Modulating the Electronic, Optical, and Transport Properties of CdTe and ZnTe Nanostructures with Organic Molecules: A Theoretical Investigation

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ABSTRACT: In this paper, we systematically investigated the electronic, optical, and transport properties of CdTe and ZnTe nanostructures before and after adsorption with benzyl viologen (BV) and tetrafluoro-tetracyanoquinodimethane (F4-TCNQ) organic molecules based on the first principles calculation. First, the band gaps of CdTe and ZnTe nanostructures obviously decrease after BV and F4-TCNQ adsorptions. Interestingly, the electronic property calculation shows that BV and F4-TCNQ can donate/accept electrons to/from the surface of CdTe and ZnTe nanostructures, leading to an effective n-/p-type doping, respectively. Second, the optical absorption in a broad spectral range (from visible to near-infrared) of CdTe and ZnTe is significantly improved by adsorption of BV and F4-TCNQ molecules, offering great opportunities for the use of CdTe and ZnTe nanostructures in renewable energy fields. Lastly, the electrical transfer characteristics on CdTe and ZnTe nanostructure-based field-effect transistors clearly showed that the conduction of the nanostructures can be rationally tuned into n- and p-type conductivity with BV and F4-TCNQ adsorptions, respectively. Our work clearly demonstrates that the electronic, optical, and transport properties of CdTe and ZnTe nanostructures are effectively modulated by adsorption of BV and F4-TCNQ, which can be used to construct high-performance electronic and optoelectronic devices.

1. INTRODUCTION

Belong to II–VI binary compound semiconductors, CdTe and ZnTe are widely applied in electronic and optoelectronic devices ascribe to their extraordinary properties.1–10 However, due to the native defects (such as Cd and Zn vacancies) and self-compensation effects, CdTe and ZnTe exhibit p-type conductivity with low carrier concentrations, which is not conducive to high-performance optoelectronic devices based on CdTe and ZnTe nanostructures. Despite the great progress, the lack of understanding and controllability on the electrical and optical properties of CdTe and ZnTe nanostructures severely impede their practical applications. CdTe and ZnTe can be doped into both n- and p-type conductivity, but it is difficult to achieve in practice due to the high concentration of native acceptors, such as (Tei) and (VZn).11–13 Therefore, it is necessary to modulate the electronic, optical, and transport properties of CdTe and ZnTe nanostructures for development of high-performance electronic and optoelectronic devices.

Recent investigations14–26 have demonstrated that the electronic, optical, and transport properties of low-dimensional materials can be effectively tuned by the adsorption of inorganic and organic molecules, which are of fundamental importance to the development of nanowire-based electronic and optoelectronic devices. For instance, by controlling the concentration of MoO3 and benzyl viologen (BV), the electron concentration and resistivity of the CdS nanoribbons can be readily modulated, which offers a feasible route to modulate the electrical and optical properties of compound semiconductor nanostructures.18 Similarly, Chen et al.20 demonstrated that graphene could be also p-type doped by modifying the surface with the electron acceptor, tetrafluoro-tetracyanoquinodimethane (F4-TCNQ). Jing et al.21,25 disclosed that F4-TCNQ and TTF (tetrathiafulvalene) could enhance the optical properties of MoS2 and phosphorene for effective light harvesting. Dynamic transport behaviors also have demonstrated that additional channels for hole transport in...
host monolayer phosphorene were generated upon the adsorption of the F4-TCNQ molecule.25

Herein, based on density functional theory (DFT) combined with the nonequilibrium Green’s function formalism (NEGF),27,28 we proved that the adsorption of BV and F4-TCNQ, can effectively modulate the electronic, optical, and transport properties of Cd(Zn)Te nanostructures. Our calculations revealed that BV and F4-TCNQ could act as the donor/acceptor to inject/draw electrons into/from Cd(Zn)Te nanostructures, resulting in the downshift/upshift of Fermi levels along with the decrease/increase in work function. Additionally, the adsorption of BV and F4-TCNQ found to be an effective way to enhance the light-harvesting capabilities of CdTe and ZnTe in the lower light energy regions. Moreover, the electrical transfer characteristics on Cd(Zn)Te nanostructures. In contrast, due to the strong electron-donating/withdrawing ability, BV/F4-TCNQ is one of the most frequently used n-/p-type dopants to tune the electronic, optical, and transport properties of low-dimensional materials.16,19–23 To explore the surface modification effects on the electronic, optical, and transport properties, we performed systematical studies on the CdTe and ZnTe nanostructures before and after F4-TCNQ/BV adsorption.

