



Electric field effects on the electronic and optical properties in C₂N/Sb van der Waals heterostructure

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ABSTRACT

Development of novel van der Waals (vdW) heterostructure is of great interest and significant to improve the performance of photovoltaic, photocatalytic and optoelectronic devices. In this work, the C₂N/ β -Sb vdW heterostructure has been investigated by the first-principles calculations. It is found that the pristine C₂N/ β -Sb vdW heterostructure is a type-II heterostructure with a direct band gap of 1.2eV, and has a number of desired optoelectronic properties that are suitable for use in a solar cell. The external electric field can effectively modulate band alignment and affect the optical properties of the C₂N/ β -Sb heterostructure. The energy conversion efficiency of the pristine heterostructure is 22.86%, and the energy conversion efficiency can be increased under the negative electric field. Our results show that the C₂N/ β -Sb vdW heterostructure possesses great potential to be high-performance optoelectronic device.

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1. Introduction

Heterostructures consisting of two types of donor and acceptor materials have been proposed to be used in photocatalytic and optoelectronic devices [1–8] due to the unprecedented performance of the materials. However, to achieve the high-performance of the devices, the heterostructures must possess a number of properties, such as chemical stability, a high carrier mobility and a direct band gap of roughly 1.2–1.6eV [1]. Organic materials consisted of polymers and small molecules have been investigated to design solar cell device [9,10]. However, it is a challenging task to tune the highest occupied molecular orbital and lowest unoccupied molecular orbital levels of the conjugated polymers; the band gaps of less than 1.5eV are hard to achieve, and thus the absorption loss in the red part of the solar spectrum can be significant [10]. The advent of two-dimensional (2D) materials with tunable optical

properties and high carrier mobility offer renewed opportunities for thin-film excitonic solar cell. Graphene received the significant attention due to its extremely high mobility as high as $2 \times 10^5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ [11]. The graphene/boron nitride heterostructure maintains the high carrier mobility under the photoinduced doping [12]. MoS₂ possesses a direct band gap [13] and exhibits high stability [14]. The type-II heterostructure composed of MoS₂ and g-C₃N₄ can easily separate the photogenerated carrier [15]. The black phosphorene possesses an inherent direct band gap and a high mobility of up to $\sim 10^3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ [16]. The tunable band gap of the black phosphorene/blue phosphorene heterostructure under the external electric field offers a practical route to application in optoelectronics [17]. The properties of the heterostructure depend on the composed materials, therefore, it is important to search new type of material to develop the high-performance photoelectronic device.

Recently, monolayer C₂N has been synthesized via a simple wet-chemical reaction [18]. The 2D C₂N sheet has a direct band gap of 2.47eV [19] and the field-effect transistor device fabricated using this material exhibits an on/off ratio of 10^7 [18]. The band gap of C₂N sheet exhibits a decreasing trend with applied electric field [20]. Few-layer C₂N has better visible light absorption than graphitic

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C₃N₄ [21], which makes C₂N a promising candidate for a metal free photocatalyst. The transition metal doped C₂N sheets show unexpected stability and have a potential application in single-atom catalyst [22]. In addition, 2D porous C₂N sheets exhibit an extremely high selectivity and large permeance favorable for H₂ [23], which can be used for hydrogen separation. Group V elemental monolayers including antimonene have been investigated widely. Both α -Sb and β -Sb possess unexceptionable stability and tunable band structure [24]. Singh et al. [25] reported that the reflectivity does not exceed 20% up to far UV in β -Sb and the maximum reflectivity reaches the values of 64% for β -Sb at the UV energy. The tensile strain can induce a nontrivial topological insulating phase in Sb thin films, indicating the possibility of realizing the quantum spin Hall state for Sb thin films on suitable substrate [26]. The As/Sb heterostructure with a tunneling barrier height of 0.21 eV is a promising candidate for the staggered gap field effect transistor [27]. In the heterostructure of Sb₂H/LaFeO₃, the substrate induces a drastic staggered exchange field in the Sb₂H film, which plays an important role for the quantum spin–quantum anomalous Hallinsulator [28].

The strategy to modulate the electronic structure is crucial to achieve the high performance of the electronic devices. The applications of an external electric field (E_{field}) and a tensile strain are the widely used engineering strategies [29–32]. For example, Guo et al. reported that the strain can transform the MXene/blue phosphorene heterostructure from type-I to type-II heterostructure [33]. Ma et al. showed that the band structure of the MoS₂/PbI₂ heterostructure can be effectively modulated by the E_{field} and the band gap varies linearly with the E_{field} [34]. However, different from the former strategies, Hu et al. constructed a heterostructure from the hydrogen- and fluorine-passivated phosphorene. The polar covalent bonds of the forms P⁺-H⁻ and P⁻-F⁻ around the edges of the phosphorene result in the type-II band alignment [35].

