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DFT study of CdSe nanotube doped with Cr atom

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Abstract: Electronic and optical properties of doped with Cr atom CdSe nanotube investigated from first principles calculations with GGA/PBE exchange correlation functional. The CdSe nanotube electronic properties were studied in terms of band structures and density of states spectrum. The DOS calculation provides the insight for the localization of charges in the valence and conduction band. It was found that, doped with Cr atoms CdSe nanotube show half metallic properties. The imaginary and real part of dielectric function were calculated for pure and Cr doped nanotube and compared. Our calculations show that Cr atom induce blue shift for spin down states and red shift for spin up states. The half metallic behavior makes Cr doped CdSe nanotube suitable to be used in spintronic devices.

Keywords: DFT, nanotube, density of state, electronic structure, optical properties

1. Introduction

Group III–V and II–VI semiconductors, due to their unique physical and chemical properties [1–9], play an important role in the field of nanodevices. Studies have shown that nanostructures are wide-gap semiconductors [10–12]. CdSe is one of the most widely studied Group II–VI semiconductors, both in one-dimensional form and its nanostructures have demonstrated versatility for new and diverse applications [13-16]. 1D CdSe nanostructures were obtained using electrochemistry, chemical reactions in solution [18-20]. Interfacial electron transfer, in semiconductor nanoparticles CdSe nanorods (NR), has significant interest and offer new opportunities in designing and optimizing hybrid photocatalysts due to their broad absorption profiles, size tunable emission, long lived excited-state lifetimes, and enhanced photostability [21-25].

The electronic, optical and elastic properties of CdSe were reported in [26–28]. Considering that the properties of nanoribbons are very sensitive to their width and edge passivation, their research opens up enormous opportunities for tuning their properties.

Among II–VI group semiconductors nanostructures doping, i.e. both n- and p-type doping, has led to the actualization of a variety of novel nanodevices, such as light emitting diodes (LEDs) [29], laser diodes (LDs) [30], photovoltaic devices [31] and so on.

The electronic and magnetic properties of nanoribbons were studied in theoretical work [32]. From the studies conducted, it was revealed that the properties of non-magnetic semiconductors for both simple and armchair CdSeNRs with hydrogen terminals turned out to be stable regardless of their width.

The magnetic properties of a monolayer of CdSe were studied in Ref. [33]. The spin polarized antisymmetric electronic band structure of doped CdSe corresponded to the magnetic properties of the monolayer. The total magnetic moment among the doped systems was: 5.620 μB when replacing one S atom with a Cr atom, 3000 μB when replacing one Cd atom with a V atom, and 7000 μB for the co-doped Cd2VCrS4 structure [33].

The binary compound nanotube materials such as CdTe nanotube [34], ZnO nanotube [35], ZnX(X=S/Se/Te) [36] were studied. Only few

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works were devoted to CdTe nanostructures [36], clusters [37], quantum dots [38] and nanoclusters [39].

From the literature survey, it is inferred that there are many works reported the electronic or structural property, synthesis and characterization of of group III–V semiconductors nanotubes. However, despite extensive research of this group, the electronic band structure of CdSe nanotube also its magnetic properties have not investigated. The novel aspect of the present work to study electronic structures and magnetic properties of Cr doped CdSe nanotube based on density functional theory which will open a new way for experimental researchers to conduct.

2. Computational Method

For electronic and optical properties investigations first principles calculations are performed using the ab initio simulation package quantumwise ATK. The generalized gradient approximation (GGA) is employed with the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional. After optimization bulk structure nanotube containing 64 atoms reconstructed. A Monkhorst–Packgrid of 1×1×15 is used for structure optimization. As pseudopotential we used HGH(d) and valence electrons were chosen as: Cd $[Kr]^{+}$ $4d^{10}5s^{2}$, Se $[Ar]^{+}$ $3d^{10}$ $4s^{2}$ $4p^{4}$ and double-zeta polarization (DZP) basis set for all of the atoms is considered. A vacuum region of about 10 Å along the nonperiodic directions was employed to avoid any interactions between adjacent supercells. The Hellman–Feynman forces were below 0.01 eV A−1 and the total energy less than 10−3eV. To reconstruct CdSe nanotube, which is formed by rolling a single layer of carbon nanoribbons into a cylinder. We use the representation accepted for carbon hexagonal nanotubes using the chirality vector $C = na_1 + ma_2$, where a1 and a2 are translation vectors of a unit cell of two-dimensional material and the tail at the adjacent zigzag end. The integer (n, m) is the number of steps of the zigzag bond.