2. RESULTS AND DISCUSSION

In order to evaluate the stability of dopant (BV and F4-TCNQ) adsorption on the surface of CdTe and ZnTe nanostructures, the adsorption energy (ΔE) was calculated as follows

$$\Delta E = E_{\text{dopant/Cd(Zn)Te}} - E_{\text{dopant}} - E_{\text{Cd(Zn)Te}}$$

(1)

where $E_{\text{dopant/Cd(Zn)Te}}$, $E_{\text{dopant}}$, and $E_{\text{Cd(Zn)Te}}$ are the total energy of the surface-modified Cd(Zn)Te systems, isolated dopant, and isolated Cd(Zn)Te nanostructure, respectively.

Due to the strong electron-donating/withdrawing ability, BV/F4-TCNQ is one of the most frequently used n-/p-type dopants to tune the electronic, optical, and transport properties of low-dimensional materials.16,19–23 To explore the surface modification effects on the electronic, optical, and transport properties, we performed systematical studies on the CdTe and ZnTe nanostructures before and after F4-TCNQ/BV adsorption.

Figure 1a,b presents the energetically most favorable configurations of BV and F4-TCNQ molecules, respectively. The most energetically favorable configurations for these two molecules on the surface of CdTe and ZnTe are presented in Figure 1c–f. It can be noted that the adsorption of BV and F4-TCNQ causes a slight distortion of the structure of Cd(Zn)Te nanostructures. In addition, the ΔE of BV/F4-TCNQ-modified CdTe and ZnTe are $-0.64/-0.94$ and $-0.47/-0.62$ eV (as shown in Table 1), respectively, suggesting a strong interaction between BV/F4-TCNQ molecules and Cd(Zn)Te nanostructures. Moreover, the adsorption energy of BV-modified systems is smaller than that of F4-TCNQ-modified systems, indicating weaker interactions between BV and Cd(Zn)Te nanostructures. The Mulliken charge analysis of bond population29,30 was employed to investigate the charge transfers between organic molecules and Cd(Zn)Te nanostructures. From the tabulated atomic charges shown in Table 1, the charge transfers (Δq) from BV molecules to CdTe and ZnTe amount to 0.14 and 0.07 e, respectively, revealing that the BV molecule acts as a donor and injects electrons into Cd(Zn)Te nanostructures. In contrast, for the F4-TCNQ-modified systems, F4-TCNQ acts as a strong acceptor and there are 0.82 and 0.68 e charge transfers from CdTe and ZnTe nanostructures to the F4-TCNQ molecule. Eventually, the adsorption of BV and F4-TCNQ molecules lead to negatively and positively charged Cd(Zn)Te nanostructures, manifesting that BV and F4-TCNQ surface modifications could be an effective approach to modulate the carrier concentrations in Cd(Zn)Te nanostructures.

Moreover, the change of carrier concentration can also be reflected by the work function variations; hence, electrostatic potential calculations are further performed to probe changes of work functions (ΔΦ) for CdTe and ZnTe nanostructures before and after BV and F4-TCNQ surface modifications. The most commonly used definition of work function is given by ΔΦ = $E_{\text{vac}} - E_{\Phi}$, where $E_{\text{vac}}$ and $E_{\Phi}$ are the vacuum level and the Fermi level, respectively. As shown in Figure 2, the calculated work functions of intrinsic CdTe and ZnTe are 3.43 and 3.84 eV, respectively. Also, the adsorption of the BV molecule on the surface of CdTe and ZnTe leads to an obvious decrease of their work functions by 0.30 and 0.44 eV (Table 1), respectively, attributing to the injection of electrons from the BV molecule into Cd(Zn)Te nanostructures. In contrast, due to the injection of holes from the F4-TCNQ molecule, the adsorption of the F4-TCNQ molecule yields an obvious increase of their work functions by 0.98 and 0.90 (Table 1), respectively. These phenomena indicate that CdTe and ZnTe nanostructures could be controlled by n- and p-type doping via...
the surface charge transfer doping (SCTD) method with BV and F4-TCNQ modifications.

