Journal of Research in Biology

An International Scientific Research Journal

ISSN No: Print: 2231 –6280; Online: 2231- 6299

Theoretical Research

In silico, structural, electronic and magnetic properties of colloidal magnetic nanoparticle $Cd_{14}FeSe_{15}$

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ABSTRACT:

Cadmium Selenide (CdSe) is a colloidal compound in groups II-VI of the periodic table that has a hexagonal and sphalerite structure under normal conditions. In this paper, the structural, electrical, and magnetic properties of nanoparticles-Cadmium, selenide in its pure form, and the form in which iron is injected in the framework of functional density theory, by improved linear plane wave method with full potential and using GGA approximation were studied. The results showed that Iron atoms entered into nanoparticles of cadmium, selenide are more stable than the iron atoms on the nanoparticle surface. In both cases, we observed the emergence of magnetism and electric polarization. The result of the study showed that the pure CdSe have very low magnetic properties and it has a half-metal property by adding Fe to this combination.

Keywords:

Functional density theory, Iron impurities, Nanoparticles, CdSe, GGA approximation.

Article Citation:
Elham Fereydouni and Rostam Moradian
In silico, structural, electronic and magnetic properties of colloidal magnetic nanoparticle $Cd_{14}FeSe_{15}$
Journal of Research in Biology (2018) 8(2): 2445-2450

Dates:
Received: 12 Jan 2018 **Accepted:** 24 Feb 2018 **Published:** 25 Mar 2018

Journal of Research in Biology

INTRODUCTION

Cadmium Selenide (CdSe) is a colloidal compound in groups II-VI of the periodic table that has a hexagonal and sphalerite structure under normal conditions. Both structures are stable in theoretical studies; but in experiments, studies have shown that hexagonal structure is more stable. This structure has a band gap of 1.57 EV. The combination of CdSe has many applications such as filters, dielectric, light emitting diodes, and solar cells. These compound nanostructures have applications in the field of nanowires and thin films. Here, we'll examine iron injection into the CdSe nanoparticles. This is done using functional density theory. In order to analyze quantum clustering and poly-electronic devices we need to Kohn-Sham equations by using the DFT method in a self-consistent form. In this research, we have used the computational code of WIEN2k for calculation (Wright, 2004).

MATERIALS AND METHODS

The theory of functional density is used mainly in the structural, optical and electronic calculations in solids. As a result of calculations in this paper, based on the full potential linearized improved plane wave method, software code of WIEN2k and GGA approximations have been used in the calculations. Muffin-tin radius selected in this compound is as follows:

R_{cd}=1.9 a.u, R_{se}=1.8 a.u

First, we introduced experimental constants of the network as input parameters for network constants. Then we let the program change these constants around the input axis and calculate the energy of the ground state of the crystal for each new volume.

Table 1. Optimized network constants

S. No	Parameters	Work	Experimental
1	a(Â)	4.51	4.30
2	c(Â)	7.36	7.01

Finally, using the data obtained, we plotted the ground state energy change by volume. From this graph, we can determine the volume for which the energy of the ground state is the lowest. At the end, network constants can be obtained. In Table 1, optimized constants of the network are reported, that the results indicate well-consistency with the experimental values (Wei, 2000).

Finally, using data obtained the graph of Ground state energy changes, according to volume. This chart can give the volume for which energy has the lowest ground state. Ultimately, it can be used to acquire network constants. Table 1 represents optimized network constants that the obtained results reveal good harmony with the reported experimental values (Al-Douri, 2003). Then, using optimized constants, the structure of CdSe is built and physical properties of this substance were studied after relaxation.

RESULTS AND DISCUSSION

The iron injection can be done in two different ways: 1) The iron replaces the Cd in the center of the nanoparticle; 2) The iron replaces the Cd on the surface of the nanoparticle. Figure 1 shows the structure of the pure nanoparticle of CdSe in two states of equilibrium and lack of equilibrium for replacement of Fe atom in the center of the nanoparticle (A), and replacement of Fe at the surface of the nanoparticle (B) (Sowa, 2005).

