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The electronic transport characteristics of hybridized hexagon beryllium sulfide and graphene nanoribbons

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ABSTRACT

Hybridized Z-$Be_xS_yC_z$ ($x+y+z=16$) systems connected by zigzag beryllium-sulfide (BeS) and graphene nanoribbons are theoretically designed, and their electronic transport characteristics are explored by first-principles approach. For the hybridized systems with unequal number of x and y, i.e. z is an odd number, an exceptional negative differential resistance (NDR) property occurs. However, for the hybridized systems including an even number of zigzag carbon chains, namely x equal to y, an interesting current-limited behavior happens. Meanwhile, the NDR phenomenon disappears. The spin transport properties of these hybridized Z-$Be_xS_yC_z$ systems with parallel magnetism configuration also reveal the above odd–even dependence conductance behavior.

1. Introduction

Graphene, already synthesized successfully in 2004 [1], is a 2-D single planar layer of carbon crystal arranged in honeycomb lattice. The unusual characteristics including high strength, long coherence length and high electron mobility at room temperature [2–4], suggest graphene as an excellent candidate of transport material for implementing future nanoelectronic devices. For realistic applications, the zero-band-gap 2-D graphene sheet needs to be tailored into quasi 1-D graphene nanoribbons (GNRs) with finite width to generate an appropriate band gap. Zigzag-edge graphene nanoribbons (ZGNRs), which are sheared along the zigzag dimmer chain, have attracted more attentions owing to their distinctive edge state in the past decades [5–8]. Many fascinating physical properties, including current switching [9], negative differential resistance (NDR) [10], magnetoresistance [11], rectification [12], and spin filtering [13], have been experimentally fabricated and theoretically predicated in ZGNRs-based devices. Among above physical features, the NDR phenomenon has become a hot research topic because it acts as a significant role in numerous applications [14,15], such as logic circuits, fast switches, memory elements, amplifiers, and high-frequency oscillators.

To get extraordinary performances beyond graphene, studies are stretched to other emerging graphene-like 2-D monolayer materials, such as molybdenum disulfide (MoS_2) [16], silicon carbon (SiC) [17], silicene [18], phosphorene [19], and natural hexagonal boron nitride (*h*-BN) [20]. As expected, these reported 2-D sheets exhibit outstanding properties [21–23], and electrons inside them also conduct like massless or massive Dirac fermions [24]. Nevertheless, compared to the widespread attention of individual 2-D atomically thin materials, hybridized systems consisting of different of single-atom-layer materials could open up new opportunities to manipulate the band gap, and hold potential to display unusual electronic properties [25,26]. In particular, planar hybridization structures composed of ZGNRs and zigzag boron nitride nanoribbons (ZBNNRs) have been successfully fabricated at an atomic scale due to their approximate in-plane crystal structures and matched lattice parameters [26], and such heteroepitaxial materials have attracted ever increasing concerns of theoretical researchers [27–30]. He et al. [27] found that the band gap of the hybridized ZGNR–ZBNNR systems could be adjusted and the transitions from insulator to semiconductor, to half-semimetal, and to metal can be achieved by altering the ratio of the zigzag chain of ZBNNR and ZGNR. Zhou et al. [28] investigated the electronic transport characteristics of a hybridized structure constructed by ZGNRs and ZBNNRs. Their calculation results confirmed that the NDR behaviors can be clearly observed in the hybridized system when the width of boron was not equal to that of nitride and the peak-to-valley ratio (PVR) of NDR could be improved by decreasing the odd numbers of ZGNRs. However, when the width of boron was equal to that of nitride, the currents in the considered bias region were nearly zero and

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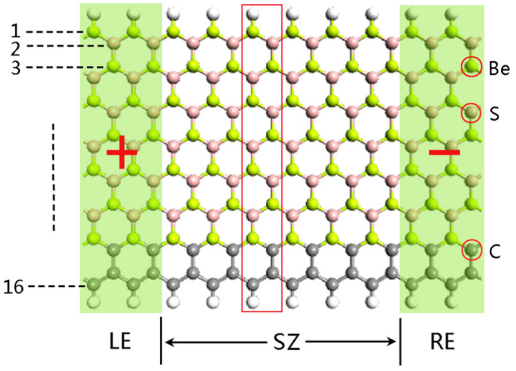

Fig. 1. Schematic drawings of the hybridized Z-$Be_7S_6C_3$ structure, simply named as C3, among the Z-$Be_xS_yC_z$ ($x + y + z = 16$) systems. SZ and LE/RE signify the scattering zone and the left electrode/the right electrode. The red solid rectangle denotes the unit cell of Z-$Be_xS_yC_z$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

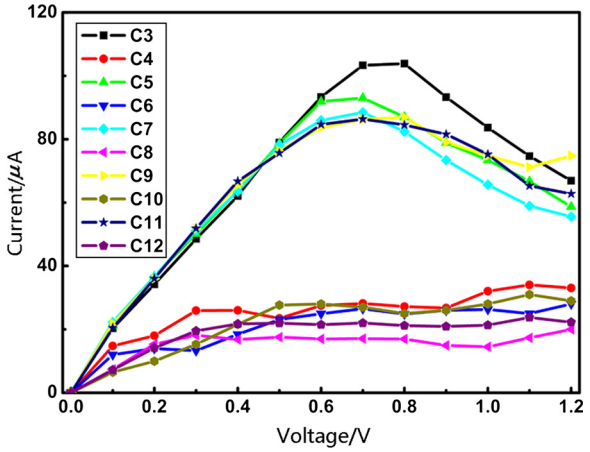

Fig. 2. The simulated current–voltage (I–V) characteristic curves for the hybridized C3–C12 systems.

the NDR feature disappeared. Zhu et al. [29] reported that ZBNNRs doped with two zigzag carbon chains (BN/C) at one edge displayed half-metal or spin-gapless semiconductor behavior by subjecting a tensile strain in its length direction.

