Journal of Alloys and Compounds 766 (2018) 215–220

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

SnS nanoribbon/graphene mixed-dimensional heterostructures: Group VII passivation and quantum size effects

Congxin Xia [a, *], Lizhen Fang [a], Xueping Li [b], Wenqi Xiong [a], Zhenduo Geng [a, **]

[a] College of Physics and Materials Science, Henan Normal University, Xinxiang, Henan 453007, China
[b] College of Electronic and Electrical Engineering, Henan Normal University, Xinxiang, Henan 453007, China

ARTICLE INFO

Article history:
Received 15 April 2018
Received in revised form
18 June 2018
Accepted 28 June 2018
Available online 30 June 2018

Keywords:
Mixed-dimensional vdWHs
p-type
Schottky contact

ABSTRACT

The mixed-dimensional van der Waals heterostructures (vdWHs) are attracting extensive attention in the electronic and optoelectronic device, while the related physics mechanisms are still unclear. Here, we study theoretically the stability and electronic properties of the SnS nanoribbon (SnSNR)/graphene mixed-dimensional vdWHs. The results show that these considered mixed-dimensional vdWHs are energetically stable, and Dirac-cone of graphene is close to the top of valence band of SnSNR and thus p-type Schottky contact is formed. Interestingly, group VII passivation can induce transformation from p-type to n-type Schottky contact. Particularly for the F-passivated case, the Fermi level is closer to the CBM of SnSNR. Also, quantum size of SnSNR slightly decreases the *p*-type Schottky barrier height (SBH). Therefore, this work understands the physics mechanism and related experiments of graphene-based mixed-dimensional vdWHs.

1. Introduction

Recently, all two-dimensional (2D) materials-based van der Waals heterostructures (vdWHs) have been developed rapidly because they possess novel properties [1–7]. Among these studied vdWHs, 2D graphene-based vdWHs are attaching extensive interesting [8–11], such as graphene/h-BN [12–14],graphene/MoS_2 [15–17] and graphene/phosphorene vdWHs [18,19]. Studies show that Schottky contact is formed in these vdWHs [8–19]. Interestingly, the Schottky contact type and the Schottky barrier height (SBH) can be adjusted by interlayer distance [20], electric field [21–25] and strain [22,26]. These publications present that they keep the characteristics of Dirac cone and semiconductor, Schottky contact can be formed and many other interesting properties far beyond those of the individual component. Thus, working on the electronic studies of graphene-based vdWHs is of great importance to understanding the related physics mechanism and device applications.

Except all 2D vdWHs, the mixed-dimensional vdWHs have also been involved intensively, which consists of 2D materials and non-2D materials (0D, 1D and 3D materials) [27–32]. For graphene-based mixed-dimensional systems, the graphene-Si mixed-dimensional vdWHs can be applied to field-effect transistors and logic devices [33]. The mixed-dimensional vdWHs of 1D ZnO nanorod and graphene exhibit some outstanding performances in ultraviolet photodetectors [34]. The 0D PbS quantum dot and graphene vdWHs can also be applied in photodetectors [35]. The spectral response can be adjusted by gate voltage and the size of quantum dot [35,36]. Moreover, in the experiment, the edges of MoS_2 nanoribbon (NR) play important role for high catalytic activity in the MoS_2NR/graphene vdWHs [37–40]. Guo et al. indicates that when the 1D MoS_2NR and 0D MoS_2 quantum dot contact graphene, the S-edges of MoS_2 materials attract electrons from graphene [41]. These can be seen that the mixed-dimensional vdWHs have some splendid properties beyond all-2D vdWHs.

In this work, we focus on the edge and size effects of SnSNR on the electronic structures in the 1D/2D SnSNR/graphene mixed-dimensional vdWHs. SnS material has been considered as a ideal optical absorber in thin film solar cells [42–45] and photocatalysts [45–48]. The 1D SnS nanowires have excellent field emission characteristics [49]. The 1D SnSNR can be used for photodetectors and has rapid photocurrent responses to illumination [50]. Hence, it is necessary to research the effect of nanoribbon size and edge passivation on the electronic structures of SnSNR/graphene mixed-dimensional vdWHs. We find that passivation edge as well as

* Corresponding author.
** Corresponding author.
E-mail addresses: xiacongxin@htu.edu.cn (C. Xia), gengzhenduo@163.com (Z. Geng).

https://doi.org/10.1016/j.jallcom.2018.06.356
0925-8388/

changing the width of SnSNR can turn effectively the Schottky contact type and change the SBH.

2. Computational method

For the calculations of this work, we use Vienna ab initio simulation package (VASP) [51,52] to simulate the electronic properties of the mixed-dimensional vdWHs of graphene and SnSNRs, which is based on the density functional theory (DFT). The exchange-correlation function is considered using the generalized gradient approximation (GGA) within Perdew-Burke-Ernzerhofer scheme (PBE) [53]. The residual force standard of smaller than 0.01 eV/Å on each atom and the energy convergence criterion of 10^{-5}eV are employed to optimize the atomic positions of configurations. A cutoff energy of 500eV and a Monkhorst-Pack k-mesh of $5 \times 5 \times 1$ are chosen for the Brillouin zone (BZ). Due to the insufficient of PBE description for non-bond interaction, we use a semi-empirical DFT-D2 method to consider the vdW interaction in the mixed vdWHs [54,55].

