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First-principles studies on electronic transport properties of CdS nanoribbon based molecular device

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Abstract

The electronic transport properties of cadmium sulfide nanoribbon based molecular device were investigated by employing first principles calculation using density functional theory. The electronic properties are discussed in terms of density of states spectrum and electron density. The density of states of charge depends on the applied bias voltage. The electron density is seen more at cadmium sites. The transport properties of CdS nanoribbon are studied using transmission coefficient spectrum and transmission pathways. The electronic transmission all along the scattering region depends on the bias voltage; depending upon the bias voltage the transmission path also gets altered. The information provided in the present study will pave way to tailor nanostructures with improved performance in nanoelectronic devices.

Keywords: Nanoribbon; Density of states; Transmission coefficient; Transport property; CdS

1. Introduction

Recent technological developments in nanoscience lead to the synthesis of nanostructured materials such as nanowires, nanoribbons, nanocages, nanorods, nanoflowers, nanosheets and nanoclusters [1–10]. Different morphologies improve the performance of nanostructured materials which finds its potential applications in photoelectric devices, sensors, solar cells, memories, semiconductor devices [11–16]. Recently, the growing interest in the field of functional nanodevice based on the one-dimensional materials is on the focus. These devices include electrically driven transistors, lasers, light emitting diodes and chemical sensors. The photoconducting properties of one-dimensional semiconducting materials are improved in ZnO [17], GaN [18], SnO_2 [19] and CdS [20] and are reported. Among the photoconducting materials cadmium sulfide (CdS) is suitable for detecting the visible light due to its band gap in the range of 2.47 eV. The enhancement of defects and trapping sites in the material strongly influence the charge carrier and the performance. CdS thin films are also used in the solid-state device application in the photodetection, photovoltaic solar energy, xerography and thin film transistors [21–23].

The objective of the present work is to study the transport properties of CdS nanoribbons which improve the performance of photoconductive property of CdS with rapid response. There are many methods reported in the synthesis of CdS nanoribbons namely, thermal evaporation [24–26], sputtering [27], chemical vapor deposition [28], physical evaporation of CdS nanopowder [29], spray pyrolysis [30] and laser ablation [31]. With this as the motive, the survey was conducted using Scirus comprehensive scientific research tool database; it is found that most of the reported work deals with the synthesis and characterization of CdS materials. There is not much work reported on the transport property of CdS nanostructured materials based on density functional theory (DFT). The present work, attempts the study of electronic transport properties of CdS nanoribbon which improves the performance in the photoconductive property.

2. Computational details

In the present work, the calculations are performed with DFT utilizing TranSIESTA module in SIESTA package [32–34]. The

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electronic wave functions are expanded with a basis set of the atom that depends on the numerical orbitals. The molecular geometry is optimized by reducing the atomic forces on the atoms to be smaller than 0.05 eV/Å. The electron–electron interactions are calculated using generalized gradient approximation (GGA) through Perdew–Burke–Ernzerhof (PBE) exchange correlation functional is used throughout the calculation [35–37]. In the present two probe system the Brillouin zones are sampled with $3 \times 3 \times 50$ k points. The electrostatic potentials in the real-space grid are determined with the mesh cut-off energy of 10^{-5} eV which is used to achieve the balance between the efficiency and calculation accuracy. To calculate the electronic properties of cadmium sulfide nanoribbon and to neglect the interaction of the nanoribbon with its periodic images a vacuum padding of 10 Å is modeled along the x and y axis. The nanoribbon structures are optimized in a self-consistent way. The atoms in the nanoribbon are free to displace along their positions until the convergence criteria is obtained with a force less than 0.05 eV/Å on every atom in the whole nanoribbon. The optimization of the molecules and the electronic properties of nanoribbon based molecular device is carried out by the double zeta plus polarization (DZP) basis set for CdS molecule and double zeta plus polarization for the electrode region is used.

3. Results and discussion

3.1. Structure of CdS nanoribbon

CdS nanoribbon is constructed with reference to the international centre for diffraction data (ICDD) card number 89-2944 exhibits hexagonal structure. CdS nanoribbon is constructed along (200) plane. CdS nanoribbon has 42 sulfur atoms and 42 cadmium atoms in order to maintain stoichiometry in the structure. CdS nanoribbon is held between two electrodes. The CdS acts as scattering region between two electrodes. The potential difference is maintained between the left electrode and right electrode, the density of states (DOS) and the transmission spectrum of the scattering region is studied and the results are reported. Fig. 1 represents the schematic diagram of CdS nanoribbon with electrodes.

