

How to cite
Hüseyin Yasin Uzunok; (2020), The Effect of Spin-Orbit Interaction On Structural and Electronic Properties of ScIr2. Sakarya University Journal of Science, 24(2), 406-411, DOI: 10.16984/saufenbilder.680230
Access link
http://www.saujs.sakarya.edu.tr/tr/issue/52471/680230

Sakarya University Journal of Science 24(2), 406-411, 2020

The Effect of Spin-Orbit Interaction On Structural and Electronic Properties of $ScIr_2$

Hüseyin Yasin UZUNOK[1]

Abstract

The structural and electronic properties of face-centred cubic ScIr2 compound is investigated by using a generalised gradient approximation scheme of density functional theory with and without spin-orbit interaction. The structural results show that the spin-orbit interaction has a negligible effect for the crystallizing of $ScIr_2$ compound. The Fermi surface calculations suggest considerable nesting along $\Gamma - X$ direction that could affect the vibrational properties.

Keywords: intermetallics, density functional theory, electronic structure, spin-orbit interaction

1. INTRODUCTION

Laves phase cubic $MgCu_2$-type (C15) intermetallic compounds are taken interest from a long time due to their interesting features such as heavy fermion behaviour, Kondo effect, interesting thermodynamic properties and especially favouring superconductivity [1-8]. The superconducting properties are studied by our group for these kind of compounds such as $CaIr_2$ and $CaRh_2$ [9]. In this study, it is observed that the spin-orbit interaction has to be taken account when the transition-metal d states dominate Fermi level region. First Compton and co-workers [10], then Geballe and co-workers [11] are successfully synthesized and studied cubic Laves $ScIr_2$ compound. They found that this compound is a superconductor with a 2.07 K superconducting transition temperature. In 2000, Goncharuk and colleagues [12] are investigated $ScIr_2$ compound for its thermodynamic features by using electromotive force measurements. They have obtained Gibb energies, enthalpies, and entropies for this compound. Shrivastava and Sanyal [13] are studied structural, electronic and elastic properties of $ScIr_2$ YIr_2, and $LaIr_2$ compounds by using full-potential linearized augmented plane wave (FP-LAPW) method. The results show that all studied compounds are showing ductile properties due to the elastic analysis. In 2019, also Chowdhury and Saha [14] have investigated the physical properties of $ScIr_2$ superconductor using *ab initio* technique. They have found that the

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electronic band structure reveals metallic conductivity and the major contribution comes from Ir-5d states. Even though there are several theoretical studies on structural and electronic properties of $ScIr_2$, there is no study included the spin-orbit interaction (SOI) for this properties.

Due to its interesting features, in this study, the structural and electronic properties of $ScIr_2$ is studied by using generalised gradient approximation (GGA) scheme implemented in Density Functional Theory with and without SOI. Since the compound has transition metal in its structure, the SOI effect on its electronic structure has to be researched. The structural lattice constants, bulk modulus and its pressure derivative B' are obtained by fitting the total energy as a function of the lattice parameter to the Murnaghan equation of states [15]. The electronic properties are calculated by using full-relativistic norm-conserving pseudopotentials for including SOI and compared by the results obtained via scalar-relativistic norm-conserving pseudopotentials without SOI.

2. METHOD

The first principles calculations are performed by using the Quantum Espresso package [16, 17]. The exchange-correlation calculations are determined by using the norm-conserving GGA scheme [18, 19]. While the full-relativistic norm-conserving pseudopotentials are employed for a description of interaction between the ionic cores and valence electrons with SOI, scalar relativistic norm-conserving pseudopotentials are used for the same calculations without SOI [18]. The wave function was expanded in plane waves with the energy cut-off of 60 Ry and the default charge-density value of 240 Ry is used for the norm-conserving pseudootentials. For the sampling of the Brillouin zone to obtain structural optimization, we have used a $(8 \times 8 \times 8)$ Monkhorst-Pack [20] $\vec{k}$-point mesh. For the electronic structure and the electronic density of states calculations $(24 \times 24 \times 24)$ Monkhorst-Pack [20] $\vec{k}$-point mesh is used.

