Theoretical insight into the intrinsic electronic transport properties of graphene/biphenylene/graphene nanosheet and nanoribbon: a first-principles study

Cheng Luo[a], Tong Chen[*ab], Xiansheng Dong[a], Luzhen Xie[a], Danfeng Qin[a], Lin Huang[a], Huili Li[c], Xianbo Xiao[*c]

a. Energy materials computing center, Jiangxi University of Science and Technology, Nanchang 330013, PR China

b State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, PR China

c. School of Computer Science, Jiangxi University of Chinese Medicine, Nanchang 330004, PR China

E-mail addresses: chentong@jxust.edu.cn (T. Chen), 20101034@jxutcm.edu.cn (X. Xiao).

Supplementary material

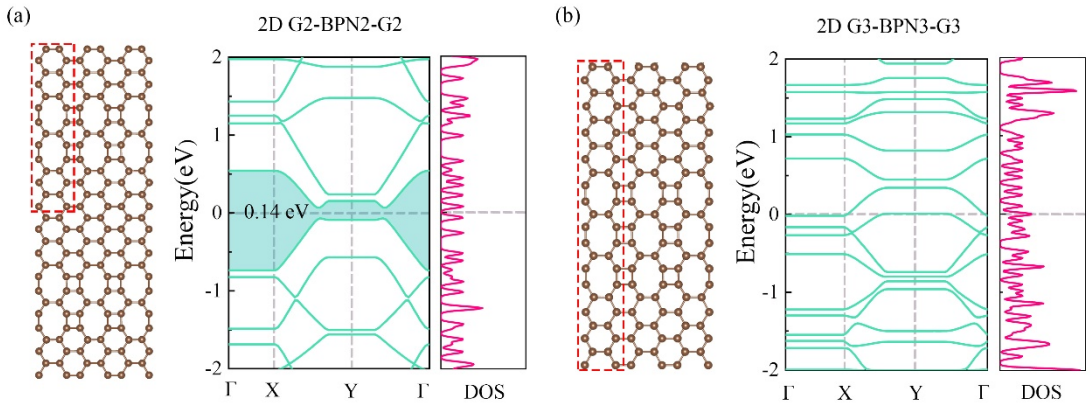

Figure S1: Top view, energy band and density of states of G2-BPN2-G2 (a) and G3-BPN3-G3 (b) heterostructure monolayer. The zero of the energy is set to Ef displayed by a level dotted line. Inside the red dotted rectangle delegates the structural unit of the heterojunction.

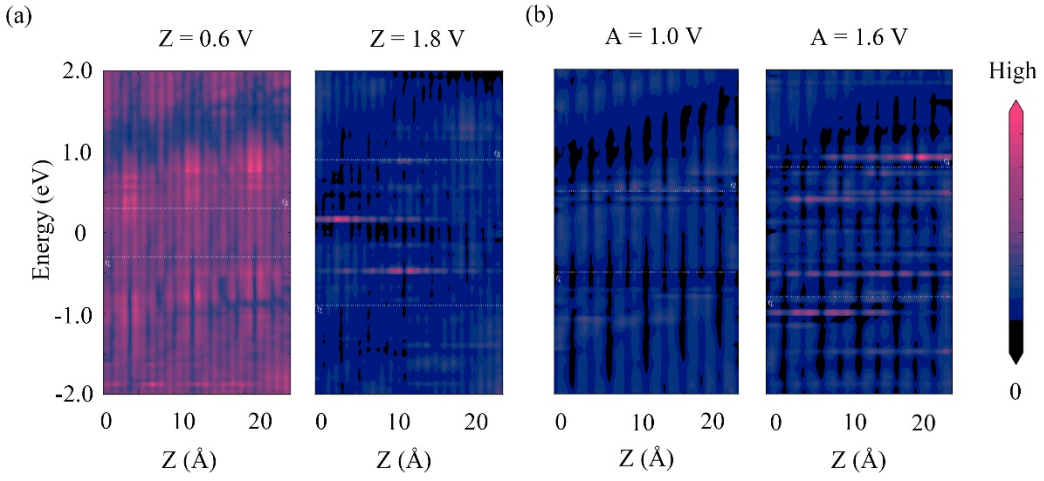

Figure S2: (a) PLDOS along the armchair direction at a bias of 1.0 V and 1.6 V. (b) PLDOS along the serrated direction at a bias of 0.6 V and 1.8 V. The color bar shows the data from 0 (black) to high (red).

