# Electronic Structure and Optical Properties Of EuIn 2 P 2

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# Electronic Structure and Optical Properties Of $EuIn_2P_2$

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**Abstract.** The electronic structures and, optical and magneto-optical properties of a newly found Zintl compound $EuIn_2P_2$ have been investigated within the density-functional theory using the highly precise full-potential linear-augmented-plane-wave method. Results of detailed investigation of the electronic structure and related properties are reported.

**Keywords:** Magneto-optical properties, $EuIn_2P_2$, density-functional theory.
**PACS:** 71.20.Eh, 78.20.-e, 78.20.Bh, 78.20.Ci,

## INTRODUCTION

Since the first presentation of the Zintl concept in the early 1990s by Eduard Zintl, Zintl-phase compounds have received a great deal of interest because of their fascinating structural variety and their useful synthetic and material applications[1]. Zintl compounds containing rare-earth ions have a variety of physical properties, such as peculiar magnetic orders, superconductivity, and colossal magneto-resistance[2-4].

There are several Eu containing Zintl phases that show unusual magnetic and magneto-transport properties. These phases are typically antiferromagetic at low temperature, while often showing a positive Weiss constant which suggests ferromagnetic correlations in the paramagnetic region. Recently, a new Eu-containing Zintl compound $EuIn_2P_2$ has been discovered[5]. The compound crystallizes in the hexagonal structure (space group $P6_3/mmc$) and contains Eu and $In_2P_2$ layers alternating along the c-axis. It exhibits a magnetic order at magnetic-transition temperature $T_C$~24K. Above $T_C$, magnetic susceptibility shows a Curie–Weiss behavior with Weiss temperature of $\theta_w$~27K. The temperature-dependent resistivity measurements show that the resistivity of $EuIn_2P_2$ is in the order of $10^{-5}$ Ω m, indicating that $EuIn_2P_2$ is in a semimetal regime. Interestingly, the electrical resistivity measurement shows a semi-conducting behavior with a small band gap of 3.2 meV[5]. The specific heat of $EuIn_2P_2$ at high magnetic field studied by Hidaka *et al*.[7]

$EuIn_2P_2$ is a newly discovered compound, having large magneto-resistance, we thought it worthwhile to investigate its electronic structures and related properties in detail. Since the experimental data of optical conductivity of $EuIn_2P_2$ exits as well, we carry out the calculations of optical properties in connection with the electronic structures. We have performed spin-polarized full-potential linearized-augmented-plane-wave (FP-LAPW) calculations, including spin-orbit coupling (SOC) with local-

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spin-density approximation (LSDA) and LSDA plus Hubbard parameter *U i.e.* LSDA+*U*.

$EuIn_2P_2$ crystallizes in the hexagonal structure (space group P 6(3)/mmc) with a unit cell of a=4.0829 Å, c=17.5955 Å. The lattice consists of Eu layers in the ab plane, separated by $In_2P_2$ layers alternating along the c axis [5]. The spin-polarized calculations, including SOC, have been performed using the FPLAPW method as implemented in WIEN2K code[14]. The LSDA+*U* method is used for better account of the correlation between the 4*f* electrons in rare-earth compounds. For the Eu *4f* electrons in LSDA+*U*, *U*=2.0 to 7.0 eV with interval of 0.5 eV is used. The value of *U*=7.0 was also reported in the previous LSDA+*U* calculations for another europium compound[16], to obtain correct energy position of 4*f* bands. To provide a reliable Brillouin zone integration, a set of 480 **k**-points in the irreducible wedge of the Brillouin zone (IBZ) was used. The convergence was also checked with a large **k**-points refined mesh in IBZ with no appreciable change in energy or properties. A broadening of 0.1 eV is taken to simulate the experimental finite life-time effects.

We have performed the calculations of $EuIn_2P_2$ in two directions of magnetization (i) along *a* axis, and (ii) along *c* axis, and found that the *a* axis (energy favorable) is the easy axis, in agreement with the experiment[5]. The calculated total magnetic moment of $EuIn_2P_2$ is almost same in both cases i.e. $6.99\mu_B$/Eu which is close to the experimental value and expected value for the free $Eu^{+2}$ ions, suggesting that the $Eu^{+2}$ moments localized. We have presented the results for band structure, optical and magneto-optical properties, by considering the magnetization along the easy axis.

Jiang *et al* [5] observed very small resistivity in the scale of $10^{-5}\Omega$ m which comes in the semi-metallic range and it drops quickly at the magnetic-transition temperature. They also reported a band gap of 3.2 meV, which is very small and two or three orders smaller than those of normal semiconductors. We have performed the spin polarized calculations by using LSDA and LSDA+*U* approaches however, not able to open the energy gap, even though, we have used different *U* values from 2.0 eV to 7.0 eV.

