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Research Article

A DFT STUDY OF STRUCTURAL AND ELECTRONIC PROPERTIES OF SPINEL FERRITE $CdFe_2O_4$

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Abstract

A density functional theory (DFT) study of structural and electronic properties of Spinel ferrite $CdFe_2O_4$ is done here by using computer code WIEN2k. Structural characteristics like lattice constant, bulk modulus, ground state volume and ground state energy are determined by using exchange correlation approximations LDA, PBE-GGA and WC-GGA. Lattice constant measured by PBE-GGA is agreed well with the experimental results. All three types of approximations reveal that $CdFe_2O_4$ has simple cubic structure. Density of States (DOS) and band structure are determined by using Full Potential Linearized Augmented Plane Wave (FP-LAPW) method within generalized gradient approximation PBE-GGA. The values of lattice constant, ground state energy and bulk modulus using the approximations PBE-GGA are 8.7030 Å-33770.2312 Ry and 168.7308 GPa, respectively. Total density of states (TDOS) and partial density of states (PDOS) are determined for both spin-up and spin-down. Energy band gap (1.2 eV) shows that Cadmium Ferrite has half metallic nature and has indirect band gap. Cadmium Ferrite is low gap semiconductors and widely used in electronics such as in magnetic and magneto-optic recording devices and in data storage devices. This work provides first comprehensive DFT study to understand the properties of Cadmium Ferrite ($CdFe_2O_4$) with LDA, PBE-GGA and WC-GGA.

Keywords:
DFT, DOS, PDOS, cadmium ferrite.

1. Introduction

Ferrites are generally has resistivity in between those of conductors and insulators. Electronic properties of ferrites have made them more attractive and interesting for both scientists and engineers. These properties of ferrites have made them able to play an important role in manufacturing of magnetic switches, transformer cores, microwave devices, micro electric devices, sensors, electromagnetic circuits and in the field of medicines [1, 2]. General Formula for spinel ferrites is MFe_2O_4, here M is a divalent metal ion e.g., Magnesium ($_{12}$Mg), Manganese ($_{25}$Mn), Nickel ($_{28}$Ni), Copper ($_{29}$Cu), Cadmium ($_{48}$Cd) etc., Fe is cation (+ve ion) and O is an anion (-ve ion). Spinel ferrites have simple cubic structure, their space group is 227 ($Fd\bar{3}m$) [3]. Lattice constant for spinel ferrites is about 8.38 Å and their curie temperature is 668 K. Resistivity of spinel ferrites is about $1\times106\ \Omega$ m. The crystal structure of spinal ferrites is cubic and has two interstitial sites called tetrahedral site and octahedral site. Each unit cell of spinel ferrites consist of eight units (cube) and therefore written as $M_8Fe_{16}O_{32}$. Bragg and Nishikawa were the first who determined the cubic structure of spinel ferrites [4].

Among all types of ferrites spinel-ferrites are very important because of their wide range of applications in many fields. Spinel ferrites are very useful materials for magnetic recording media and computer memory devices. They are also used in components of magnetic switches, electronic filters and microwave devices. For memory and switching devices they are used in form of thin films. They are extensively used in manufacturing of rod antenna and radio frequency coil [5, 6]. Spinel ferrites are used to make sensors which have definite and sharp Curie temperature and can be used for temperature control. These ferrites can also be used for humidity sensitivity, they have large surface area, open pore formed on bulk surface and have high surface charge density [7, 8].