In such a situation, we can let the atoms of the

Table 2. Bond lengths (Å) for CdSe pure nanoparticles and to inject Fe atom in the center of nanoparticles and at the surface of nanoparticle and the stack mode

S. No	The combination	Pure nanoparticle		Nanoparticle with Fe
		Center (Cd-Se) (Å)	Surface (Cd-Se) (Å)	Fe @ Center (Fe-Se) (Å)
1	Bond length	2.53	2.44	2.40

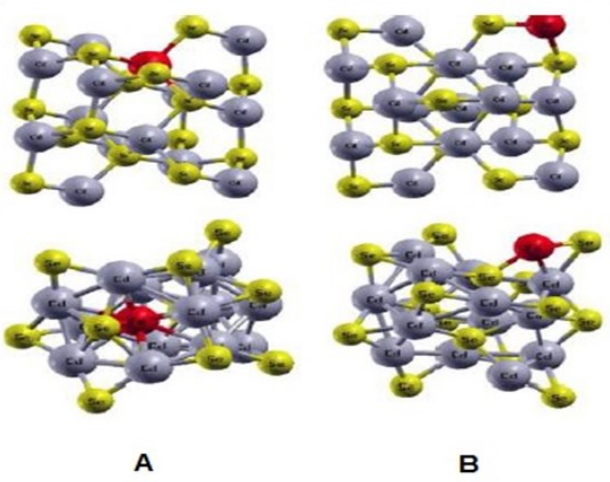

Figure 1. Non-relaxed (top) and relaxed (down) structures for (A) CdSe and iron injection in the center; and (B) replacement on the surface

Table 3. Magnetic moment values in terms of the Bohrmagneton (μB) and energy in electron volts (eV) in three cases: pure CdSe nanoparticle; CdSe nanoparticle with injected Fe in centre; CdSe nanoparticle with injected Fe in surface

S. No	Type	$\mu_{tot}(\mu_B)$	$\mu_{Fe}(\mu_B)$
1	Pure nanoparticle	-0.01	----
2	Fe in surface of nanoparticle	4.00	3.30
3	Fe in center of nanoparticle	4.01	2.46

nanoparticle find their right place such that the force reaches the lowest level. Results are presented in table 1. The energy of the CdSe in which iron is injected to the center is more stable than in another state (Hu, 1987). As can be seen in Table 2, in studying the structural properties, the bond length (Cd-Se) of central atoms, and also of surface atoms in the pure state of CdSe nanoparticle is more in comparison with the bond length of Fe-Se.

The calculation indicates that the bond length for CdSe stack is 2.71 Å which is bigger than the length of the nanoparticle. It is seen that the presence of impurities causes decreasing in the bond length of the desired structure. As it has been indicated in Table 2 bond lengths in the pure nanoparticles at the surface came lower than the bond length in the center state (Erbarut, 2003).

Magnetism

Atoms have the highest magnetic moment when they are isolated but the magnetic moment is reduced when placed in conjunction with other atoms. According to Table 3 the total magnetic moment in Fe injected into the center of CdSe nanoparticle is lower than the total magnetic moment in Fe injected into the surface of CdSe nanoparticle and this is due to the more links of Fe atoms with Se and Cd atoms in the center of the nanoparticle. In another hand, the Fe atom which has been replaced instead of Cd atom has a more magnetic moment because of dangling bonds. This suggests that the presence of Fe causes magnetism in the structure (Tomimoto, 2010).

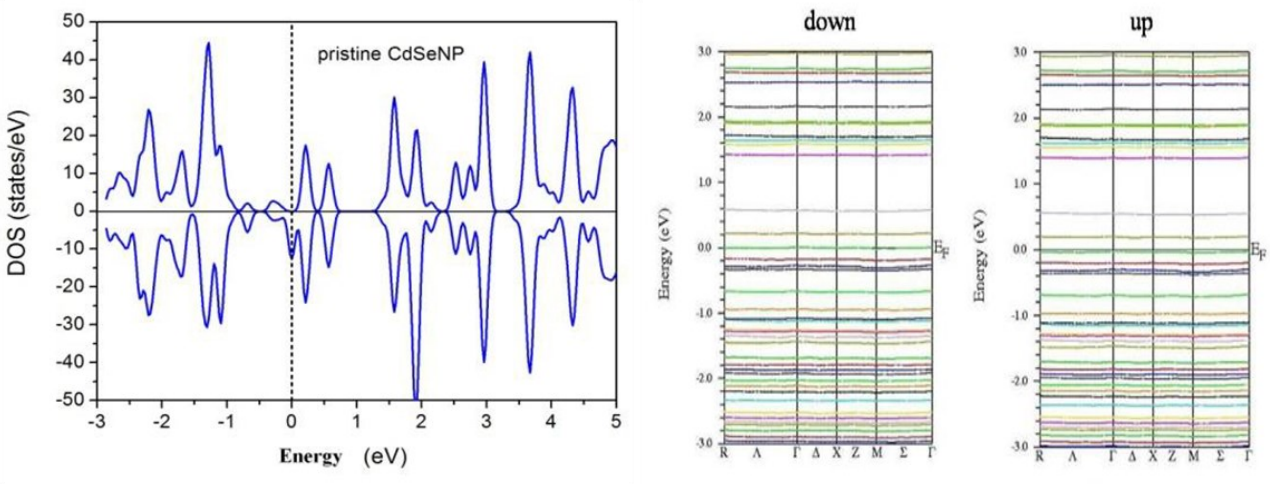

Figure 2. Density figure of electron states and band structure for pure nanoparticle of CdSe in both, up and down channels