Recently, Yu et al. [31] theoretically predicted a new graphene-like hexagonal beryllium sulfide (h-BeS) 2-D sheet that can appear excellent thermodynamic stability up to 1000 K and a wide energy gap of 4.26 eV, which is close to that of the hexagonal boron nitride (h-BN). An et al. [32] demonstrated that zigzag beryllium sulfide nanoribbons (ZBeSNRs) can display a remarkable NDR behavior, and such NDR effect was independent of the ZBeSNRs width. Their research further showed that the hydrogen-passivated ZBeSNRs presented interesting current-limited feature owing to the localized band near the Fermi energy (E_F) blocked the electron transferring. So far, no attempt has been made to explore the charge transport features of hybridized Z-$Be_xS_yC_z$ systems constructed by the zigzag beryllium-sulfide (BeS) and the graphene nanoribbons. Herein, we conduct a theoretical simulation on Z-$Be_xS_yC_z$ ($x + y + z = 16$) by gradually doping carbon atoms at one edge. Surprisingly, it is found that the current–voltage (I–V) curves are intensively dependent on the width of doped graphene nanoribbons or the remainder BeS nanoribbons. For Z-$Be_xS_yC_z$ with an odd number of z, i.e. the number of x unequal to y, a significant NDR effect is observed. Specially, for Z-$Be_xS_yC_z$ containing an even number of zigzag carbon chain, namely the number of x equal to y, the NDR effect no longer exists, instead of which is an amusing current-limited behavior similar to the ZGNRs with an even number of zigzag chain [33]. We further computed the spin transport features of these hybridized Z-$Be_xS_yC_z$ structures under parallel magnetism configuration. Interestingly, we can also observe above odd–even dependence conductance property.

2. Models and computational methods

The designed hybridization device Z-$Be_xS_yC_z$ (referred to as Cz hereafter) is illustrated in Fig. 1, where $x + y + z = 16$, and x, y, and z denote the row number of beryllium, sulfur, and carbon, respectively. The optimized C–C, Be–S, and C–S (C–Be) bond length is 1.46 Å, 1.95 Å, 1.76 Å (1.78 Å), respectively, which is close to previous calculations of C–C and Be-S bond length [8,31]. All Z-$Be_xS_yC_z$ systems keep the planar structure after their geometry optimization, and a little deformation appears in the connected region between the ZGNRs and ZBeSNRs. Each system consists of three regions: the left electrode (LE), the right electrode (RE), and the scattering zone (SZ). A pair of semi-infinite electrodes is modeled by a super-cell with two repeated unit cells of hybridized Z-$Be_xS_yC_z$ nanoribbon (indicated by the green shaded areas) along the electronic transport direction, and the SZ contains six unit cells of Z-$Be_xS_yC_z$ nanoribbon. Both of beryllium and carbon atoms at the two edges of Z-$Be_xS_yC_z$ nanoribbons are all inactivated by one hydrogen atom.

So-proposed two-probe systems are modeled and their electronic transport properties are simulated utilizing the software package Virtual NanoLab-Atomistix Toolkit (VNL-ATK), which implements the density functional theory (DFT) combined with the fully self-consistent non-equilibrium Green's function (NEGF) method so as to avoid phenomenological parameters [34]. In our practical calculations, the local density approximation (LDA) [35] is chosen as the exchange correlation potential. Numerical atomic orbital of all atoms are expanded with single-zeta plus polarization (SZP) basis set. The real space grid with a plane wave mesh cutoff energy is fixed at 150 Ry in numerical integrations, and both the electrodes temperature is set to 300 K. A 12 Å vacuum layer is added for each system to eliminate lateral interplay. To realize the calculation balance of flexibility and accuracy, the device structures are relaxed until the residual force exerted on each atom is small than 0.02 eV/Å. The 1-D Brillouin zone (BZ) of the two electrodes is sampled with $1 \times 1 \times 100$ k-points following the Monkhorst–Pack grids, and Troullier–Martins norm-conserving pseudo potentials [36] are selected. When the convergence of self-consistency simulation is attained, the Landauer-Büttiker formula $I(V_b) = \frac{2e}{h}\int_{-\infty}^{+\infty}[f_L(E-\mu_L) - f_R(E-\mu_L)]T(E,V_b)dE$ [37] can be used to calculate the current through a two-probe system. In this formula, $\mu_{L/R}$ indicates the Z-$Be_xS_yC_z$ electrode chemical potential, $f_{L/R}$ denotes the LE/RE Fermi–Dirac distribution function, and $T(E, V_b)$ stands for the bias-determinative transmission coefficient at energy E under applied bias V_b. Considered that the average E_F is fixed at zero, the range for the energy integral bias window in fact is $[-V_b/2, V_b/2]$.

3. Results and discussion

The self-consistently computed current–voltage (I–V) curves for the hybridized Z-$Be_xS_yC_z$ nanoribbons in the bias voltage range [−1.2 V, 1.2 V] with a 0.1 V increasing step are displayed in Fig. 2. For Z-$Be_xS_yC_z$ with an odd-numbered z, as can be seen clearly that these devices present an evident NDR behavior in a certain bias voltage region. For instance, the currents pass through model C3 have a rapid growth with the bias voltages increasing from 0 V to 0.7 V (maximum current) and displays a metal characteristic, hut its current declines sharply when the bias voltage beyond 0.7 V and until reaching 1.2 V (minimum current). As compared with the hybridized Z-$B_xN_yC_z$ ($x+y+z=16$) systems in reference [28], the PVR and the bias voltage region of NDR effects in our Z-$Be_xS_yC_z$

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