Supplementary Information

Ballistic transport simulation of acceptor-donor C_3N/C_3B double-wall hetero-nanotube field-effect transistors

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Fig. S1 Equilibrium structures of single-wall (a) (6,0) C₃N, (b) (6,0) C₃B with smaller diameters, and (c) (12,0) C₃N, (d) (12,0) C₃B with larger diameters, respectively. The black frame indicates the unit cell.

Fig. S1 shows the atomic structures of single-wall zigzag C₃N and C₃B nanotubes with different diameters. The (n, m) nanotube describes how to roll up C₃N or C₃B sheet to form single-wall C₃N or C₃B nanotube, in which the integer *n* and *m* are unit vectors along two directions in the crystal lattice of C₃N or C₃B sheet. In our work, m = 0, the rolled nanotube is called zigzag nanotube. The diameters of (6,0) C₃N and (6,0) C₃B are approximately 4.83 Å and 4.94 Å, respectively, which are almost halved compared to those of (12,0) C₃N and (12,0) C₃B. Thus, when the integer *n* becomes larger, the diameter of nanotube increases gradually.



Fig. S2 Band structures (left panels) and PDOS (right panels) of (a) (6,0) C₃N, (b) (6,0) C₃B, (c) (12,0) C₃N, and (d) (12,0) C₃B, respectively. The red dashed line denotes the position of the Fermi level.

To characterize the electronic properties of C_3N and C_3B nanotubes with various sizes, we calculated their band structures. As shown from the band structures in the left panels of Fig. S2, it is obvious that there are two bands cross the Fermi level along Z- Γ direction in (6,0) C_3N and (6,0) C_3B , respectively, indicating their metallic properties along axial direction.^{1, 2} PDOS for B, C, and N atoms in the right panels of Fig. S2

validates the contributions of various atoms in the band structures of nanotubes with different diameters.



Fig. S3 (a-c) Schematic structures of the simulated GAA (6,0) $C_3N/(12,0) C_3B dwHNT$ FETs with various wrapping units in the central channel region. The number of wrapping units within the dashed frames increases from 0, 2, to 4, which is represented by E0, E2, and E4, respectively. The C₃N and C₃B nanotubes in the source and drain leads are repeated semi-infinitely. (d-f) Output characteristic, rectifying ratio, and transfer characteristic for (6,0) $C_3N/(12,0) C_3B dwHNT$ FET as a function of the wrapping unit number. Inset in (f) shows the enlarged transfer characteristic of E0.

To check the effect of different entrapping lengths on the device performance of $(6,0) C_3N/(12,0) C_3B dwHNT$ FET, we increased the number of entrapping units in the central channel from 0 to 4 with an interval of 2. The corresponding devices are labeled as E0, E2, and E4, respectively, as shown in Fig. S3a-S3c. The output characteristic curves in Fig. S3d demonstrate that I_{DS} of $(12,0) C_3N/(6,0) C_3B dwHNT$ FET increases almost linearly under a low V_{DS} , indicating the Ohmic contact between $(6,0) C_3N$ and $(12,0) C_3B$, irrespective of the wrapping unit number.^{3, 4} E2 possesses the highest conductivity, among all devices with different wrapping unit number. It is assumed that two entrapping units is favorable to promote the transport efficiency between $(6,0) C_3N$

and (12,0) C_3B . The rectifying ratio in E0 is 0.12, whereas that in E4 has risen to 0.90, indicating a weakened rectifying effect. This is because the A-D asymmetry of (6,0) $C_3N/(12,0)$ C_3B *dw*HNT along the axial direction has been reduced spontaneously, when the wrapping unit increases from E0 to E4. In addition, it is noted that the p-type conductance in E0 has been transformed into n-type in E4, as shown in Fig. S3f. In other words, the hole-dominated transport behavior in E0 can be tuned into electron-dominated transport in E2, by increasing the overlapping area between (6,0) C_3N and (12,0) C_3B .

References

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