The difference in electron density (Δρ) was calculated to visualize the charge transfer between the adsorbed molecules (BV and F4-TCNQ) and Cd(Zn)Te nanostructures, which illustrates how the electron density changes during the adsorption process. Δρ is defined as

$$\Delta \rho = \rho_{\text{dopant/Cd(Zn)Te}} - \rho_{\text{dopant}} - \rho_{\text{Cd(Zn)Te}}$$

in which \( \rho_{\text{dopant/Cd(Zn)Te}} \), \( \rho_{\text{dopant}} \), and \( \rho_{\text{Cd(Zn)Te}} \) denote the electron density of the organic molecule-modified systems, the isolated dopant, and the isolated Cd(Zn)Te, respectively. Figure 3 shows the isosurface of the charge density difference after BV and F4-TCNQ modifications, and the blue and red regions denote the depletion and accumulation of electrons, respectively. It can be noted that the electrons transfer from the BV molecule to the surface of Cd(Zn)Te nanostructures, which validates that the BV molecule can act as an electron donor and donate electrons to Cd(Zn)Te nanostructures. In contrast, the adsorption of F4-TCNQ leads to an obvious electron depletion on the surface of CdTe and ZnTe nanostructures but enrichment around the F4-TCNQ molecule, revealing that F4-TCNQ acts as a strong acceptor and accepts the electrons from Cd(Zn)Te nanostructures. All these results verify that there is an obvious charge transfer between BV/F4-TCNQ and Cd(Zn)Te nanostructures, which is consistent with the Mulliken charge-transfer analysis in Table 1.

Due to the significant charge transfer, the electronic properties of Cd(Zn)Te nanostructures at the GGA/PBE level are consistent with the literature report.31 Remarkably, the band gaps of the BV- and F4-TCNQ-modified systems are significantly decreased in comparison with those of the intrinsic systems. For the electron-donating molecule (BV)-modified systems, the new flat bands derived from the BV molecules, appear below Fermi levels (\( E_F \)). The original Fermi levels of CdTe and ZnTe in the new systems are upshifted due to the occupation of new flat bands by electrons, which decrease the work functions. The new flat bands can serve as the donor states and are beneficial to the charge transfer between BV and Cd(Zn)Te nanostructures.

Figure 2. (a, b) Plots of calculated work functions of intrinsic and different organic molecule-modified (a) CdTe and (b) ZnTe at the GGA/PBE level.

Figure 3. (a, b) Difference in electron densities of BV and F4-TCNQ organic molecule-modified (a) CdTe and (b) ZnTe. A loss of electrons is indicated in blue, while electron enrichment is indicated in red.

Figure 4. (a–c) Band structures of (a) intrinsic, (b) BV-, and (c) F4-TCNQ-modified CdTe and ZnTe at the GGA/PBE level. The dashed lines indicate the \( E_F \). The acceptor and donor states from the adsorbed molecules (F4-TCNQ and BV) are indicated by the flat line.

Figure 5. (a, b) Total DOS (red lines) and PDOS of organic molecules (green lines) and Cd(Zn)Te nanostructures (blue lines) for BV- and F4-TCNQ-modified (a) CdTe and (b) ZnTe at the GGA/PBE level. The dashed lines indicate the \( E_F \). The acceptor and donor states from the adsorbed molecules (BV and F4-TCNQ) are indicated by orange arrows.
attributed to the F4-TCNQ molecules. The appearance of the new empty flat bands in the band gaps shifts the original $E_g$ in Cd(Zn)Te nanostructures to the lower energy regions, thus increasing the work functions. The new flat levels can act as acceptor states in F4-TCNQ-modified systems, which are in favor of the charge transfer from the Cd(Zn)Te nanostructures to the F4-TCNQ molecules.

