Interactions between the edge states of bilayer zigzag SiC nanoribbons

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Graphene nanoribbons (GNRs) have been studied intensively because its extraordinary electronic properties can be modified by the geometrical structure. As one kind of GNRs, zigzag graphene nanoribbons (ZGNRs) are confirmed to have peculiar localized state near the zigzag edge, the so-called edge state with spin polarization, consisting of non-bonding p_z orbitals [1]. Considering the van der Waals (vdW) interaction, recent study has indicated that the AA-stacked bilayer ZGNRs exhibit nonmagnetic ground state, resulting from the interaction between the edge state [2]. Although SiC-based nanoribbons have the similar structure with GNRs, the electronic states are quite different. It has been reported that monolayer zigzag SiC nanoribbons (SiCNRs) exhibit a half-metallic state because the two edges are terminated by different edges [3].

In this research, we investigate the edge-edge interactions of bilayer zigzag SiCNRs using the first-principles calculations based on the density functional theory with the vdW parameters. For the SiCNRs with the ribbon width of 7, the AB_α stacking is more stable than AA one ($\Delta E = 0.246$eV) and AB_β one ($\Delta E = 0.339$eV) because the AB_α stacking can receive the energy gain through the edge-edge interaction. The structural stability for bilayer SiCNRs is dominated by the trade-off between the edge-edge interaction and the vdW interaction, which is similar with bilayer ZGNRs. However, the edge states of bilayer SiCNRs are quite different with ZGNRs. We will discuss the details in the presentation.

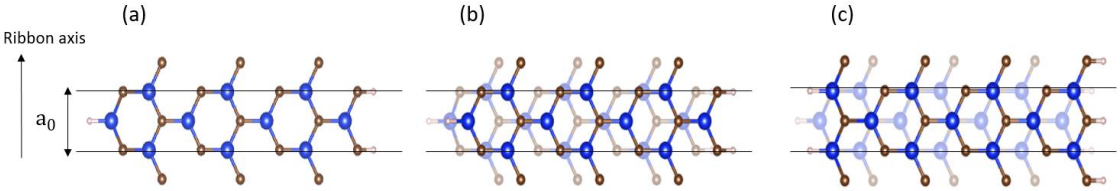

Fig.1 Optimized structure for the (a) AA- (b) AB_α- and (c) AB_β-stacked bilayer SiCNRs

[1] M. Fujita, K. Wakabayashi, K. Nakada, & K. Kusakabe, *J. Phys. Soc. Jpn.* **65,** 1920 (1996)

[2] T. Asano, J. Nakamura., *ACS omega,* **4,** 22035 (2019)

[3] Sun, Lian, et al. *J. Chem. Phys.* **129,** 174114 (2008)