Research Article

Revisiting the Zinc-Blende/Wurtzite Heterocrystalline Structure in CdS

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The band offset at CdS zinc-blende (ZB)/wurtzite (WZ) heterocrystalline interface was revisited using the first principles calculations with the local density approximation (LDA), generalized gradient approximation (GGA), and Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional. It was revealed that, unlike most IV, III-V, and II-VI semiconductors, the band alignment at CdS ZB/WZ heterocrystalline interface was of type-I with straddling lineup of band edges, which was irrespective of the exchange-correlation energy functional, the thickness of ZB and WZ segments, and the ZB/WZ interface location. The partial charge densities of VBM and CBM states were separated around two adjacent interfaces in one unit cell of heterocrystalline superlattice. This type of carrier localization was mainly attributed to the spontaneous polarization occurring in the WZ segment rather than the band offset at the interface.

1. Introduction

The zinc-blende (ZB)/wurtzite (WZ) heterocrystalline structure can form a new type of superlattice [1]. This type of superlattice had the potential to produce the “anomalous photovoltaic effect” [2, 3] and thus may be applied in the solar energy conversion and utilization. As a prototypical example, ZB/WZ heterocrystalline structure in SiC has been extensively studied [4–7]. It has been established that the spontaneous polarization, valence band offset, and quantum confinement effect were three key effects in the heterocrystalline superlattice which should be considered [8]. The band alignment of type-II at ZB/WZ interface was determined by density functional theory (DFT) calculations on ZB and WZ bulk IV, III-V and II-VI semiconductors [9], and confirmed by the Photoluminescence measurements and tight-binding calculations on InP and GaAs [10–12]. It has also been reported that this type of band alignment can be tuned by the diameter of ZB/WZ superlattice nanowires [13].

CdS is an important energy material in photovoltaic cells, photoelectrochemical, or photocatalytic water splitting [14–19]. Li et al. found that phase junctions on TiO_2 and Ga_2O_3

can significantly improve the efficiency for hydrogen production [20, 21]. Thus, it is meaningful to introduce the concept of phase junction into the design of CdS photocatalyst. Murayama and Nakayama calculated the valence band offset at CdS ZB/WZ heterocrystalline interface using a plane wave pseudopotential method without considering the ZB/WZ interface effect [9]. Wei and Zhang calculated the valence band offset with the interface dipole using a linearized augmented plane wave method [22]. Both studies gave a band alignment of type-II with staggered lineup of band edges at CdS ZB/WZ interface. However, we noticed that the spontaneous polarization occurring in the WZ structure was not taken into consideration in determining the valence band offset. Such an effect was important to determine the band offsets at the interface and carrier distribution in the superlattice.

In this paper, the band offset at CdS ZB/WZ heterocrystalline interface was determined with the first-principles calculations. Three exchange-correlation energy functionals, different number of ZB or WZ atomic layers in one unit cell and different interface locations were considered to verify the reliability of calculated results. The carrier distribution

FIGURE 1: Schematic diagram of one unit cell in CdS ZB/WZ heterocrystalline superlattice with 6 zinc-blende (ZB) and 6 wurtzite (WZ) atomic layers. Empty circle represents S atom and solid circle represents Cd atom. Vertical dashed and dotted lines indicate the locations of abrupt interfaces I and II, respectively.

in ZB/WZ heterocrystalline superlattice was explained by the effect of spontaneous polarization.

2. Computational Methods

The unit cell in CdS ZB/WZ heterocrystalline superlattice was made up of a number of ZB and WZ atomic layers along ZB (111) and WZ (0001) directions, as shown in Figure 1. The calculations were carried out by using the Vienna *ab initio* Simulation Package (VASP) [23, 24]. The plane wave and projector augmented wave potentials (PAW) method [25] were employed in the framework of DFT. Local density approximation (LDA-PZ-CA) [26, 27], generalized gradient approximation (GGA-PBE) [28], and HSE06 hybrid functionals [29, 30] were used to examine the effect of the exchange-correlation energy on the band alignment at the interface. For HSE06 hybrid functional, 30% of Hartree-Fock exchange was used to produce a band gap agreeing well with the experimental value. The kinetic energy cutoff was chosen as 380 eV. The Monkhorst-Pack k-point meshes [31] were $9 \times 9 \times 9$ for bulk ZB phase CdS, $9 \times 9 \times 5$ for bulk WZ phase, and $9 \times 9 \times 1$ for the heterocrystalline superlattice. When the hybrid functional was used, these k-point meshes were somewhat reduced to save the computational cost.

The method to determine the band offset [32] was described in the following three steps: first, to calculate the energy difference between the valence band maximum (VBM) and macroaveraged electrostatic potential through bulk calculations; second, to calculate the difference in the macroaveraged electrostatic potential across the ZB/WZ interface through the interface calculations; third, to determine the valence band offset (VBO) by combining the energy differences in bulk calculations and the potential difference across the interface, and furthermore the conduction band offset (CBO) from VBO and the difference in band gap between ZB and WZ phase CdS.

