Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Materials

Section I

In this section, using nonequilibrium Green's functions (NEGF) and density functional theory (DFT), we will give some discussions on the two hererojunctions based on ZGNRs and s-triazine-based g-C3N4 nanoribbons with nitrogen atoms terminated by hydrogen atoms. The devices are labeled by HGGN and HGNN as shown in Fig. 1. The calculated transmission spectrums of HGGN and HGNN at bias 0.1V are shown in Fig. 2. We can conclude that the spin polarization behavior is not obvious compared with that of GGN and GNN. For the corresponding transmission pathways shown in Fig. 3, it can be seen that the edge effect is less important than that of GGN and GNN.

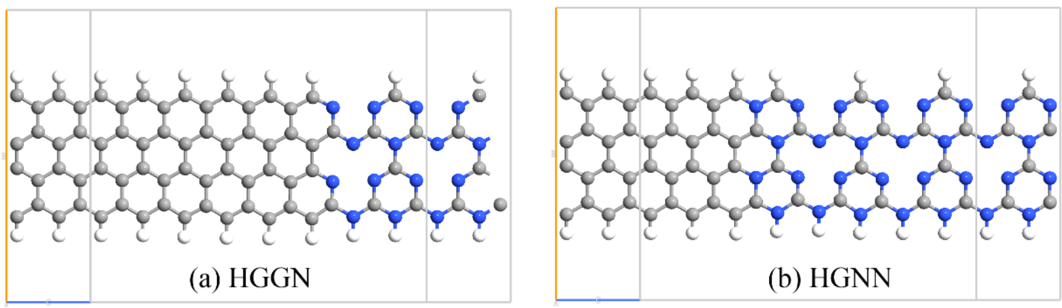


Fig.1 (color online) (a) and (b) Correspond to the two heterojunctions based on ZGNRs and s-triazine-based g-C3N4 nanoribbons with nitrogen atoms terminated with hydrogen atoms.