3. RESULTS

3.1. Structural Properties

The $ScIr_2$ compound crystallizes in $MgCu_2$-type face-centred cubic (fcc) structure with the space group $Fd\bar{3}m$ (Wyckoff no:227). The structure is presented in Fig. 1. In this crystal structure, atomic positions are taken as Sc at 8b (0.375, 0.375, 0.375) and Ir at 16c (0.00, 0.00, 0.00). The ground state properties have been determined by calculating the total energy as a function of lattice constant (a (Å)) and fitted to the Murnaghan equation of state [15] for defining the equilibrium lattice, the bulk modulus (B), and the pressure coefficient (B') [15]. Table 1 presents the calculated values of a, B, B' and the distance between atoms along with available previous experimental and theoretical studies.

Table 1.The calculated structural properties for fcc $ScIr_2$ with available previous studies.

	$\boldsymbol{a}$(Å)	$\boldsymbol{d_{Sc-Ir}}$ (Å)	$\boldsymbol{d_{Ir-Ir}}$ (Å)	$\boldsymbol{B}$ (GPa)	$\boldsymbol{B'}$
This Work (With SOI)	7.450	3.1176	2.6587	209.3	4.39
This Work (Without SOI)	7.520	3.1201	2.6654	208.5	4.52
Experimental	7.348				
FP-LAPW[13]	7.399			224.2	5.02
GGA[14]	7.449			225.8	

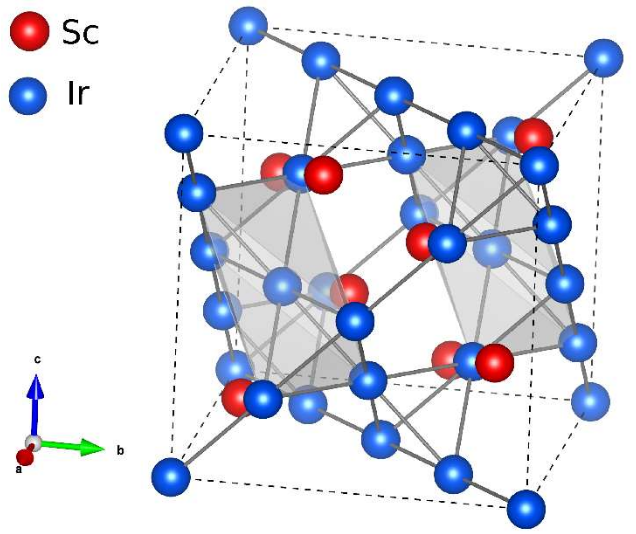

Figure 1. The fcc $MgCu_2$-type crystal structure of $ScIr_2$

The calculated results in this study are in accordance with previous experimental and theoretical results. More importantly, the results with and without SOI are very close to each other. This result is a sign for the spin-orbit interaction does not effect on the structural properties of studied $ScIr_2$ compound. The distance between Ir atoms is shorter than the sum of their covalent radii which suggest a covalent bonding between Ir atoms while the electronegativity difference between Sc and Ir atoms suggest an ionic bonding. It could be said that the $ScIr_2$ compound contains an interplay between covalent, ionic and metallic bonds.

3.2. Electronic Properties

The electronic structure of $ScIr_2$ compound without SOI is presented in Figure 2 (a). The electronic structure in this figure clearly shows the metallic nature of the studied compound because of the electronic bands that are crossing the Fermi energy level (E_F). Dispersive bands are crossing the E_F along all the symmetry directions that shows there is no insulated direction along the studied high symmetry points. The bands show nondispersive character along the $\Gamma - X$ direction which suggest the density of states at the Fermi level ($N(E_F)$) have a higher value because of this behaviour.

Figure 2 (b) is presented the electronic band calculations with (solid red lines) and without (dashed black lines) SOI for comparison. Even though there is some splitting effect occurred for six-fold and four-fold degenerated bands, since the compound is centrosymmetric, there is no splitting seen for the two-fold degenerated bands. The six-fold degeneration around -0.26 eV at the Γ high-symmetry point is split into two- and four-fold degenerated electronic band with a 0.1 eV energy difference. The split two-fold degenerated band stays under the E_F along $\Gamma - X$ direction and does not contribute the $N(E_F)$ value. Along the $\Gamma - L$ direction the SOI splitting make the split band get closer to E_F that makes more contribution to the $N(E_F)$. The SOI split four-fold degeneration into two-fold degenerated bands with a 0.04 eV difference at the W high symmetry point. Even though this splitting is quite small, the split bands get close to E_F. Overall, the SOI effect on the electronic band structure is negligible.