3. Results and discussion

After structural optimization (our structure parameters were in good agreement with previous results [40, 41]) electronic band structure and density of state of bulk CdSe structure was calculated.

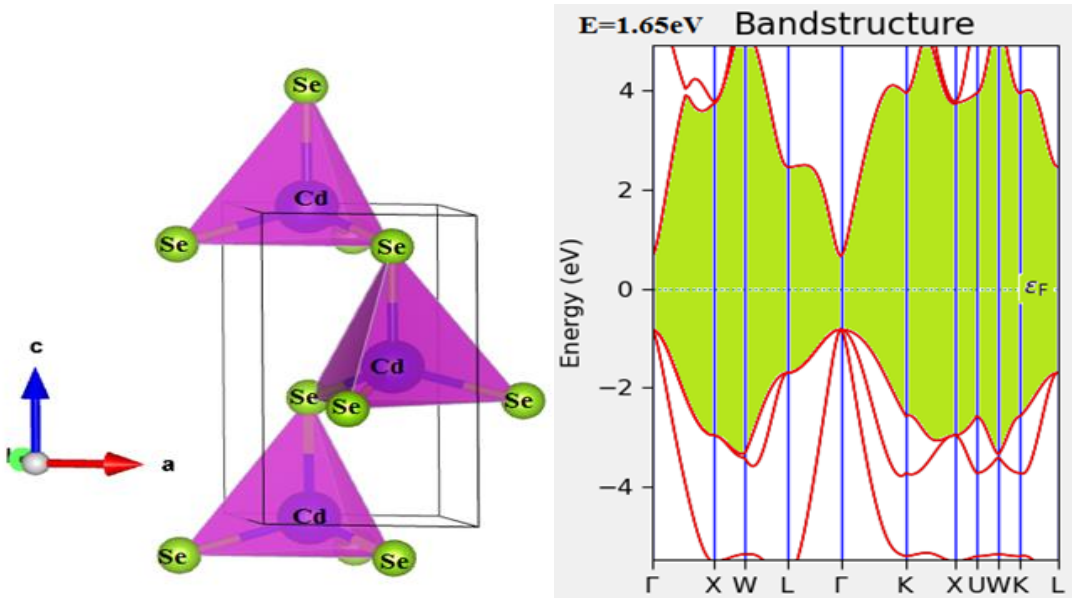

Figure 1 Primitive cell and calculated electronic band structure of CdSe bulk.

From band structure (Figure 1) it was obvious that forbidden gap of bulk CdSe formed by a direct transition at *Γ* point and value for forbidden gap was 1.65 eV which is in good agreement with [42 - 45].

For reconstruction nanotube we used optimized bulk structure CdSe. The chirality dimension of CdSe nanotube are n = 4 and m = 3 with the repetition along c-axis as one. The length of CdSe nanotube is around 13.27Å and the tube diameter is 5.9 Å.

Calculated density of state of CdSe nanotube presented in Fig.2. As can be seen from the Fig.2 spin up and spin down states is symmetrical which

mean CdSe nanotube is nonmagnetic. It was obvious that band gap for CdSe nanotube increased and equal to 2.05eV. This behavior is typical for nanostructures [46-48].