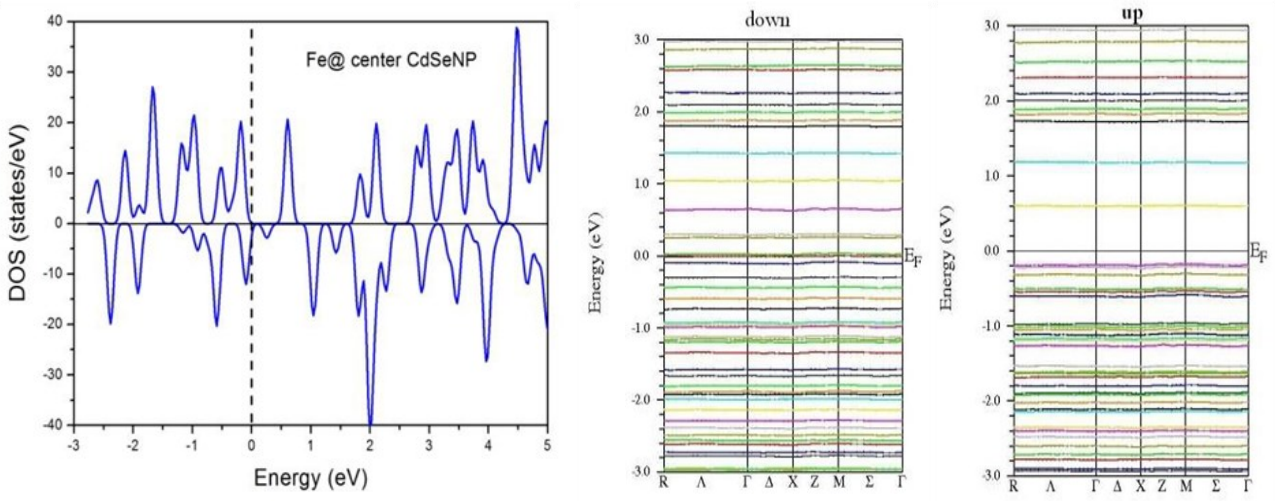

Figure 3. Density figure of electron states and band structure for pure nanoparticle of CdSe in both, up and down channels

The electronic properties

The density of electronic states which is provided in this section is obtained according to the density functional theory and by using GGA Approximation and WIEN2k. Here we reviewed and compared three different electronic state and band structure for the nanoparticle.

Scrutinizing the density diagram of electronic states in pure CdSe nanoparticle

Figure 2 illustrates tape structure and the density diagram of electron state for pure Nano-particle in both majority spin channel (up) and minority spin channel (down). According to Figure 2, the density of electronic state is clear which this instruction with high spin electron has a 0.20 EV gap. It has no gap for a low spin electron in surrounding the Fermi energy. It states that this compound has a half-metallic property. In fact band structure shows the special graph of amounts of energy in terms of wave vector in the first Brillouin zone. According to the figure, Half-metal band structure properties could be observed and the amount of energy gap is obvious in the high spin channel (Salles *et al*., 2009).

Reviewing the electron density plot of CdSe Nanoparticle which the iron was injected into its center

In the electron density plot of CdSe nanoparticle which the iron was injected into its center, according to