The appearance of the acceptor and donor states, originating from the dopant molecules (BV and F4-TCNQ), reduces the band gaps of Cd(Zn)Te nanostructures. The narrowed band gaps between the new flat bands and the conduction band minimum (CBM) are defined as $E_g$ for BV-modified systems, while $E_f$ is used to denote the reduced band gaps between the valence band maximum (VBM) and the new flat bands. As shown in Figure 4b, the new flat band below the Fermi level is close to the CBM ($E_g = 0.103$ and $0.17$) for BV-modified Cd(Zn)Te nanostructures, confirming that it can form a shallow donor state and leading to a typically controlled n-type doping in Cd(Zn)Te nanostructures. Meanwhile, the new flat band above the Fermi level is very close to the VBM ($E_f = 0.102$ and $0.099$ eV) in the F4-TCNQ-modified systems (Figure 4c), verifying that it acts as a shallow acceptor state for controlled p-type doping. The total DOS of the molecule-modified systems and the PDOS for both dopant molecules (BV and F4-TCNQ) and Cd(Zn)Te nanostructures in these adsorption systems were also computed (Figure 5), validating that the results from the band structures and confirm that the new flat energy levels are generated by the dopant molecules. The above results collectively demonstrate that the electronic property of CdTe and ZnTe nanostructures can be modulated by the adsorption of BV and F4-TCNQ molecules.

SCTD has been proven to be a simple, nondestructive, and effective method to modulate the electronic, optical, and transport properties of low-dimensional semiconductors. In this approach, through controlling the Fermi level ($E_F$) misalignment of surface dopants with respect to underlying semiconductor nanostructures, electrons can be extracted from (or injected into) the nanostructures forming an electron-deficient (or electron-rich) surface layer. Carrier concentration and even conduction type of the semiconductor nanostructures can be readily tuned by varying the types and densities of surface dopants, leading to effective n- and p-type doping on the nanostructures. Therefore, BV with low ionization potential and F4-TCNQ, with high electron affinity are chosen as n- and p-type dopants to control n- and p-type doping of CdTe and ZnTe nanostructures in this work, respectively, because these n- and p-type surface dopants can be deposited onto the semiconductor surface via solution-processing methods like spin-coating and drop-casting or vapor-based technologies like evaporation. Energy level alignment between the semiconductor and surface dopant offers an intuitive physical picture for understanding the SCTD process. Figure 6 illustrates the energy versus vacuum energy of Cd(Zn)Te semiconductors and surface dopants (BV and F4-TCNQ), and the energy level of Cd(Zn)Te semiconductors and surface dopants (BV and F4-TCNQ) is obtained from the literature studies. It can be noted that the highest occupied molecular orbital (HOMO) of BV lies a little above the conduction band minimum (CBM) of ZnTe while much higher than the CBM of CdTe, which impels electron transfer from the HOMO of BV to the CBM of the Cd(Zn)Te semiconductor due to the energy difference and strong electron-donating ability of BV. Thus, the large downward band bending with electron accumulation near the Cd(Zn)Te semiconductor surface is achieved at thermal equilibrium, corresponding to n-type doping in the semiconductor. In contrast, the lowest unoccupied molecular orbital (LUMO) of p-type surface dopant F4-TCNQ lies slightly below the valence band maximum (VBM) of the Cd(Zn)Te semiconductor, which drives electron transfer from the VBM of the Cd(Zn)Te semiconductor to the LUMO of F4-TCNQ when they are placed into contact with each other until thermal equilibrium is reached. This leads to a large upward band bending with hole accumulation near the Cd(Zn)Te semiconductor surface, corresponding to p-type doping in the semiconductor. These relative energy level positions of the HOMO/LUMO of the BV/F4-TCNQ organic molecule to those of the Cd(Zn)Te semiconductor determine the doping type, which agrees well with calculated results of electronic properties for CdTe and ZnTe before and after surface modification as aforementioned (Figures 4 and 5). Therefore, to some extent, the adsorption of BV and F4-TCNQ is important for doping of CdTe and ZnTe nanostructures.

