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Study the Band Structure and Density of State Of Co Using Density Functional Theory

Saeedeh Arabzadeh, Mohamad Reza Benam
Department of physics, Payamenor University of Mashhad, Mashhad, Iran

Abstract

We have studied the properties of CO-hcp in its bulk state . The Calculations were performed in the framework of density functional theory (DFT),using full-potential linearized augmented plane wave (FP-LAPW) method with generalized gradient approximation (GGA) for exchange – correlation potential. We have calculated the Energy band structure and total density of state of Co. In order to study the magnetic properties of Co,The calculation was performed in spin polarized situation. The result shows that the Co-hcp is a ferromagnetic and the electrons of localized d-orbital have a predominant contribution on its magnetic behavior. We obtained 3.147μ_B for magnetic moment per unit cell which is comparable to its experimental value i.e.3.42 μ_B.

I. Introduction

Cobalt is an essential element for life in minute amounts. It is found naturally only in chemically combined form. The free element, produced by reductive smelting, is a hard, lustrous, silver-gray metal. The most common ores of cobalt are cobaltite smaltite , chloranthite and linnaeite .The major suppliers of cobalt in the world are Zambia ,Canada ,Russia, Australia ,Zaire and Cuba.

Cobalt has a valence of 2 or 3. Cobalt is a hard, brittle metal .Its is similar in appearance to iron and nickel .Cobalt has a magnetic permeability around 2/3 that of iron [1]. The magnetic moment is 1.7 Bohr magneton per atom [2].Cobalt is found as a mixture of two allotropes over a wide temperature range .Nowadays Cobalt is used in the preparation of permanent magnetic devcices. Cobalt forms many useful alloys. It is alloyed with iron, nickel and other metals to form Alnico, an alloy with exceptional magnetic strength. Cobalt is used in magnet steels and stainless steels. A cobalt chloride solution is used to make a sympathetic ink. Cobalt is essential for nutrition in many animals. Cobalt-60 is an important gamma source, tracer, and radio therapeutic agent [3].The most important application is in the production of super alloys. Super alloys primarily consist of iron, cobalt or nickel with small amounts of other metals, such as chromium ,tungsten, aluminum and titanium[4].Super alloys are resistant to corrosion (rusting) and retain their properties at high temperatures .Cobalt's use in magnetic alloys is critical for devices that must hold a magnetic field, such as electric motors .Cobalt is one of only three naturally occurring magnetic metals. The other two are iron and nickel .The magnetic properties of cobalt are even more obvious in alloys. In medicine , it is used to find and treat diseases . Cobalt is needed for the production of vitamin B12.Vitamin B12 is necessary to ensure that an adequate number of red blood cells are produced in the body[5].

II. Method of Calculation

The calculation were performed in the framework of density functional theoty (DFT)[6], using the full linearized augmented plane wave (FP-LAPW) method as implemented in Wien2k codes .The generalized gradient approximation(GGA) of Perdewet al was selected for the exchange-correlation energy in ourcalculations . The wave function were expanded into spherical harmonics within atomic muffin-tin (MT) spheres and in the form of plane waves in the remaining space .The MT spheres are supposed not to overlap with each other . The chosen radii of MT spheres for Co atom is RMT(Co)=2.26Å.The cut –off energy ,which defines the separation of the valence and core states, was chosen to be about -6. Ryd.The space group for our unitecell was chosen to be 194-P63 mmc for hexagonal phase . The lattice constants after optimizing were obtained as a=b=4.66Å and c=7.5492Å.

For solving the Kohn–Sham equations , the relativistic effects have been taken into account and also .The iteration process was stopped after the calculated total energy converged to less then 0.0001 Ryd . A total of 12 iterations were necessary to achieve self – consistency in our calculations.