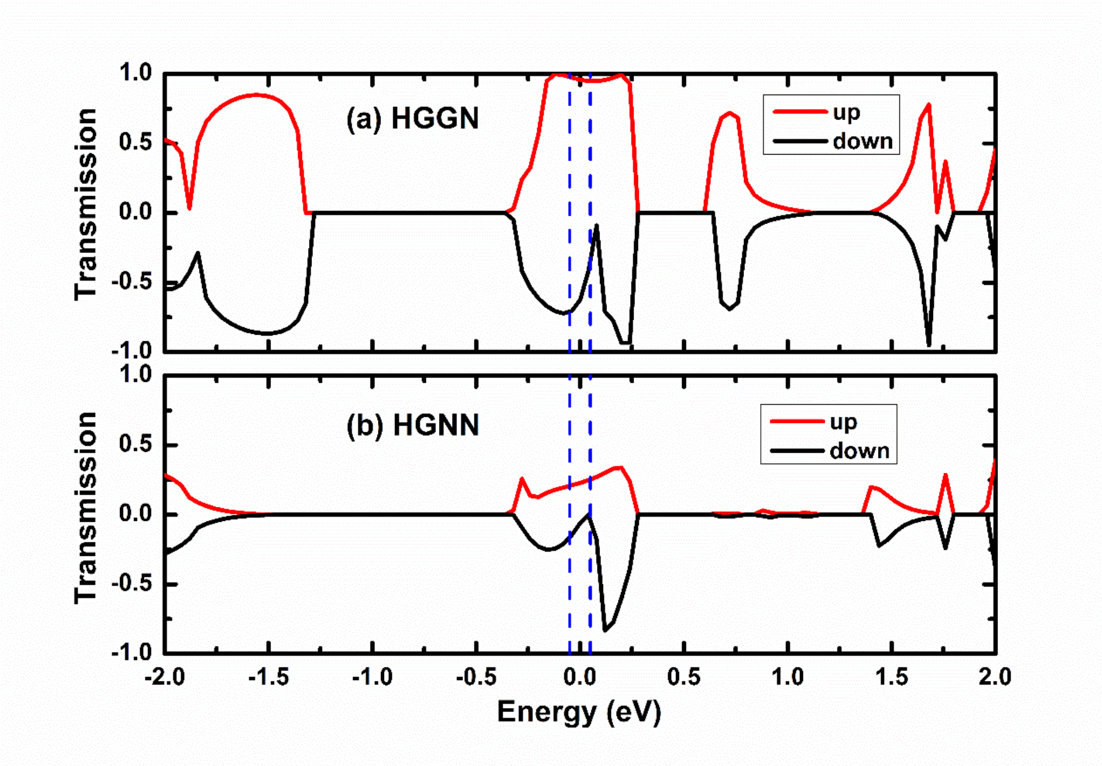


Fig. 2 (color online) The transmission spectrums of (a) HGGN, (b) HGNN at bias 0.1V. The blue dashed lines indicate the bias window.

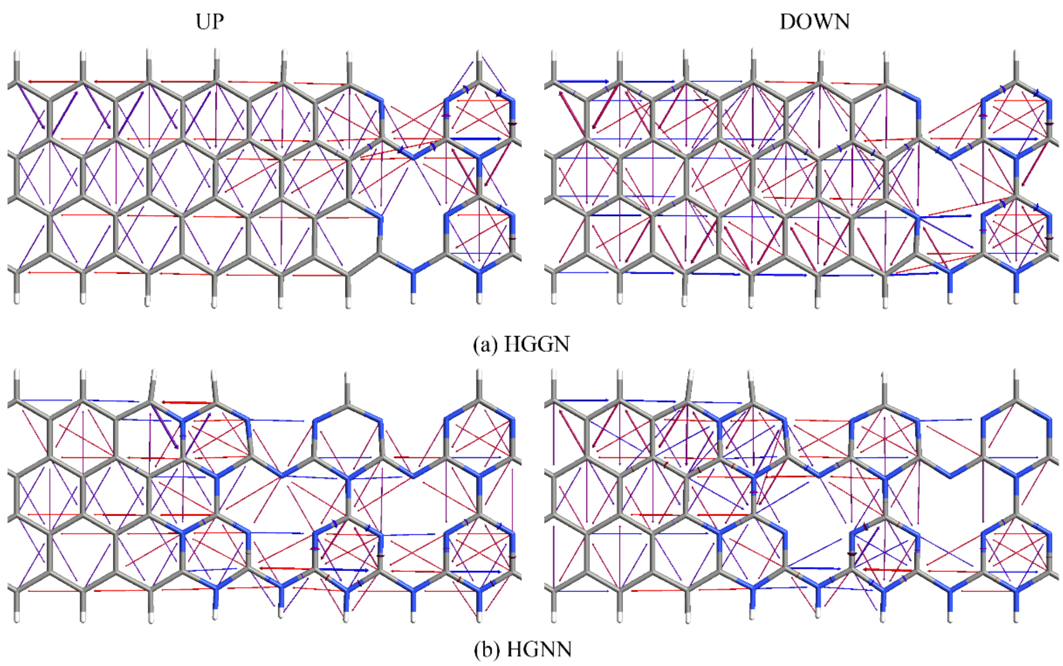
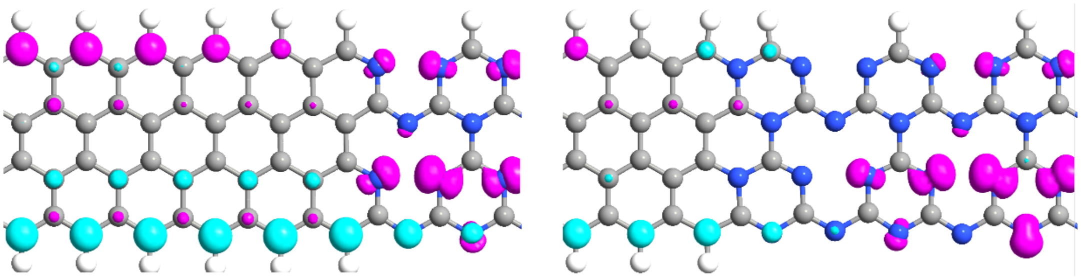


Fig. 3 (color online) The transmission pathways of (a) HGGN, (b) HGNN at bias 0.1V. The left column indicates the spin up channel and the right column indicates the spin down channel.

