Supplementary Information

Rectification inversion in the oxygen substitution graphyne-graphene-based heterojunctions

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Section. 1

The geometry of left electrode of system A has been characterized in Figure S1 and Table S1. According to our simulation models, the carbon atom is bonded to oxygen using a double bond, which can be inferred by the bond length of C_1-O. For graphyne nanoribbon, there are two types of hybridized forms for carbon atoms according to hybrid orbital theories. All the carbons contained in the six-membered ring are sp2- hybridization (named C_1-C_6), and two carbons between the six-membered ring are sp- hybridization (named C_7-C_8). Consequently, the framework of six-membered ring is constructed by C_1 (sp2)-C_2 (sp2) sigma orbital. C_4 (sp2)-C_7 (sp) and C_7 (sp)-C_8 (sp) sigma orbitals constitute the joint of six-membered ring. The hydrogen is bonded to the carbon through C_1 (sp2)-H_1 (s) sigma orbital. On the

vertical direction of current in the backbone, C_1 (pz)-C_2 (pz), C_4 (pz)-C_7 (pz) and C_7 (pz)-C_8 (pz) stand side by side, which form large pi conjugated orbital. When a hydrogen is substituted by an oxygen, carbon atom and oxygen atom will form double bond. One of them is a stronger sigma orbital, and the other O (pz) will form extended pi conjugated orbital with originally formed carbon large pi conjugated orbital.

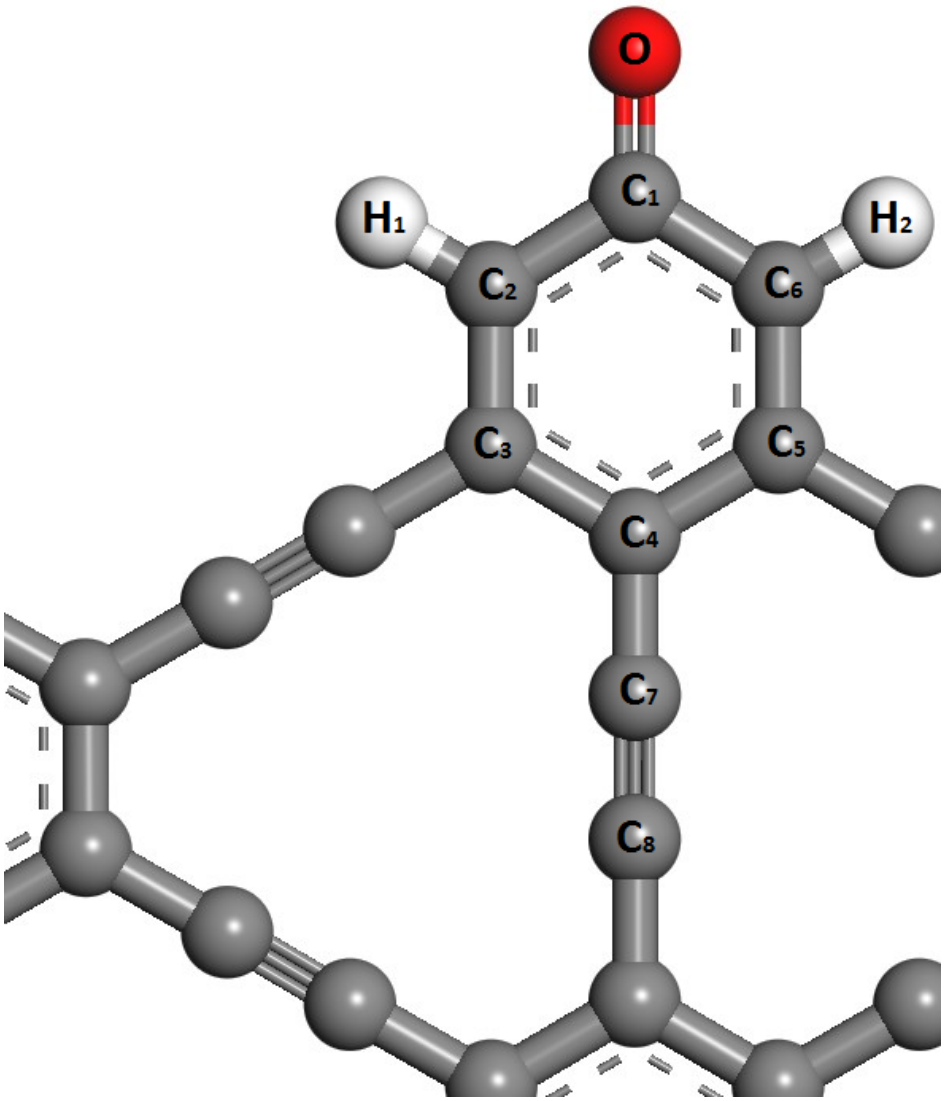

Figure S1. Schematic diagram of the left electrode of system A

Table S1: Some selected geometric parameters of the left electrode of system A. the unit of Bond length is angstrom (Å)