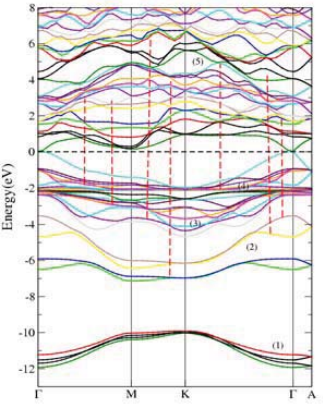


**Figure 1**. The calculated band structure of $EuIn_2P_2$

We present here the LSDA+$U$ ($U$=7.0) results for the BS and DOS with the partial DOS of $EuIn_2P_2$. The BS for the majority spin is shown in Fig. 1. The BS for minority spin is similar to that for the majority spin except that the Eu unoccupied *f* states lie as high as ~7eV above the Fermi level ($E_F$). The total DOS along with the partial DOS is shown in Fig. 2. From the partial DOS, we are able to identify the angular momentum character of the states. The calculated BS and DOS of the $EuIn_2P_2$ can be divided in to five groups of band. The first group of bands lies in the energy range 12 to 10 eV below $E_F$ is mainly due to the P-*s* with some amount of In-*s* states. The large depth from $E_F$ ensures that these bands retain their atomic character and do not attain the conventional large bandwidth. The second group of bands from 7.0 eV to 4.0 eV below $E_F$ are due to the occupied In-*s*, P-*p* states. These bands are degenerate and less dispersive in comparison with the conduction bands. The third and fourth group of bands lie between -4.0 eV to $E_F$. The sharp peak at -3.0 eV originates from the occupied Eu-*f* states. The last structure of bands above $E_F$ is mainly derived from the hybridization between Eu-*d* states and In-*s* and *p* and P-*d* states.

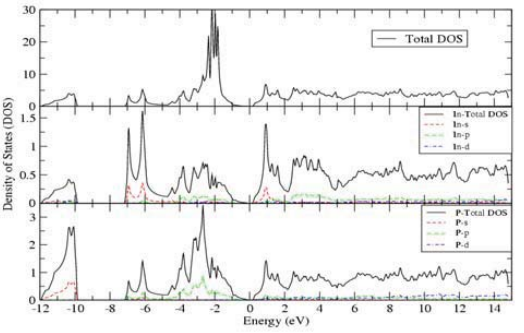


**Figure 2.** The calculated total density of states of $EuIn_2P_2$ along with projected density of states of In and P.

Our results of the optical conductivity produce a strong shoulder at ~0.4 eV and peak at 0.85 eV, similar to its experimental counterparts. The calculated spectrum also shows structures between 2 to 4 eV, which are due to the transitions between In-*p* states to Eu-*d* states. The structures at higher energy range 3 to 6 eV belongs to the transitions between groups band (2 and 3) to group of bands above $E_F$. The magnitude of calculated optical conductivity is larger than experimental one. If we increase the broadening the magnitude comes closer to the experimental but lost the structures.

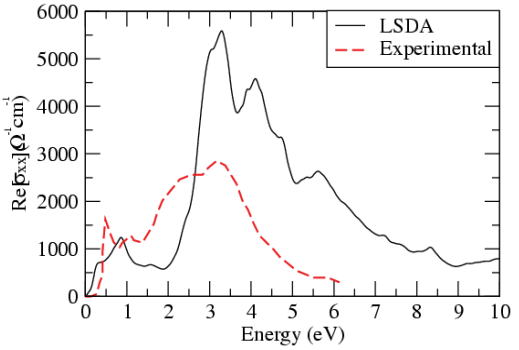


**Figure 3.** The calculated real part of diagonal optical conductivity Re $[\sigma_{xx}]$, along with corresponding experimental data, of $EuIn_2P_2$

In conclusion, the spectral features of the optical-conductivity tensor in the 0–10 eV energy range were analyzed in terms of the BS and DOS. The experimentally observed energy gap 3.2 meV is too narrow to extract a meaningful data and also difficult to produce this small gap by using DFT. Therefore, we argue that the apparent 'semiconducting' behavior observed in the range of 29-60K is just an accidental coincidence, but not a 'real' semiconducting one. We found that different types of interband transitions contribute in shaping the conductivity tensor. The dipole matrix elements play a key role greatly affecting the optical spectra in the low as well as high energy ranges. Further studies are needed in order to better explain how the proper electronic structure can be achieved (i.e., by making use of alloying, pressure, strain field) in order to enhance the minima of Re $[\sigma_{xx}]$.

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