Due to the outstanding properties of the type-II heterostructures, a number of monolayer materials have been investigated to construct the 2D heterostructure [36–46] in both experimental and theoretical fields. However, to our knowledge, the study is rare in C₂N (Sb)-based 2D heterostructure. In light of the superior electronic properties of C₂N monolayer and Sb monolayer, it is necessary to investigate the C₂N/Sb heterostructure. It is worth noting that band edges of β -Sb can locate at the gamma point [24], and the band edges of C₂N monolayer also locate at the gamma point, the electronic structure of the C₂N/ β -Sb heterostructure may be interesting. Therefore, in this paper, we systematically investigate the electronic structure of the C₂N/ β -Sb vdW heterostructure. The results show that the C₂N/Sb vdW heterostructure is a type-II heterostructure. The tunable band alignment and band gap of the C₂N/Sb heterostructure originate from the various band edges under the E_{field} . The Fermi level (E_F) of C₂N and Sb monolayer diverge under the E_{field} , which promotes the electrons transfer. The optical absorption edge is shifted to lower (higher) energy region under the positive (negative) electric field. Finally, the high power conversion efficiency (PCE) of the C₂N/Sb heterostructure has been predicted. Owing to the tunable electronic properties and large PCE, the C₂N/Sb vdW heterostructure will has a tremendous opportunities to be applied in the photo-electronic device.

2. Methods

Our calculations were based on Density Functional Theory (DFT) in conjunction with projector augmented wave (PAW) potentials, as implemented in the Vienna *ab initio* simulation package (VASP) [47–50]. For the exchange–correlation functional, the generalized

gradient approximations (GGA) of Perdew–Burke–Ernzerhof (PBE) [51] was employed for the structural relaxation. The k-points of $9 \times 9 \times 1$ and $11 \times 11 \times 1$ automatically generated by the Monkhorst–Packscheme [52] were used for structural optimization and self-consistent calculations, respectively. The cutoff energy was set to be 500 eV and the dipole correction has been employed. The DFT-D3 method [53] was employed to describe the interlayer vdW interactions. The vdW interaction is important to investigate the interface distance. Many methods, such as DFT-TS, vdW density functionals (vdW-DF) and random phase approximation (RPA) [54], can get reasonable results. However, given the computational cost, we selected the DFT-D3 method [53] to describe the interlayer vdW interactions. The thickness of the vacuum region was taken to be at least 20 Å to avoid artificial interactions between the layer and its periodic images. In order to obtain a more accurate description of the electronic states, all of the results were calculated using the hybrid functional (HSE06) [55,56]. The convergence criteria for energy and force were set to be 10^{-5} eV and 0.005 eV/Å, respectively. The number of band was set to 300 (241 for unoccupied bands) and the frequency grid was set to 301 in optical property calculations.

3. Results and discussion

The optimized structures of monolayer β -Sb and C₂N are illustrated in Fig. 1(a) and (b), respectively. The monolayer C₂N has a planar framework, which is different from silicene and germanene. The optimized lattice constants of monolayer C₂N and Sb are 8.33 Å and 4.12 Å, and the bond lengths of C–N, C–C(1) and C–C(2) are 1.337 Å, 1.428 Å and 1.471 Å, respectively, which agree with previous studies [57,58]. Fig. 1(c) and (d) plot the projected band structure of monolayer Sb and monolayer C₂N, respectively. In the C₂N monolayer, the band edges are contributed by the C-2p orbital and N-2p orbital, the valence band maximum (VBM) and conduction band minimum (CBM) both locate at the Γ point, indicating the C₂N monolayer is a direct band semiconductor with a band gap (E_g) of 2.46 eV, which is in agreement with previous study [19]. In Sb monolayer, the band edges are contributed by Sb-5p orbital, the VBM locates at the Γ point and CBM locates at the area adjoined M point, indicating the Sb monolayer is an indirect band semiconductor with a E_g of 1.95 eV. The lattice match is crucial for the heterostructure. To minimize the lattice mismatch of the heterostructure, the stacking sheet is composed by 1×1 unit cell of C₂N and 2×2 unit cell of Sb. The lattice mismatch is less than 1.1%, which is desirable to fabricate the vdW heterostructure. We consider three typical stacking configurations, which are labeled by A-type, B-type and C-type, respectively, as shown in Fig. 2. It is clear that stacking models can transform each other by horizontal layer sliding and the interlayer distances are identical. The binding energy of C₂N/Sb vdW heterostructure is evaluated according to the equation,

$$E_b = E_C + E_S - E_T \quad (1)$$

where E_T , E_C and E_S are the total energy of the C₂N/Sb vdW heterostructure, C₂N monolayer and Sb monolayer, respectively. The results are listed in Table 1, which indicate the A-type is the most stable stacking configuration. In order to check the dynamic stability of A-type stacking configuration, we perform *ab initio* molecular dynamics (AIMD) under the canonical (NVT) ensemble, using a $2 \times 2 \times 1$ supercell containing 104 atoms. The simulations are carried out using a Nosé thermostat at 300 K for 6 ps. Fig. 3 shows the fluctuation of total energy and temperature as a function of the simulation time. After 6 ps, no structure distortion is found in the heterostructure, and the amplitude of fluctuation for total energy is small during the AIMD process, which confirms that

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