Section II

In this section, the spin density distributions (after the self-consistent calculations) of device GGN and GNN in the antiferromagnetic (AFM) state are shown in Fig. 4. The transmission spectrums and total density of states of both devices at zero bias in the AFM state are shown in Fig. 5. Compared with the FM state, the difference would be obvious.



(a) GGN (b) GNN

Fig. 4 (color online) (a) and (b) Correspond to the spin density distributions of device GGN and GNN in the AFM state.

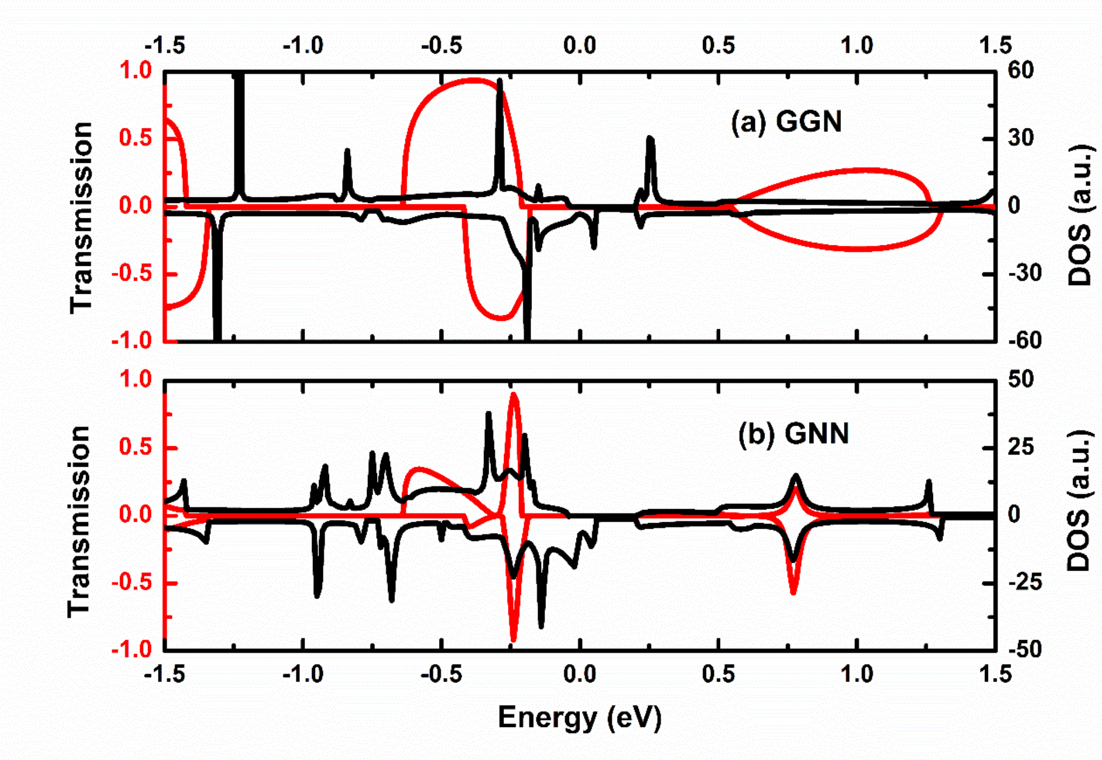


Fig. 5 (color online) The transmission spectrums and total density of states of (a) GGN and (b) GNN at zero bias in the AFM state. The red line represents the transmission spectrums and the black line represents the total density of states.