$CdFe_2O_4$ is an important spinel ferrite, it has many applica-

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tions in bulk form as well as in nanoparticle form. $CdFe_2O_4$ is a semiconductor oxide. It has an ability to resolve the many environmental and energy problems. $CdFe_2O_4$ can use solar energy to eliminate serious pollutants in air as well as in water, it can also effectively detect toxic gases in atmosphere of Earth and can protect the living organisms from harmful impacts of various pollutants present in our surrounding[9, 10]. $CdFe_2O_4$ is a normal spinel ferrite and like other ferrites it also shows magnetic properties[11]. $CdFe_2O_4$ in bulk form shows ferromagnetic properties but below 10K it shows antiferromagnetic behavior [12]. Cadmium ferrite ($CdFe_2O_4$) has a number of electronic, magnetic, catalytical and electrical switching properties. $CdFe_2O_4$ has cubic structure belonging to space group 227 i.e. Fd3m. In Cadmium ferrite Cd is tetrahedral cation, Fe is octahedral cation, here the unit cell dimensions (Lattice Constant) a = 8.7050Å, anion positional parameter ucalc = 0.2685Å, tetrahedral bond length R_{tet} = 0.780Å, octahedral bond length R_{oct} = 0.645Å, electronegativity of tetrahedral cation χ_{tet} = 1.690, electronegativity of octahedral cation χ_{oct} = 1.830 [13]. In bulk form $CdFe_2O_4$ has X- ray density ρ = 5.81x 103 Kg m-3, force constant K=1.00 x102 Nm-1 , bulk modulus B = 206 GPa , young modulus E = 185 GPa , rigidity modulus G = 68 GPa , PoissonÂ´s ratio σ = 0.35 , Debye temperature θ = 499 k [14]. Experimentally it is noted that Cadmium ferrite has conductivity in between the conductors and insulators, at standard temperature the experimental values of band energies for $CdFe_2O_4$ are given as, conduction band energy ECB = 0.55 eV , valance band energy EVB = 2.85 eV, energy band gap Eg = 2.3 eV, these values show that Cadmium ferrite is electrically semiconductor material [15]. This research is an attempt to find out structural and electronic properties of spinel ferrite $CdFe_2O_4$ based on DFT and then compares them with already existing experimental results.

2. Materials and Methods

Density Functional Theory is the theoretical tool to investigate solids by finding the density of electrons in the material. DFT is an ab-initio method to solve the Schrodinger equation for many body problems. In this theoretical technique a number of suitable approximations are made to solve the Schrodinger equation and an attempt is made to reach to the reasonable suitable results of the given materials. The first step to solve Schrodinger wave equation for complex matter is the Born-Oppenheimer approximation. This approximation separates the motion of nuclei and the electrons. Hartree proposed that Schrodinger equation for many electron system can be rewrite as a single-electron equation, and this electron is considered as moving in a mean potential from all the other electrons. According to Hartree-Fock approximation the exact wave function of many-body system needs to be anti-symmetric function by exchange of electrons. InHartree-Fock technique the exchange is treated exactly but the correlation is ignored [16, 17].

DFT is based on charge density of electrons rather than wave function of electrons, i.e., $E(\Psi_\circ) = E(\rho_\circ)$. DFT is a successful and an efficient technique to investigate a solid. It is the most reliable method to find the properties of condensed matter. It is the theory which reduced the many-particle Schrodinger equation to single-body independent Schrodinger equation. Modern DFT found its roots in 1964 AD by Hohenberg and Kohn. They gave two landmarks theorems which provided a base to investigate a material theoretically by using DFT [18]. Kohn and Sham played an important role to make DFT more suitable to measure the exact value of electron density. By applying the Kohn-Sham ideas the single electrons equations are formed. These single electrons Schrodinger equations are known as Kohn-Sham equations. i.e.

$$\widehat{H}_{KS}\Phi_i = \left[-\frac{1}{2}\nabla^2 + V_{eff}\left[\rho\left(\overrightarrow{r}\right)\right]\right]\Phi_i\left(\overrightarrow{r}\right) \quad (1)$$

Here $\widehat{H}_{KS}$ is single electron Hamiltonian and $V_{eff}(r)$ is effective potential formed by all other electrons in which single electron moves. This effective potential can be written as,

$$V_{eff}\left[\rho\left(\overrightarrow{r}\right)\right] = V_{ext}\left(\overrightarrow{r}\right) + \widehat{V}_H\left[\rho\left(\overrightarrow{r}\right)\right] + V_{xc}\left[\rho\left(\overrightarrow{r}\right)\right] \quad (2)$$

The Kohn-Sham equations are needed to be solved self-consistently. An initial charge density is supposed and then by using this initial guessed the Hamiltonian for this charge density is set up and then diagonalized the resulting approximate Hamiltonian. The main purpose of Kohn-Sham theory is to find the exact results for many-body system by making reasonable approximations to calculate $\frac{E_{xc}}{V_{xc}}$ [19].