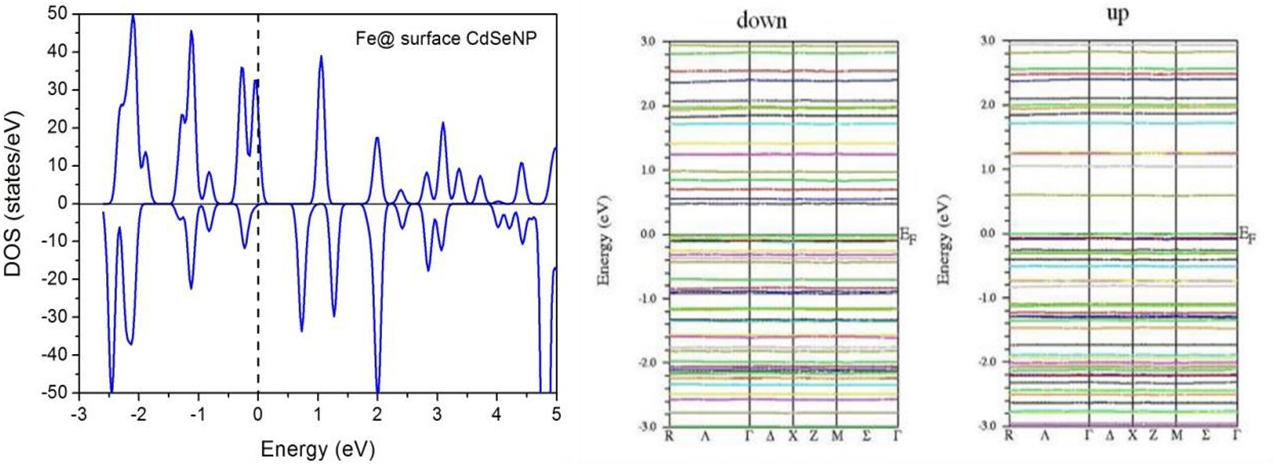

Figure 4. Density figure of electron states and band structure for pure nanoparticle of CdSe in both, up and down spin channels

the Figure 3 which it has 0.43 EV for high spin electrons indicate that this combination has Half-metal band structure properties. The amount of this energy gap is obvious in band structure diagram (Figure 3) (Kohn and Sham, 1965).

According to Figure 4, there is no electron with high spin in surrounding the Fermi energy. For electron with low spin there is 0.50 EV in surrounding the Fermi energy and this issue illustrate that this combination obtains the half-metal properties. It should be considered that here the gap energy occurred in low spin states of electrons and it is the opposite of two previous estates which the energy gap happened in density states of electrons with high spin (Blaha *et al*., 2001).

The general conclusion that we could gain is that in each three states the nanoparticles obtained half-metal properties meanwhile the aggregate of this particle has semi-conductive properties with 1.70 EV energy gap. We can explain this situation in this way that the atoms in surface of each nanoparticle loss some neighbors and as a result some rogue charge is produced.

These rogue electrons act like free electrons and cause half-metal properties and 100% polarization in these nanoparticles. It is expected that by increasing the size of the nanoparticles the effects of nanoparticles decline and physical properties of nanoparticles come close to the properties of aggregate properties of nanoparticles (Peter and Cardona, 2001).

CONCLUSION

The result of the study showed that the pure CdSe have very low magnetic properties and it has a half-metal property and with adding Fe to this combination we will see a lot of magnetic and half-metal properties. Also, for CdSe nanoparticle with Fe impurities we saw the reduction in bond length and increasing in energy gap. The dangling bonds in the compound are the reason of magnetism in pure nanoparticle which act like rogue electrons and cause half-metal and Spin polarization properties. But with Fe impurities in addition to rouge electrons half-metal and Spin polarization properties plays an important role as a transition metal.

REFERENCES

Al-Douri Y. 2003. The pressure effect of the bulk modulus seen by the charge density in CdX compounds. *Materials Chemistry and Physics*, 78(3): 625-629.

Blaha P, Schwarz K, Madsen GKH, Kvasnicka D and Luitz J. 2001. Wien2k, An augmented plane wave+ local orbitals program for calculating crystal properties. Vienna University of Technology, 188 p.

Erbarut E. 2003. Optical response functions of ZnS, ZnSe, ZnTe by the LOM method. *Solid State Communications*, 127(7): 515-519.

Hu JZ. 1987. A new high pressure phase of CdTe. *Solid State Communications*, 63(6): 471-474.

Kohn W and Sham LJ. 1965. Self-consistent equations including exchange and correlation effects. *Physical Review*, 140(4A): A1133-A1138.

Peter YYU and Cardona M. 2001. Fundamentals of Semiconductors; Physics and Materials Properties. 3rd ed., Springer-Verlag, Berlin and Heidelberg.

Salles BR, Kunc K, Eddrief M, Etgens VH, Finocchi F and Vidal F. 2009. Hexagon-on-cube versus cube-on -cube epitaxy: The case of ZnSe(111) on $SrTiO_3$ (001). *Physical Review B*, 79(15): 1-5.

Sowa H. 2005. On the mechanism of the pressure-induced wurtzite-to NaCl-type phase transition in CdS: an X-ray diffraction study. *Solid State Sciences*, 7(1): 73-78.

Tomimoto S, Nozawa S, Terai Y, Kuroda S, Takita

K and Masumoto Y. 2010. Anisotropic spin dynamics of confined electrons in CdTe/ZnTe quantum structures. *Physical review B*, 81(12): 1-10.

Wei SH and Zhang SB. 2000. Structure stability and carrier localization in Cd X (X= S, Se, Te) semiconductors. *Physical Review B*, 62(11): 6944.

Wright K and Gale JD. 2004. Interatomic potentials for the simulation of the zinc-blende and wurtzite forms of ZnS and CdS: Bulk structure, properties, and phase stability. *Physical Review B*, 70(3): 035211.