In order to investigate the nature of electronic bands, the total and partial density of states (DOS) with and without SOI of $ScIr_2$ are presented in Figure 2 (c), and a comparison between total DOS values with and without SOI is presented with an inset figure. From this inset figure, it is found that the effect of SOI on the total DOS of $ScIr_2$ is very small and negligible even though the $N(E_F)$ value with SOI seems higher than without SOI one. This feature could be related with the splitting effect that cause the electronic bands get near the E_F. The value of $N(E_F)$ with SOI is calculated to be 4.78 states/eV that decreases to 4.61 states/eV by turning off the SOC. These results are in accordance with previous FL-LAPW result of 4.64 states/eV [13]. The value of $N(E_F)$ consists of roughly 82 % of Ir electronic states and 18% Sc electronic states. In particular, Ir 5d state alone contribution to the $N(E_F)$ is up to 74%. This result signs that Ir 5d electrons are most influential in consisting the free electrons around the developing the E_F.

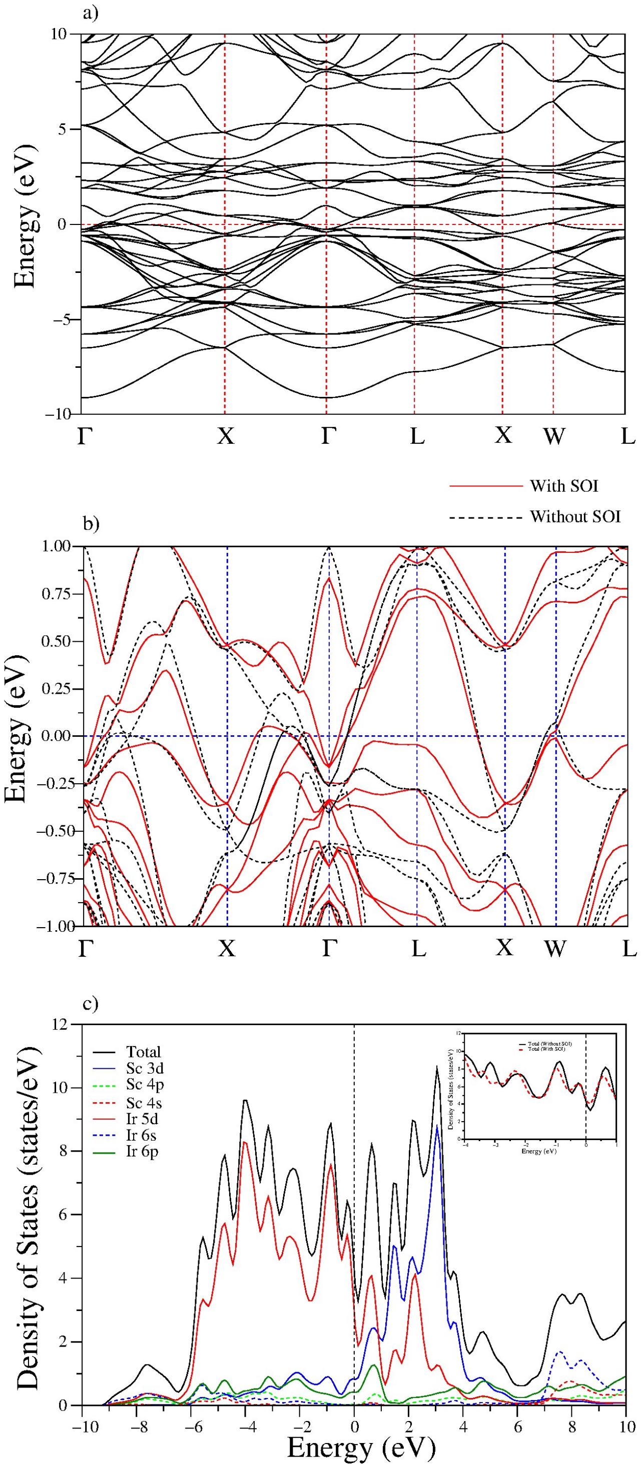

Figure 2. (a) The electronic structure of $ScIr_2$ compound without SOI, (b) The comparison between the electronic structure with (solid red lines) and without (dashed black lines) SOI, and (c) electronic DOS. The inset figure in (c) is presenting a comparison between total DOS values with and without SOI