Here in these calculations we used three different approximations LDA, PBE-GGA and WC-GGA to find the structural and electronic properties of $CdFe_2O_4$. WIEN2k is a computer software which is being used here, WIEN2k works on the bases of DFT [20, 21]. WIEN2k is an excellent scheme to find out the structural, electrical, magnetic, optical and elastic properties of solid materials. The computer code WIEN2k is followed the method of Full Potential Augmented Plane-Wave (APW) + local orbitals (Lo). Here in this method the crystal unit cell is divided into two main regions, one is non-overlapping Muffin-Tin sphere and the second is the remaining interstitial space. WIEN2k is an all electrons method, it can made calculations for valance electrons and also for the core electrons [22].

3. Results and Discussion

3.1. Structural Properties

Structural properties of Spinel ferrite $CdFe_2O_4$ is determined here by using Density Functional Theory (DFT), structural properties is characterized by finding some important parameters such as lattice constant, bulk modulus, minimum volume, minimum energy and the pressure derivative of bulk modulus. These structural parameters are determined at different potentials by using LDA, PBE-GGA and WC-GGA. To determine the ground state energy for these two compounds, their total energy is minimized at various volumes by using the Murnaghan's equation of state [23] which can be given as,

$$E(V) = E_\circ + \frac{9V_\circ B_\circ}{16}\left[\left\{\left(\frac{V_\circ}{V}\right)^{\frac{2}{3}} - 1\right\}^2 B'_\circ + \left\{\left(\frac{V_\circ}{V}\right)^{\frac{2}{3}} - 1\right\}^2 \left\{6 - 4\left(\frac{V_\circ}{V}\right)\right\}^{\frac{2}{3}}\right] \quad (3)$$

Here $B'_\circ$ is the pressure derivative of bulk modulus $B_\circ$ and it is given as,

$$B'_\circ = \frac{dB_\circ}{dP} \tag{4}$$

Where $E_\circ$ is the minimum energy and $V_\circ$ is the minimum volume By taking minimum energy the graphs are drawn between total energy and the volume for all three approximations i.e. LDA, PBE-GGA and WC-GGA. In each case approximations having values of structural parameters nearly equal to that of experimental values are selected. Our calculated structural parameters by using PBE-GGA are completely agreed with experimental values. Atomic positions of cadmium (Cd), iron (Fe), and oxygen (O) in Cadmium ferrite which are used to calculate the optimized lattice constants are given in table 1. Each unit cell of optimized $CdFe_2O_4$ crystal is cubical belonging to space group 227 (Fd3m), cubical crystal structure of $CdFe_2O_4$ is shown in figure 1.

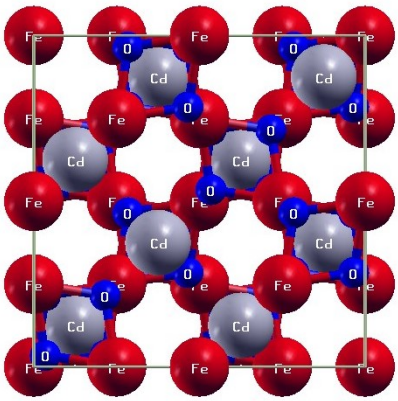

Figure 1: Crystal structure of $CdFe_2O_4$

By using Local Density Approximation (LDA) calculated ground state energy is $E_\circ$ = -33725.3212 Ry, minimum optimum volume is $V_\circ$=1034.4154 a.u3, the stiffness of the material (Bulk Modulus) is B = 214.1811 GPa, the pressure derivative of bulk modulus is BP = 5.0000. Calculated Lattice Parameters by LDA and relative % error by comparing with experimental data is shown table 2. Optimized curve volume vs energy for CdFe2O4 by using LDA is shown in figure 2.

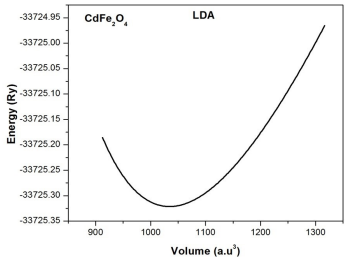

Figure 2: Volume vs Energy Plot for $CdFe_2O_4$ within LDA

By using PBE-GGA calculated ground state energy is $E_\circ$ = -33770.2312 Ry, minimum optimum volume is $V_\circ$= 1112.1083 a.u3, the stiffness of the material (Bulk Modulus) is B = 168.7308 GPa, the pressure derivative of bulk modulus is BP = 5.0000. Calculated Lattice Parameters by PBE-GGA and relative % error by comparing with experimental data is shown table 3. Optimized curve volume vs energy for $CdFe_2O_4$ by using PBE-GGA is shown in figure 3.

