

In silico, structural, electronic and magnetic properties of colloidal magnetic nanoparticle $\text{Cd}_{14}\text{FeSe}_{15}$

Authors:

Elham Fereydouni¹ and Rostam Moradian²

Institution:

1. Department of Physics, Imam Khomeini International University, Qazvin, Iran.

2. Department of Physics, Faculty of Sciences, Razi University, Kermanshah, Iran.

Corresponding author:
Elham Fereydouni

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.