For doing calculation, we should optimize lattice constant and the necessary number of k-points in the first Briloen zone .In order to obtain the theoretical equilibrium cell parameters. We have calculated and drawn the total energy with respect to lattice parameter

with this condition that the c/a be constant and equal to 1.62 . The equilibrium lattice parameter at minimum energy was obtained about a=4.66Å and therefore c=7.5492Å (see Figure 1).

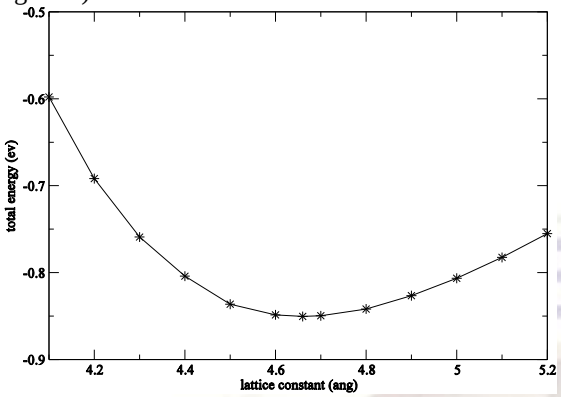


Figure 1:The change of total energy with respect to lattice parameter.

In order to obtain optimum number of k-points, we have calculated and drawn the total energy with respect to k-points in the first Briloen zone which has been shown in Figure 2. According to this diagram we chose the optimum number of k-points to be 2000.

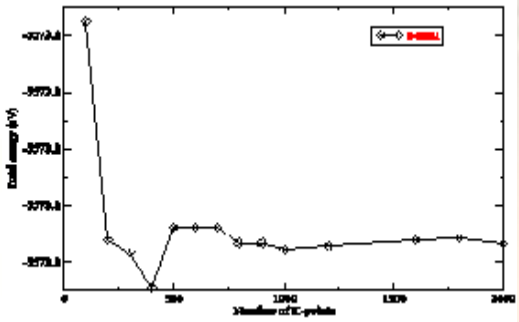


Figure 2: The change of total energy respect to number of k-points in the first Briloen zone

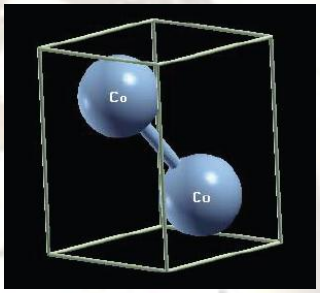
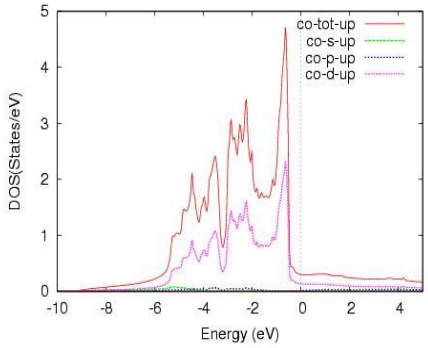


Figure 3: unitecell of Co

Image of unitecell of Co along the lines of high symmetry inside the first Briloen Zone (BZ) have been shown In fig. 3. The total Density of State for the spin up and down situation of Cowith the calculations of partial DOS(P-DOS) for spin up and down polarization has been shown in Figures 4 and 5.

In this Figures we see that the population of electrons in majority and minority spin are not equal which means that Co should be a ferromagnetic material . In fact the Fermi energy passes through the total DOS of spin down state which meansit is a metal and has ferromagnetic characteristic.