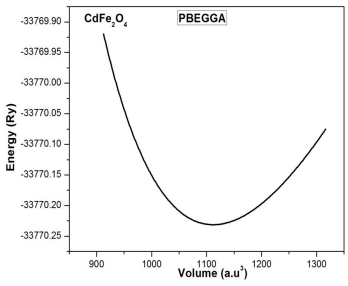

Figure 3: Volume vs Energy Plot for $CdFe_2O_4$ within PBE-GGA

By using WC-GGA calculated ground state energy is $E_\circ$= -33762.4552 Ry, minimum optimum volume is $V_\circ$ =1071.3152 a.u3, stiffness of the material (Bulk Modulus) is B = 181.9959 GPa, the pressure derivative of bulk modulus is BP = 5.0000. Calculated Lattice Parameters by WC-GGA and relative % error by comparing with experimental data is shown table 4. Optimized curve volume vs energy for $CdFe_2O_4$ by using WC-GGA is shown in figure 4.

Table 1: Atomic positions for $CdFe_2O_4$

Atoms	X	Y	Z
Cd	0.125	0.125	0.125
Fe	0.5	0.5	0.5
O	0.2847	0.2847	0.2847

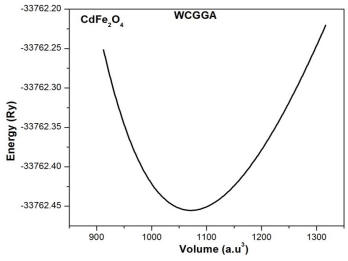

Figure 4: Volume vs Energy Plot for $CdFe_2O_4$ within WC-GGA

3.2. Electronic Properties

In complex matter physics the density of states (DOS) of a material are described as, “number of states per interval of

Table 2: Calculated Lattice Parameters by LDA for $CdFe_2O_4$

Lattice parameter	Calculated values	Experimental Data [14]	% Error
Lattice Constant $a_\circ$(Å)	8.4954	8.7000	2.35
Minimum Volume $V_\circ(a.u^3)$	1034.4154	1033.215	0.12
Minium energy $E_\circ(Ry)$	-33725.3212	-33720.416	0.014
Bulk Modulus B (GPa)	214.1811	206	3.97
BP	5.000	5.000	0.0

Table 3: Calculated Lattice Parameters by PBE-GGA for $CdFe_2O_4$

Lattice parameter	Calculated values	Experimental Data [14]	% Error
Lattice Constant $a_\circ$(Å)	8.7030	8.7000	0.034
Minimum Volume $V_\circ(a.u^3)$	1112.1083	1033.215	7.6
Minium energy $E_\circ(Ry)$	-33770.2312	-33720.416	0.15
Bulk Modulus B (GPa)	168.7308	206	18.09
BP	5.000	5.000	0.0

energy at each energy level available to the occupied". In crystalline structure of a material electron waves can propagate only in one direction i.e. only certain states are permitted. Therefore it can be possible that in any specific energy level a number of states are available for occupation and on another energy level it can also be possible that no states are available. In three dimensional system the units of DOS is Energy-1 Volume-1 , in two dimensional system units of DOS is Energy-1 Area-1 , in one dimensional system the units of DOS is Energy-1 Length-1 [24].

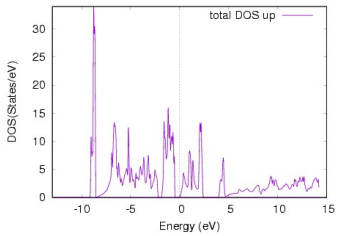

Figure 5: TDOS of $CdFe_2O_4$ for up spin within PBE-GGA

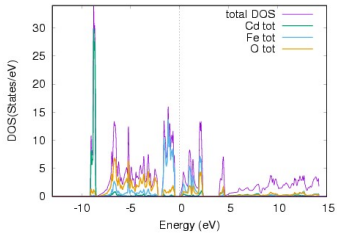

Figure 6: TDOS of $CdFe_2O_4$ for down spin within PBE-GGA

We computed total density of states (TDOS) and partial density of states (PDOS) for $CdFe_2O_4$ crystal by using exchange correlation approximation PBE-GGA. Total density of states for spin up and spin down are shown in figures 5 and 6 respectively. TDOS for spin up shows that band gap calculated by PBE-GGA corresponds to three parts in valance band of energy range -9.2 eV -8.4 eV, -8.2 eV 3.0 eV and -1.8 eV -0.4 eV.