	C_1-C_2	C_2-C_3	C_3-C_4	C_4-C_7	C_7-C_8	C_1-O
Bond length (Å)	1.456	1.378	1.447	1.369	1.235	1.236

Section. 2

In order to investigate whether the widths of the nanoribbon have effective influences to the transport properties, we build two kinds of different widths of Graphyne and Graphene nanoribbons as shown in Figure S1. Here, geometrical structures of b and d possess mirror symmetry under the xz midplane mirror operation. The corresponding energy bands and Γ-point Bloch wave functions are plotted in Figure S2 and S3. The structure of energy bands of system a, b and D (in Figure 4(a)) are distinctly different. But there is only trivial difference between system c and d. Meanwhile, the b_2- and b_3- subbands have even parity, and b_1- subbands have odd parity, which are different from system D in Figure 5. Therefore, the transport properties will vary with the widths of the graphyne nanoribbon.

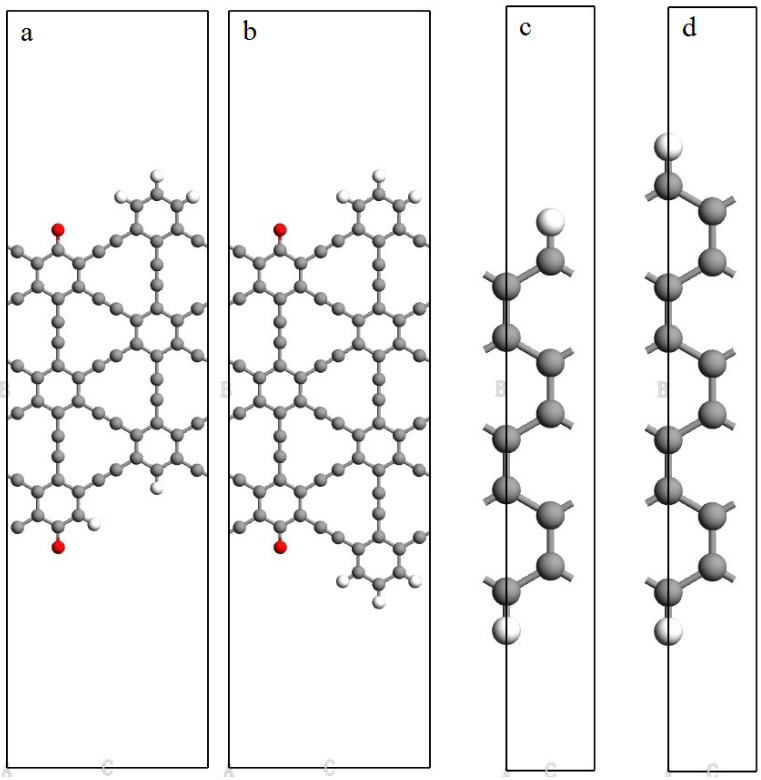

Figure S2. Different widths of graphyne nanoribbons (a, b) and graphene nanoribbons (c, d).