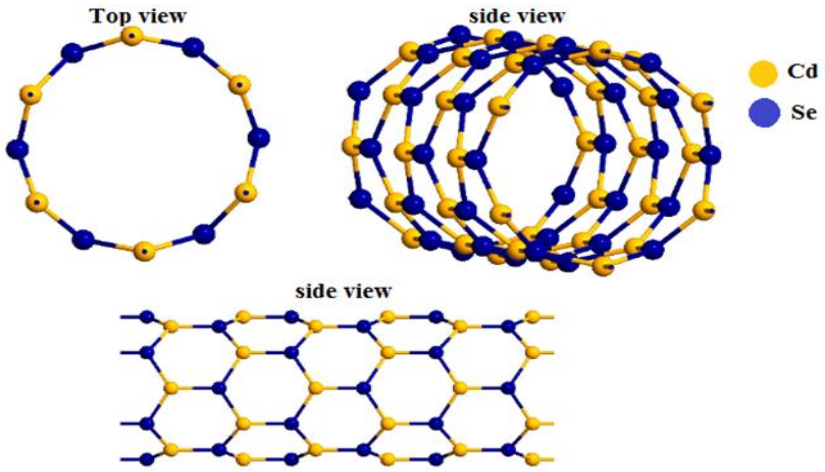

Figure 2. Top and side view of CdSe nanotube

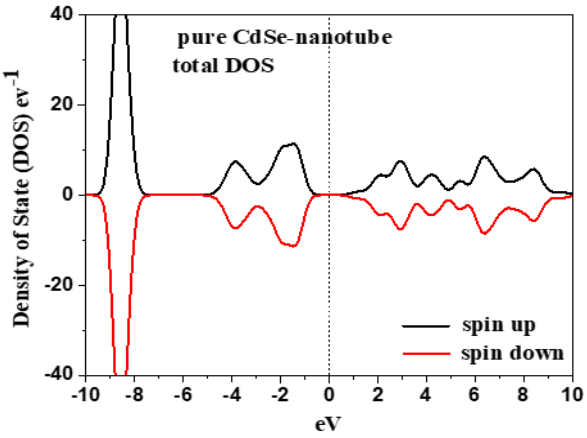

Figure 3. Calculated density of state of pure CdSe nanotube

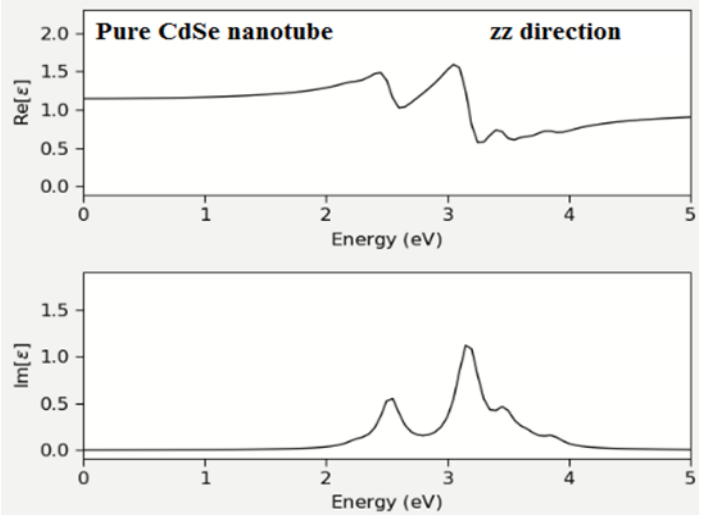

Figure 4. Calculated imaginary and real part of dielectric function of pure CdSe nanotube