For a better understanding the electronic properties with SOI, the Fermi surfaces of $ScIr_2$ is illustrated with and without SOI in Figure 3. The Fermi surfaces without SOI are illustrated in Figure 3 (b)-(c)-(d) and the Fermi surfaces with SOI are illustrated in Figure 3 (e)-(f)-(g)-(h). It is clear that the Fermi surfaces are divided into split sheets because of SOI. The Fermi surface in Figure 3 (b) has a hole characteristic and barely consists because the electronic band that constitute this surface is barely touched the E_F along $\Gamma - X$ direction. This Fermi surface does not consist when the SOI considered because SOI move this band away from the E_F. The Fermi surface presented in Figure 3 (c) without SOI is split into two Fermi surfaces that are given in Figure 3 (e) and Figure 3 (f). This Fermi sheets make a closed curves around the Γ and X high symmetry points which show a high nesting features [21-23] along $\Gamma - X$ direction. Similar to this feature, the Fermi surface calculated without SOI that presented in Figure 3 (d) is split into two different Fermi surfaces when the SOI taken into account. These surfaces are given in given in Figure 3 (g) and Figure 3 (h). The Fermi sheets without SOI show complex features when the SOI simplified them.

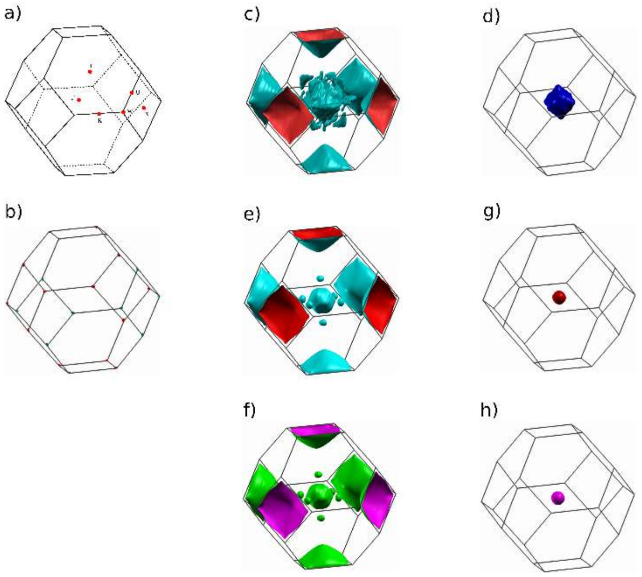

Figure 3. (a) High symmetry points of Brillouin zone of fcc structure, the Fermi surface sheets (b)-(c)-(d) without SOI, and (e)-(f)-(g)-(h) with SOI for $ScIr_2$ compound.

4. SUMMARY

The structural and electronic properties of face-centred cubic $ScIr_2$ compound is investigated by using a generalised gradient approximation scheme of density functional theory with and without spin-orbit interaction. The structural results show that the spin-orbit interaction has a negligible effect for the crystallizing of $ScIr_2$ compound. The distances between the atoms are also suggest an interplay between different kind of bonding features exist.

The electronic structure calculations are in good accordance with previous calculations[13, 14]. The SOI has a negligible effect on the electronic features of this compound even though the Fermi level is occupied by transition metal’s d orbital electrons. The Fermi surfaces are shown a considerable nesting and could affect the vibrational properties of studied $ScIr_2$ compound. Hence the lattice dynamical properties have to be examined with detail.

ACKNOWLEDGMENTS

I want to thank Prof. Dr. Hüseyin Murat Tütüncü and Dr. Ertuğrul Karaca for their invaluable support.

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