As mentioned above, the adsorption of BV and F4-TCNQ on the surface of CdTe and ZnTe nanostructures has an obvious effect on the electronic properties of intrinsic nanostructures. Therefore, to further characterize the impact of BV and F4-TCNQ adsorptions on the optical properties of CdTe and ZnTe nanostructures, we calculated the optical spectra of the intrinsic and surface-modified Cd(Zn)Te nanostructures, as shown in Figure 7. The imaginary part of the dielectric functions ($\varepsilon_2$) is an effective parameter to measure the optical absorption ability of materials. As we know, the peaks in $\varepsilon_2$ are caused by the absorption of incident photons and the interband transition of electrons. It can be noted that there are obvious absorption peaks in the visible light region for intrinsic CdTe and ZnTe, which is in good agreement with previous report and verifies the light-absorbed materials of CdTe and ZnTe. For the BV-modified systems, a significant redshift in absorption peaks is observed in CdTe and ZnTe.
new peak appears at ∼1200 nm in the near-infrared region and the intensity of the absorption peak in the visible light region is enhanced compared to those of intrinsic CdTe and ZnTe peaks. Similarly, in the F4-TCNQ-modified systems, new absorption peaks appear in the near-infrared region. All these phenomena suggest that both BV and F4-TCNQ surface modifications can induce an increase in the optical absorption range and the absorption intensity of intrinsic CdTe and ZnTe nanostructures, leading to the enhanced light absorption in the long wavelength direction. This will be of great importance to the application of CdTe and ZnTe in high-performance optoelectronic devices, such as photovoltaics and photodetectors.

The above static electronic properties reveal that SCTD can achieve an effectively controlled n- and p-type doping of CdTe and ZnTe nanostructures. Therefore, to explicitly evaluate the effects on the performance of Cd(Zn)Te nanowire (NW) devices and the change of their electronic transport behaviors, we employed the NEGF method to calculate the electrical transfer characteristics of Cd(Zn)Te NW devices before and after surface modification (BV and F4-TCNQ), as shown in Figure 8.

Figure 8a,b depicts the simulated CdTe FET before and after F4-TCNQ modification in which the bottom-gate geometry provides high gate-controlled electrostatics. Qualitatively, the drain–source currents ($I_{DS}$) of Cd(Zn)Te NW FETs decrease exponentially with the rise in gate voltage ($V_G$) (in Figure 8c), indicating their intrinsic p-type conductive characteristics. By comparison, $I_{DS}$ of the CdTe NW FET is $10^3$–$10^5$ times higher than that of the ZnTe NW FET, revealing the higher conductivity of CdTe, which might be attributed to the narrower band gap in intrinsic CdTe. Because the amount of calculation of both CdTe and ZnTe NW FETs before and after surface modification is very large, we take the CdTe NW FET as an example to clarify the effect of surface modification on the electrical transfer characteristics, as presented in Figure 8d. The electrical transfer characteristics of F4-TCNQ-modified CdTe NW FET also present a p-type conductivity. Meanwhile, it is observed that $I_{DS}$ of the CdTe NW FET can be dramatically enhanced by the adsorption of F4-TCNQ by more than $10^3$ times. The reason for this phenomenon is that the charge transfer from CdTe NWs to the adsorbed F4-TCNQ can further increase the amount of hole carriers into CdTe NWs, which is a positive factor to improve the conductivity of p-type CdTe NWs. However, after the adsorption of the BV molecule, the tendency of $I_{DS}$ changes to increase with the rise in $V_G$, which obviously shows an n-type conductive characteristic. It is indicated that the adsorption of the BV molecule can not only exhaust the hole carriers from the intrinsic p-type CdTe NWs but also inject electrons into CdTe NWs, thus effectively tuning the conduction type of CdTe NWs from p-type into n-type, owing to the strong n-type doping effect of the BV molecule. According to the above device performance of surface-modified CdTe NW FETs, it is possible to modulate the electronic transport behavior in the ZnTe NW FET via the surface adsorption of BV and F4-TCNQ molecules. Therefore, these results indicate that SCTD with BV and F4-TCNQ molecules can effectively modulate the transport property of CdTe and ZnTe NWs.