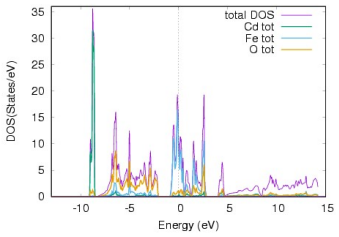

Figure 7: PDOS of $CdFe_2O_4$ for up spin within PBE-GGA

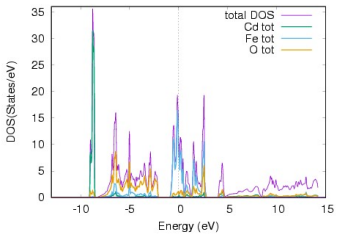

Figure 8: PDOS of $CdFe_2O_4$ for down spin within PBE-GGA

In valance band region the energy range -9.2 eV -8.4 eV has DOS value 38, -8.2 eV 3.0 eV has DOS value 13.5 and -1.8 eV -0.4 eV has DOS value 16. Highest valance band peak occurs in region -9.2 eV -8.4 eV. Total density of states (TDOS) of CdFe2O4 for up-spin within PBE-GGA shows that conduction band corresponds to 0 eV 2.5 eV, 4.2 eV 4.8 eV and 5.0 eV 14.2 eV. In conduction band region the energy range 0 eV 2.5 eV has DOS value 13.8, energy range 4.2 eV 4.8 eV has DOS value 7.6 and 5.0 eV 14.2 eV has DOS value

Table 4: Calculated Lattice Parameters by WC-GGA for $CdFe_2O_4$

Lattice parameter	Calculated values	Experimental Data [14]	% Error
Lattice Constant $a_\circ$(Å)	8.5953	8.7000	1.20
Minimum Volume $V_\circ(a.u^3)$	1071.3152	1033.215	3.7
Minium energy $E_\circ(Ry)$	-33762.2312	-33720.416	0.12
Bulk Modulus B (GPa)	181.9959	206	11.6
BP	5.000	5.000	0.0

4. Highest peak in conduction band region is occurred between 0 eV 2.5 eV. Partial density of states (PDOS) of Cadmium Ferrite ($CdFe_2O_4$) for spin up and spin down within PBE-GGA are shown in figures 7 and 8 respectively.

PDOS for spin up shows that on valance band region the contribution made by Cadmium (Cd) is from -9.2 eV to -8.4 eV at DOS value 30 and Cd contributes on conduction band side from 0 eV to 2.5 eV at DOS value 1.2. Contribution made by Fe in valance band region is from -7.6 eV to -2.2 eV at DOS value 3 and from -1.8 eV to -0.4 eV at DOS value 14. Fe has its contribution in conduction band region from 0 eV to 2.5 eV at DOS value 8. Oxygen (O) contribute from -9.2 eV to -8.4 eV at DOS value 1.5, from -8.0 eV to -3.0 eV at DOS value 6.5 and from -1.8 eV to 0.4 eV at DOS value 2 in valance band region. O made contribution from 0 eV to 2.5 eV at DOS value 4.5 and from 4.2 eV to 4.8 eV at DOS value 2 in conduction band region.