3. Results and Discussions

The calculated structural parameters and band gaps of bulk ZB and WZ CdS were shown in Table 1. The structural parameters from LDA and GGA-PBE calculations slightly deviated from those experimental values. The hybrid functional HSE06 calculations used the crystal structure optimized by GGA calculations and showed a large improvement on the band gap with respect to LDA and GGA calculations. When building the ZB/WZ interface, the structural parameter in the

TABLE 1: Calculated and experimental structural parameters (a , c , and u) and band gap (E_g) of zinc-blende (ZB) and wurtzite (WZ) CdS.

Properties	LDA	GGA-PBE	HSE06	Experiment ^a
$a_{\text{ZB}}/\text{\AA}$	5.770	5.944		5.818
$a_{\text{WZ}}/\text{\AA}$	4.087	4.210		4.136
$c_{\text{WZ}}/\text{\AA}$	6.668	6.856		6.714
$(c/a)_{\text{WZ}}$	1.632	1.628		1.623
u_{WZ}	0.3758	0.3762		0.3730 ^b
$E_g(\text{ZB})/\text{eV}$	0.96	1.04	2.29	2.37 ^c
$E_g(\text{WZ})/\text{eV}$	1.03	1.10	2.36	2.48 ^d

^a[22], ^b[34], ^c[35], and ^d[36].

interface was taken to be the average value of $a_{\text{ZB}}/\sqrt{2}$ and a_{WZ} in the planes perpendicular to ZB (111) and WZ (0001) direction. The lattice mismatch at this interface was estimated within 0.1% and thus the lattice strain was very small.

3.1. Band Offset. The spontaneous polarization occurring in the WZ segment in the heterocrystalline superlattice resulted in a macroaveraged electrostatic potential with the sawtooth-like shape, as shown in Figure 2. The potential difference at the ZB/WZ interface cannot be estimated straightforwardly because of the spontaneous polarization which was not remarkable in the conventional heterojunction. The method proposed by Qteish et al. [4] was employed to exclude the effect of the spontaneous polarization on the determination of band offsets. The potential difference can be regarded as the discontinuity in the electrostatic potential at the ZB/WZ interface which was determined by linearly extrapolating the macroaveraged electrostatic potentials on both sides of the interface. There are two ways to define the abrupt interface, which were reported in the literature. Interface I was defined from the viewpoint of local environment “seen” by the interface [33], and interface II was located according to the analysis of charge distribution [4]. Both types of interfaces were examined in this paper. The macroaveraged valence charge density around the interface significantly deviated from that in the bulk region, reflecting the effect of the interface.

The calculated band offsets at CdS ZB/WZ heterocrystalline interface were summarized in Table 2. A clear band alignment of type-I was manifested from all of our results, regardless of the exchange-correlation energy functional, the

FIGURE 2: (a) Macroaveraged valence charge density and (b) macroaveraged electrostatic potential in CdS ZB/WZ heterocrystalline superlattice. For empty and solid circles and vertical dashed and dotted lines, please see Figure 1.

TABLE 2: Band offset (VBO and CBO) at CdS ZB/WZ heterocrystalline interface (values in parentheses without considering the interface dipole) and band gap (E_g) with different zinc-blende (ZB) and wurtzite (WZ) atomic layers.

Properties	Murayama ^a	Wei ^b	ZB/WZ layers	LDA	GGA-PBE interface		HSE06
					I	II	
VBO/meV	(19)	46 (-1)	6/6	-23 (-31)	-38 (-18)	-17 (-18)	-36 (-18)
			12/12		-43 (-18)	-20 (-18)	
			24/12		-40 (-18)	-17 (-18)	
CBO/meV	(73)	115 (68)	6/6	44 (36)	25 (45)	46 (45)	35 (53)
			12/12		20 (45)	43 (45)	
			24/12		23 (45)	46 (45)	
E_g /eV			6/6	0.964	1.025		2.268
			12/12		0.875		
			24/12		0.727		

^a[9]; ^b[22].