3. CONCLUSIONS

In conclusion, based on the first principles calculations, the electronic, optical, and transport properties of CdTe and ZnTe nanostructures were systematically investigated before and after adsorption with BV and F4-TCNQ organic molecules. The calculated results showed that the surface of CdTe and ZnTe nanostructures tends to accumulate the electron/hole after the adsorption of BV/F4-TCNQ, respectively, leading to the downshift/upshift of the Fermi level. Also, the difference in charge density analysis also proved the remarkable surface charge transfer between Cd(Zn)Te nanostructures and organic molecules. In addition, the adsorption of BV and F4-TCNQ resulted in a new flat band appears close to the CBM/VBM of Cd(Zn)Te nanostructures, confirming that it can form a shallow donor/acceptor state for n-/p-type doping, respectively. Moreover, the optical property calculation suggested that the adsorption of BV and F4-TCNQ on Cd(Zn)Te nanostructures not only induced new adsorption peaks in the near-infrared region but also strengthened the absorption intensity in the visible light region, enhancing the light absorption at a longer wavelength direction. Also, the transport
calculation revealed that the conduction type of the Cd(Zn)Te NWs can be rationally modulated by the adsorption of BV and F4-TCNQ, thus forming the basis for a variety of high-performance electronic and optoelectronic nanodevices. Our work demonstrated that the electronic, optical, and transport properties of CdTe and ZnTe nanostructures can be efficiently modulated by organic molecules (BV and F4-TCNQ), opening up the opportunities to construct high-performance optoelectronic devices, widening the applications of CdTe and ZnTe nanostructures in the electronic and optoelectronic device fields.

4. COMPUTATIONAL METHODS

Our first principles calculations were performed by employing the DFT as implemented in the Cambridge sequential total energy package (CASTEP) program\textsuperscript{37} in Materials Studio 7.0 package of Accelrys Ltd. The interactions between the ions and electrons were treated by the generalized gradient approximation (GGA) in the form proposed by Perdew, Burke, and Ernzerhof (PBE) with Vanderbilt ultrasoft pseudopotential.\textsuperscript{38–40} The zero-damping vDW-D3 correction proposed by Grimme\textsuperscript{41} was used to describe the long-range interaction between the organic molecules and Cd(Zn)Te nanostructures. The cutoff energy of 500 eV and 8 × 8 × 1 Monkhorst–Pack\textsuperscript{42} k-points in the first Brillouin zone were used. Both the cutoff energy and k grid were tested to be converged in the total energy. The initial surface models of CdTe and ZnTe nanostructures were built from an ideal bulk CdTe and ZnTe phase, and the native defects (vacancies, interstitials, etc.) were not considered in this study.

Electron transportation behavior was calculated by the DFT coupled with the NEGF formalism implemented in the SIESTA package.\textsuperscript{43} The simulated bottom-gate field-effect transistor (FET) structure consisted of BV- and F4-TCNQ-adsorbed Cd(Zn)Te NWs as the intrinsic channel material, the two end sides of which were assumed to act as the source and drain contacts. In the BV-adsorbed system, the whole simulated region was embedded above a BN (k = 4) dielectric layer with a thickness of 1.5 Å and a metallic gate electrode with a thickness of 2.3 Å was attached to the dielectrics below layer with a thickness of 1.5 Å and a metallic gate electrode. In the BV-adsorbed system, the whole simulated region was embedded above a BN (k = 4) dielectric layer with a thickness of 1.5 Å and a metallic gate electrode with a thickness of 2.3 Å was attached to the dielectrics below layer with a thickness of 1.5 Å and a metallic gate electrode with a thickness of 2.3 Å was attached to the dielectrics below layer with a thickness of 1.5 Å and a metallic gate electrode with a thickness of 2.3 Å was attached to the dielectrics below layer with a thickness of 1.5 Å and a metallic gate electrode.

\begin{align}
I(V_G, V_D, V_D) &= \frac{2e}{h} \int_{-\infty}^{+\infty} \left[ T_{V_G}(E, V_D, V_G) \right. \\
&\left. \left[ f_s(E - \mu_s) - f_D(E - \mu_D) \right] \right] dE
\end{align}

where $T_{V_G}(E, V_D, V_G)$ was the transmission probability at a given gate voltage $V_G$ and drain–source voltage $V_D$. $f_s$ and $f_D$ are the Fermi–Dirac distribution function for the source/drain electrode, and $\mu_s/\mu_D$ is the electrochemical potential for the source/drain electrode. Effects of gate were calculated by solving the Poisson equation self-consistently.

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