3. Results and discussion

3.1. The stability of 1D/2D SnSNR/graphene mixed-dimensional vdWHs

To simulate the 1D/2D SnSNR/graphene mixed-dimensional vdWHs, we investigate the geometrical structures of 2D SnS and graphene unit cell. SnS is a phosphorene analogue including two S atoms and Sn atoms in a unit cell. The calculated lattice parameters of SnS unit cell are $a = 4.25$ Å and $b = 4.03$ Å, and the lattice parameter of graphene is $a = 4.26$ Å. Then, we put 1×3 SnS supercell on the top of 1×5 graphene supercell to build the SnS monolayer/graphene vdWHs possessing the lattice mismatches of 0.1% and 0.9% along the x and y directions, respectively. By cutting the SnS monolayer along zigzag edge (y direction) into SnSNRs, thus the SnSNR/graphene mixed-dimensional vdWHs can be obtained as shown in Fig. 1. The vacuum layer around 20 Å is left to avoid atomic interactions in x direction for upper SnSNR.

One edge of zigzag SnSNR is S-terminated, but the other edge is Sn-terminated. In order to equilibrate the calculate time and accuracy of results, we take the width of SnSNR of 2, 3, and 4 as the considered models, which are marked as bare_W2, bare_W3, and bare_W4, respectively. Then we use F, Cl and Br atoms to passivate the edge of SnSNR in bare_W2, bare_W3 and bare_W4, which are named as F_W2, F_W3, F_W4, Cl_W2, Cl_W3, Cl_W4 and Br_W2, Br_W3, Br_W4, respectively. After relaxed all atoms, the minimum distance of two counterparts in these vdWHs is 2.726 Å, which is larger than the sum of maximal radius of interfacial atoms (2.63 Å), so these vdWHs is dominated by vdW attraction.

To prove the feasibility of these 1D/2D mixed-dimensional vdWHs in practice, we study their stability by calculating the binding energy as follows [56,57]:

$$E_b = \frac{E_{complex} - E_{Gra} - E_{SnS}}{n_S} \quad (1)$$

where $E_{complex}$, E_{Gra} and E_{SnS} are the energies of the SnSNR/graphene mixed-dimensional vdWHs, individual graphene and SnSNR supercells, respectively. The n_S is the number of S atom. In view of the contact area difference between SnSNR and graphene in the SnSNR/graphene mixed-dimensional vdWHs considering different width of SnSNR, the value is normalized to each S atom (unit area). Thus, the smaller value of E_b represents the energetically favorable bond between two counterparts. Table 1 finds that for bare and passivated cases, the binding energies are negative, which indicates that these considered mixed-dimensional vdWHs are energetically stable and may be fabricated under equilibrium conditions. Moreover, for the same width, passivating SnSNR can induce that the synthesis of mixed-dimensional vdWHs become easier.

3.2. Electronic properties of bare 1D/2D SnSNR/graphene mixed-dimensional vdWHs

Because the band structure engineering of semiconductor is

Table 1
Binding energy of SnSNR/graphene mixed-dimensional vdWHs.

Binding energy (eV per S atom)	W2	W3	W4
SnSNR/graphene	−0.825	−0.859	−0.831
F-passivated SnSNR/graphene	−1.485	−1.070	−0.987
Cl-passivated SnSNR/graphene	−1.207	−1.034	−0.975
Br-passivated SnSNR/graphene	−1.258	−1.080	−1.006

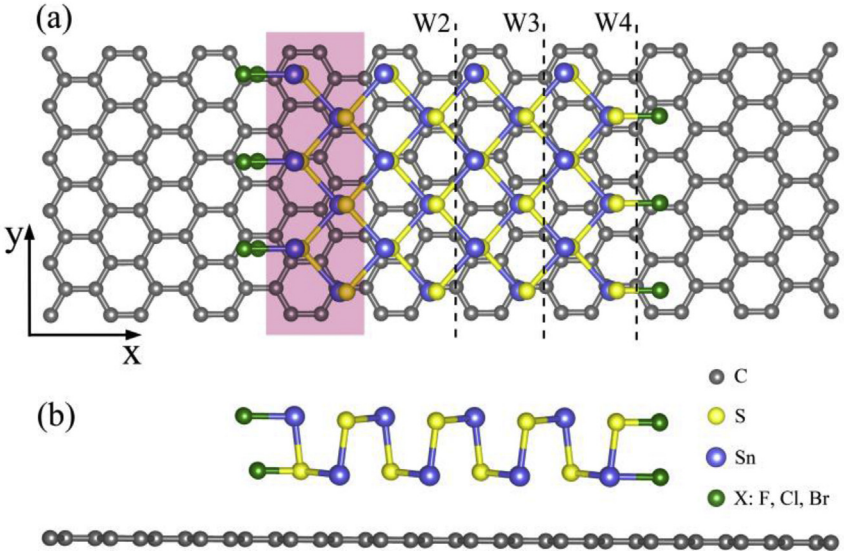

Fig. 1. The top view (a) and the side view (b) of the mixed-dimensional vdWHs. The shaded rectangular part stands for the unit cell of SnSNR/graphene mixed-dimensional vdWHs.