size of unit cell, and the interface location and dipole. GGA-PBE and HSE06 methods produced similar VBOs which were slightly larger than the value from LDA method. The thickness of ZB and WZ segments in one unit cell had a large influence on the band gap, but hardly affected the band offsets. The interface dipole changed with the choice of interface location, decreasing from interface I to II. This resulted in a larger VBO at interface I than at interface II. In order to further verify the reliability of the calculated band offsets, the well-known VBO at SiC ZB/WZ interface was examined here. A VBO of 0.12 eV was obtained at interface I with LDA, comparable with the reported values of about 0.13 eV [4, 8] and 0.14 eV [6, 37]. The previous study by Murayama and Nakayama gave a band alignment of type-II through ZB and WZ bulk calculations, which used the plane wave pseudopotential and LDA method. We deduced that the inconsistency may be due to the exclusion of d electrons in Cd and Zn atoms in their work. Inclusion of d electrons has been demonstrated to be essential to form correct VBM states [38]. Wei and Zhang reported that the band alignment between CdS ZB and WZ phases was of type-I without the interface dipole, but the band alignment turned to type-II if the ZB/WZ interface was considered [22]. We deduced that the inconsistency may be attributed to the spontaneous polarization occurring in the WZ structure which was not considered in their calculation. The effect of spontaneous polarization was obvious in CdS ZB/WZ heterocrystalline superlattice. The band gap decreased with the thickness of

ZB and WZ segments increasing, due to the spontaneous polarization [6] which may be overestimated by the current first-principles calculations [8].

In addition, the effect of atom relaxation in the supercell was considered. We found that the atom relaxation can be neglected in terms of the small interface atom movement, almost identical band offset, and consistent partial charge distribution (for partial charge, see the text below).

3.2. Carrier Localization. According to the previous reports, the type of band alignment at ZB/WZ interface can be identified by the charge density distribution of VBM and CBM states [1, 22, 39]. We would like to point out that it was a misunderstanding. Figure 3 shows the plane-averaged charge densities of VBM and CBM states in CdS ZB/WZ heterocrystalline superlattice with different thickness of ZB and WZ segments. It can be found that the partial charge densities in CdS ZB-6/WZ-6 superlattice well reproduced those presented by Wei and Zhang [22]. It seems that VBM state was localized in the WZ region while CBM state was localized in the ZB region, and thus this type of carrier distribution was attributed to the type-II band alignment at the ZB/WZ interface, just as Wei and Zhang described. However, as the thickness of ZB and WZ segments increases, we found that VBM and CBM states were actually localized around two adjacent interfaces in one unit cell of the superlattice, instead of on both sides of one single interface. The partial charge

FIGURE 3: Plane-averaged charge densities of (a) VBM and (b) CBM states in three CdS ZB/WZ heterocrystalline superlattices (ZB-6/WZ-6, ZB-12/WZ-12, and ZB-24/WZ-12). For empty and solid circles and vertical dashed and dotted lines, please see Figure 1.

FIGURE 4: The lineups of VBM and CBM in CdS and ZnS ZB/WZ heterocrystalline superlattices.

density of CBM state was more delocalized than that of VBM state because of the smaller effective mass for CBM state.

The character of carrier localization was in good accord with the lineup of VBM and CBM states in CdS ZB/WZ heterocrystalline superlattice, as shown in Figure 4. The lineup of VBM and CBM states was composed of the potential variation resulted from spontaneous polarization, band offset at the interface, and quantum confinement effect. The plane-averaged charge density of VBM state was mainly localized around the interface at the hill of electrostatic potential while that of the CBM state was mainly around the interface at the valley of electrostatic potential. In the CdS ZB/WZ heterocrystalline superlattice, the effect of spontaneous polarization played a decisive role in determining the lineup of VBM or CBM, instead of the band offset.

It has been established that “anomalous photovoltaic effect” took place only in crystals where at least some stacking disorder occurred (i.e., changes in structure from ZB to WZ) [2, 3]. The main feature of this effect was the production of a much larger photovoltage than the band gap. According to “theory of the anomalous photovoltaic effect” [40], the photovoltages produced by two opposing interfaces in one unit cell of heterocrystalline superlattice could not be cancelled completely. This was due to one interface on the hill and the other interface in the valley of the periodic potential, leading to two interfaces with different carrier concentrations and photovoltages. As a result, a net photovoltage can be generated in one unit cell, and after superposing photovoltages of these unit cells, the final large photovoltage was generated. We thought that such a large photovoltage can afford extra power to promote the photocatalytic reaction for hydrogen production. Recently, the nanowires with controlled stacking faults have been fabricated successfully [41]. This provided an opportunity to examine the effect of “anomalous photovoltaic effect” on the photocatalytic reaction.

4. Conclusions

In summary, the band alignment at CdS ZB/WZ heterocrystalline interface was revisited with careful first-principles calculations, and it proved to be of type-I. The inconsistency with previous theoretical studies may be attributed to their incomplete consideration of ZB/WZ heterocrystalline

superlattice. Such a superlattice had the ability to separate photogenerated carriers, and the separation of electrons and holes was mainly due to the spontaneous polarization occurring in the WZ structure, not merely due to the band offset. The spontaneous polarization dominated the distribution of electrostatic potential, and thus resulted in the localization of partial charge densities of VBM and CBM states in the heterocrystalline superlattice. Finally, it can be expected that “anomalous photovoltaic effect” that occurred in the ZB/WZ heterocrystalline superlattice may be applied in the photocatalytic reactions because of the large photovoltage output.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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