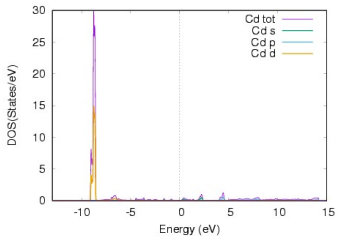

Figure 9: PDOS of Cd-atom for up spin within PBE-GGA

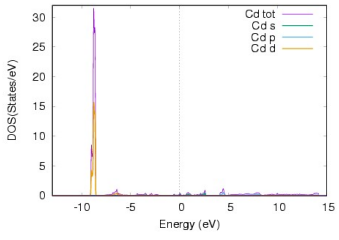

Figure 10: PDOS of Cd-atom for down spin within PBE-GGA

In total density of states (TDOS) the highest peak in valance band region with DOS value 38 is mainly contributed by Cadmium Cd-4d. In valance band region from -8.2 eV to 3.0 eV at DOS value 13.5 is contributed by Oxygen O-2p and similarly third range in valance band from -1.8 eV to 0.4 eV with DOS value 16 is mainly contributed by Fe-3d. In conduction band the highest peak with DOS value 13.8 from 0 eV to 2.5 eV is contributed by both Fe-3d and O-2p. Partial density of states (PDOS) for Cd, Fe, and Oxygen with spin up and spin down are shown in figures 9-14.

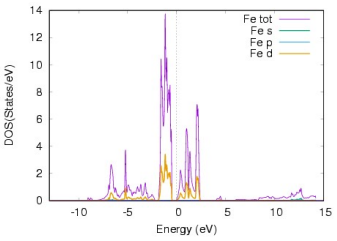

Figure 11: PDOS of Fe-atom for up spin within PBE-GGA

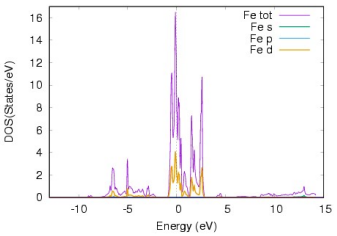

Figure 12: PDOS of Fe-atom for down spin within PBE-GGA

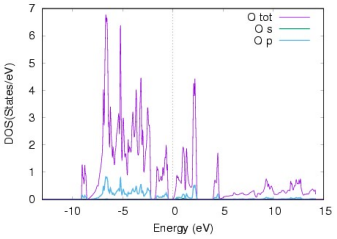

Figure 13: PDOS of O-atom for up spin within PBE-GGA

Band gap calculations for $CdFe_2O_4$ is calculated by using the exchange correlation approximation PBE-GGA between the energy range -10.0 eV to 8.0 eV. Band gap for $CdFe_2O_4$ for up-spin and down-spin within PBE-GGA are shown in figures 15

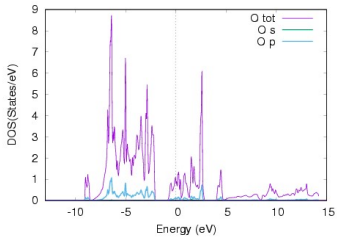

Figure 14: PDOS of O-atom for down spin within PBE-GGA

and 16 respectively. In our calculations it is found that Cadmium Ferrite has indirect band gap structure. Band structure of $CdFe_2O_4$ for up-spin shows a band gap of about 1.2 eV but for down-spin valance band and conduction band overlap each other showing zero band gap. This predicted that Cadmium Ferrite ($CdFe_2O_4$) is semiconductor in nature. At $0^{\circ}C$ or at 273K experimental value for $CdFe_2O_4$ band gap is about 2.3 eV [15].

4. Conclusion

WIEN2k computer code is used here, it applies the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method within DFT. Structural parameters such as lattice constant, bulk modulus, ground state volume and ground state energy are determined here by using three exchange correlation potentials LDA, PBE-GGA and WC-GGA. Results obtained here by using DFT are agreed with experimental results especially with PBE-GGA. These calculations show that $CdFe_2O_4$ has simple cubic structure and here Cadmium (Cd) is tetrahedral cations, and Iron (Fe) is octahedral cation. The values obtained by PBE-GGA are as follows; lattice constant 8.7030 Å, minimum volume 1112.1083 $a.u^3$, minimum energy $E_{\circ}$ -33770.2312 Ry and bulk modulus B 168.7308 GPa. PBE-GGA is used here to find the total density of states (TDOS), partial density of states (PDOS) and electronic band structure for both spin-up and spin-down. Electronic band structure for Cadmium Ferrite is indirect band gap and shows some band gap for spin-up (of about 1.2 eV), but for spin-down valance band and conduction band overlap each other (zero band gap). This shows that $CdFe_2O_4$ has semi metallic nature. This is the first ab-initio study of electronic band structure of spinel ferrite $CdFe_2O_4$ with PBE-GGA.

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