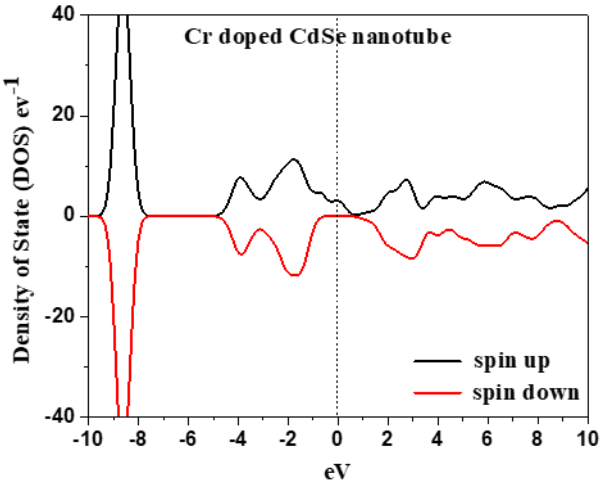

Figure 5. Calculated DOS for Cr doped CdSe nanotube

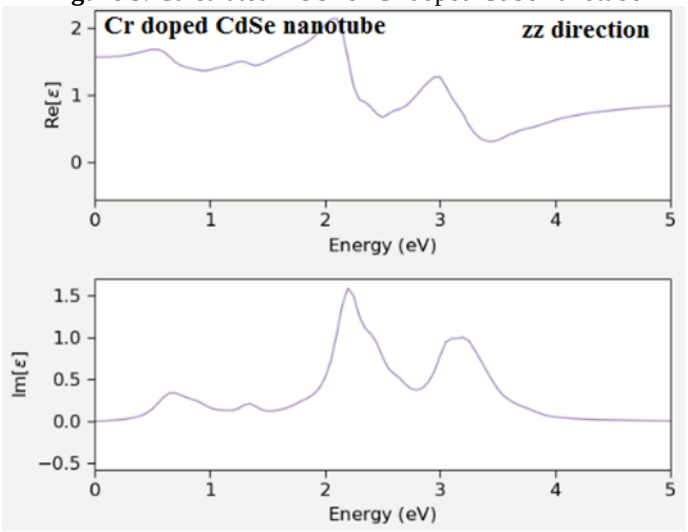

Figure 6. Calculated imaginary and real part of dielectric function of Cr doped CdSe nanotube

The imaginary and real part of dielectric function was calculated according the equation 1 and 2 and presented in Figure 3.

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega' \qquad 1)$$

$$\varepsilon_2(w) = \frac{4\pi e^2}{m^2\omega^2} \sum_{ij} \int \langle i|M|j\rangle I^2 f_i \ (1 - f_i) \delta(E_f - E_i - \omega) d^3k \qquad (2)$$

The first peak in imaginary part of dielectric function in the 2.5eV is due to transition from Cd p state in CBM to Se p state in VBM. The mean peak in 3.3 eV associated with transition from Cd s to Se p state.

In order to study influence of Cr atom on CdSe nanotube we replace two Cd atom by Cr and calculate electronic and optical spectrum of this structure. From spin polarized DOS it was obvious that Cr atom reduce band gap of CdSe nanotube also induce magnetic properties.

So, DOS for spin up and spin down states is not symmetrical. As can be seen from Fig.4 calculated spin up and spin down gaps for Cr doped CdSe nanotube is differ from each other. This indicate that this structure shows magnetic properties. The main reason of magnetic properties is associated with Cr d states. In the top of the valence new impurity level was observed for spin up state which reduce band gap of nanotube to 0 eV. In contrast to in the forbidden gap of nanotube for spin down state

band gap is larger than for pure nanotube and equal to 3.01eV. The half metallic behavior makes Cr doped CdSe nanotube suitable to be used in spintronic devices.
From imaginary part of dielectric function, it is obvious that with introduction Cr atom red shift for spin up and blue shift for spin down states were observed.

4. Conclusions

In presented work influence of Cr atom on electronic and optical properties of CdSe nanotube were studied. For this purpose, we replace two Cd atom by Cr. From spin polarized DOS it was obvious that Cr atom reduce band gap of CdSe nanotube. Our calculations reveal that spin up and spin down gaps for Cr doped CdSe nanotube is differ from each other. This indicate that this structure shows magnetic properties. The main reason of magnetic properties is associated with Cr d states. In the top of the valence new impurity level was observed for spin up state which reduce band gap of nanotube to 0 eV. In contrast to in the forbidden gap of nanotube for spin down state band gap is larger than for pure nanotube and equal to 3.01eV. The half metallic behavior makes Cr doped CdSe nanotube suitable to be used in spintronic devices.

Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Research data are not shared.

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