3.2. Density of states

The visualization of the charges in the valence band and the conduction band of nanoribbon is given by the density of states (DOS) spectrum. The DOS spectrum gives the perception of the charges present in the energy interval [38–40]. In the present work, the bias voltage is varied within the interval of 0–1.5 V across the scattering region in terms of 0.5 V. The bias windows between the electrodes are set to [−V/2, V/2], henceforth, the Fermi level (E_F) is taken as zero. The overlapping of s, p, d orbitals with different cadmium and sulfur atoms results in the DOS spectrum. The projected density of states (PDOS) arises due to the overlapping of s, p, d orbitals along the scattering region. The electronic configuration of cadmium is $4d^{10}5s^2$ and sulfur is $3s^23p^4$. Fig. 2(a) depicts the PDOS spectrum at zero bias condition, near the Fermi level

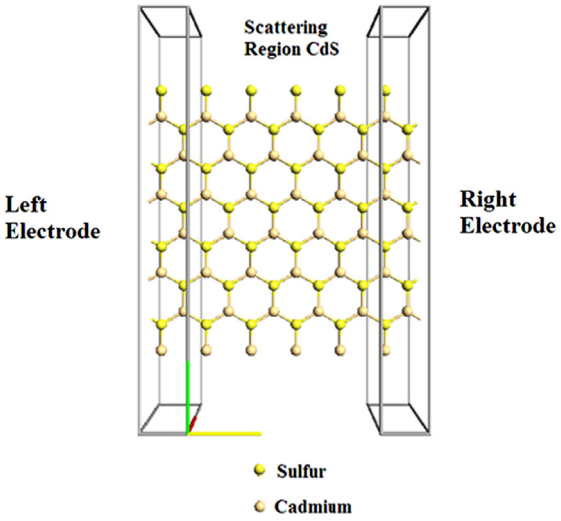

Fig. 1. Schematic diagram of the CdS nanoribbon with electrodes.

(E_F) at −0.1 eV a peak is observed in the d and s orbitals whereas there is a decrease in amplitude in p orbital. This may be due to the overlapping of $4d^{10}5s^2$ of cadmium with $3s^23p^4$ of sulfur. The increase and decrease in the amplitude in s, p, d orbitals arise with the positions of atoms in the nanoribbon. Han et al. reported electronic structure and optical properties of CdS, the major contribution arise due to $3p$ electron of sulfur atom [41]. In the present study, under no bias condition the major contribution is due to p orbital which is in agreement with the reported work. The calculated density of states by Noor et al. in ab-initio study of structural, electronic and optical properties of Be-doped CdS compounds found similar results as that of the present work [42]. Minibaev et al. calculated density of states spectrum for CdS quantum well which resembles the PDOS spectrum at 0 V in the present study [43]. Fig. 2(b) illustrates the PDOS spectrum at 0.5 V bias. Interestingly, the peak amplitude is observed around 0.6 eV in the positive energy which refers the conduction band. The reason behind this is the applied voltage cause the electrons in the valence band to move towards the conduction band and major contribution is seen in p orbital. Fig. 2(c) signifies the PDOS spectrum at 1 V bias. From this figure it is clearly inferred that the peak maximum is observed near the Fermi level and there are more number of peak observed both in valence band and conduction band. The turbulence of peaks infers that the applied voltage causes more electrons to move from valence band to conduction band. On further increasing the voltage to 1.5 V, a sharp peak is noticed at 0.3 eV as shown in Fig. 2(d). The number of peaks gets reduced in this situation in valence band and conduction band. The device density of states (DDOS) spectrum arises due to the superposition of PDOS spectrum. DDOS spectrum of CdS nanoribbon is depicted in Fig. 3. From this it is clearly evident that depending upon the bias voltage the peak maximum can be fine-tuned on different energy levels in the nanostructure.

Fig. 4 represent the electron density along the nanoribbon. The electron density is perceived more near cadmium atom, due to the metallic nature of cadmium atom the electron