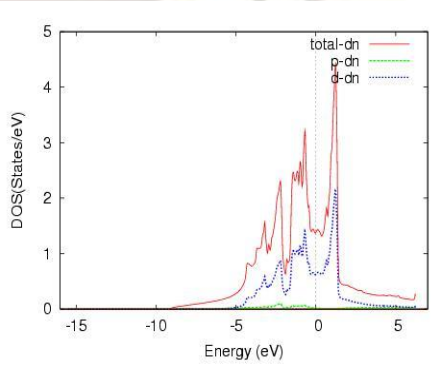


Figure 4: The total Density of State and (P-DOS) in the spin up Figure 5: The total Density of State and (P-DOS) in the spin down

The contribution to the valance band is mainly from the Co- 3d orbital which has been extended nearly from zero to - 6 in spin up and nearly from 1.5 to – 5 in spin down situations .The first

Briloen Zone (BZ) of Co and the line with high symmetry inside it has been shown in Figure 6. The spin –polarized calculations for band structure of Co have been performed for orbitals s, p, d, of Co and has been shown in Figure 7.

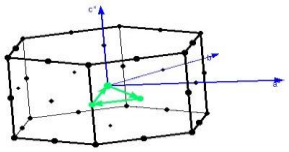
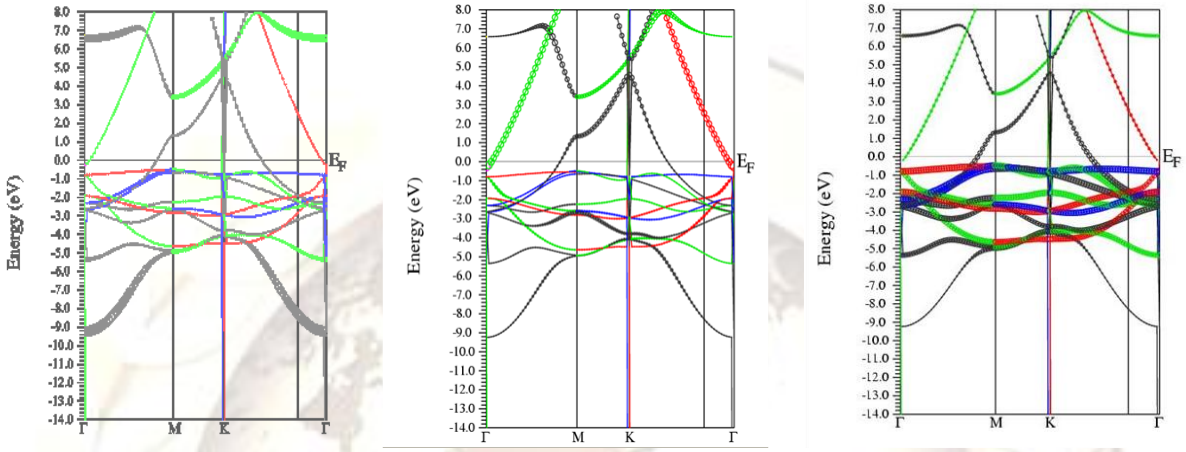


Figure 6: The first Briloen Zone (BZ) with the line of high symmetry.



(a()b()c())

Figure 7:Contribution of S-orbitals(a), P-orbitals(b) and d-orbitals (c) in the band structure.

We see in Fig7 . that Contribution of s-orbitals the band structure has been extended nearly from - 9.4 to -4.4 and also from 4.4 to 8 and the Contribution of p-orbitals has been extended nearly from - 0.4 to 8 and the Contribution of d-orbitals has been extended nearly from 0.8 to 5.4. We see that the Contribution of d-orbitals on the band structure around the Fermi energy is high and therefore the d-orbitals play a crucial rule on the electronic and magnetic properties of Co. We also have obtained 3.147 μ_B for magnetic moment per unit cell which is comparable to its experimental value i.e.3.42 μ_B [7].

III. Conclusion :

In conclusion , the Band structure and total density of state of Co for spin up and down polarization were calculated and compared with each other . There was a remarkable difference between the two spin situations. We may benefit from this calculation in spintronic and magneto-optic devices which the spin component plays a crucial rule in them. The amount of spin magnetic moment per unit cell was calculated about 3.147 μ_B. The amount of spin magnetic moment per unit cell was calculated about 3.42 μ_B.

IV. Acknowledgment

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