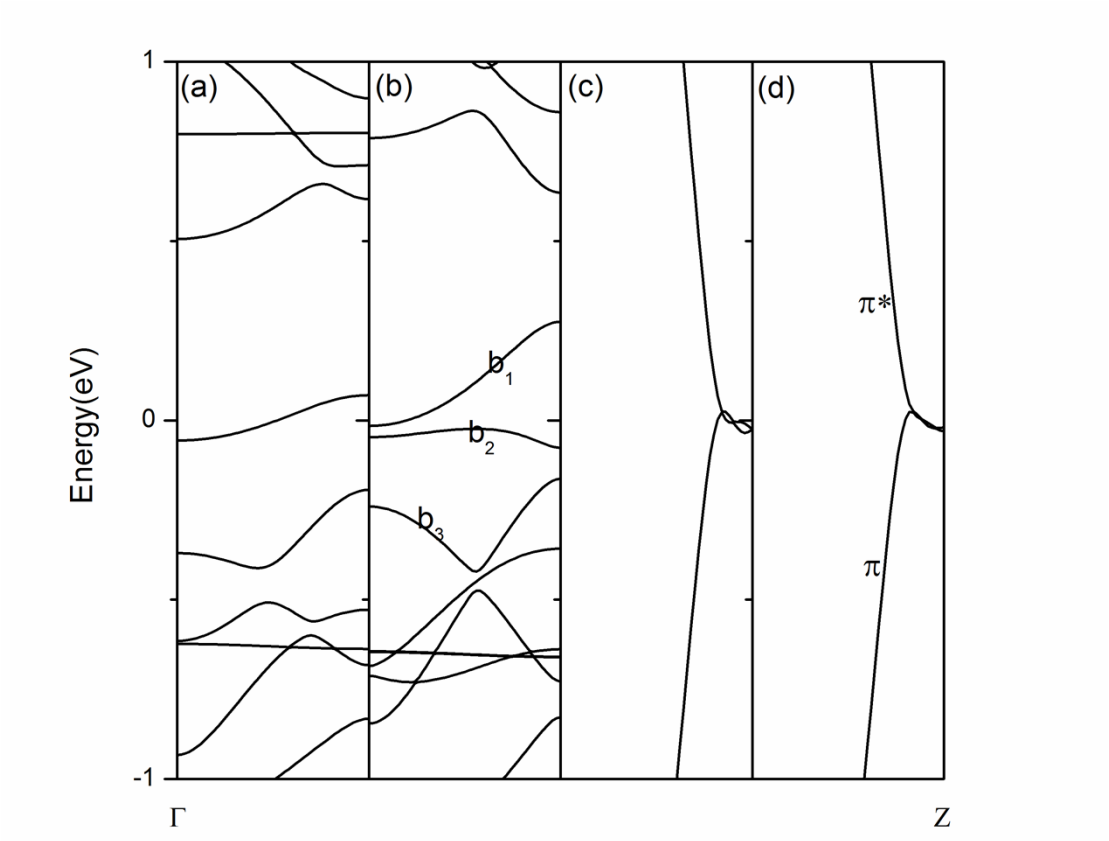

Figure S3. The calculated energy band of the four structures in the Figure S1.

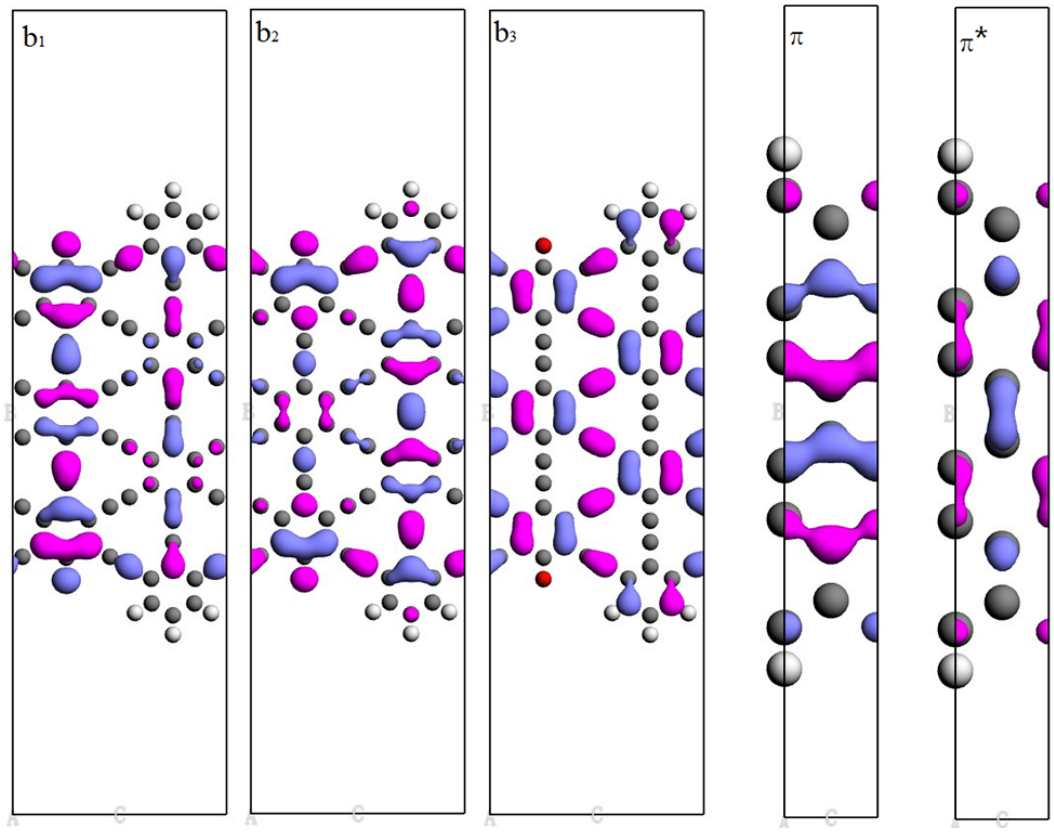

Figure S4. Isosurface plots of the Γ-point Bloch wave functions of b_1-, b_2-, b_3-, π*-

and π- subbands of the structures in Figure S2 (b) and (d). Different colors represent different phase.