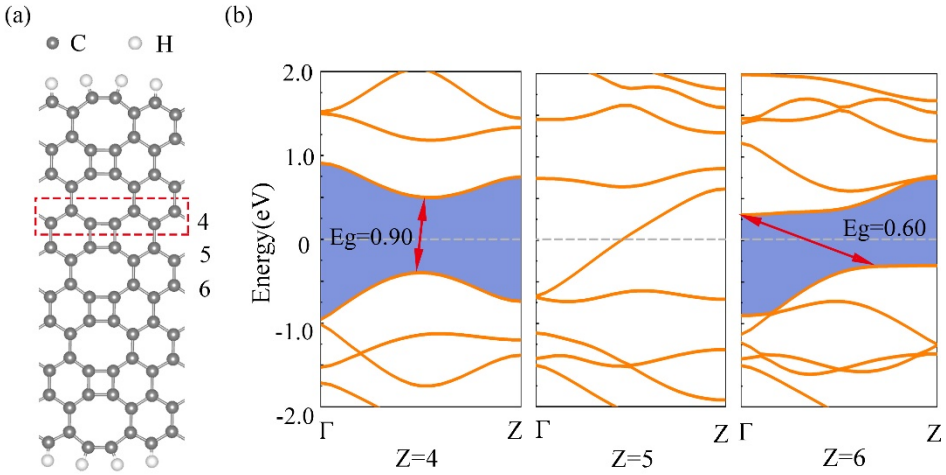

Figure. S3 (a) Structures along the zigzag direction. The red rectangular dashed line indicates the changing unit structure of 4 to 6. (b) Energy bands of different structures from 4 to 6. The red arrow indicates the width of the band gap and the gray dashed line represents the Fermi energy level.

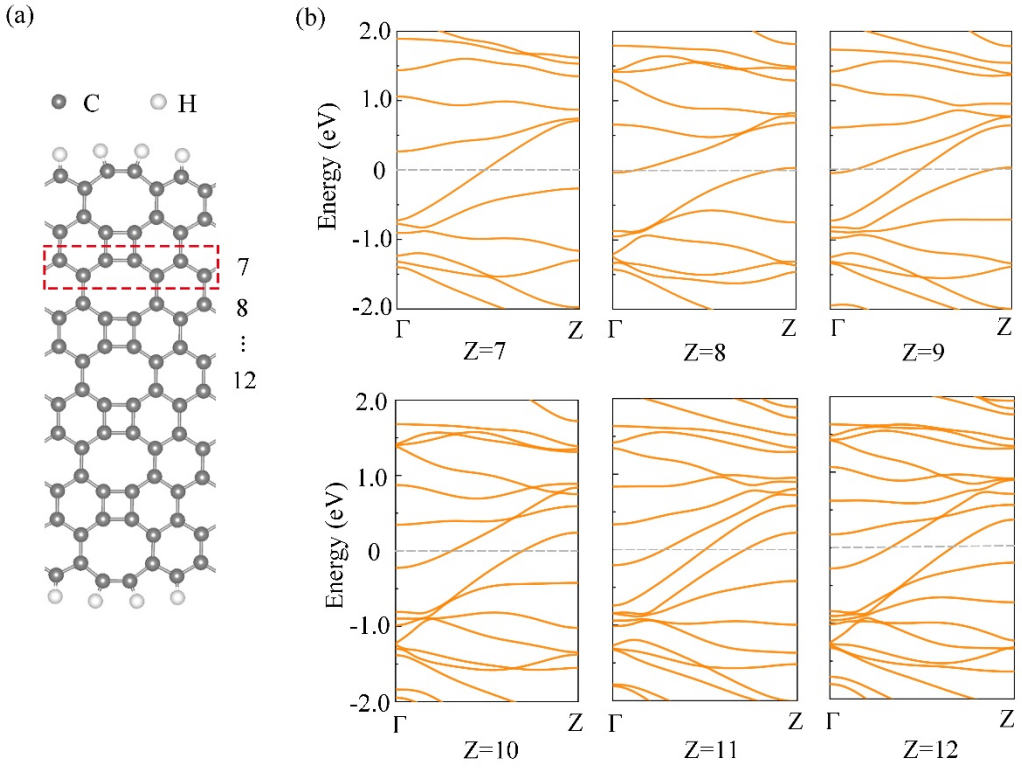

Figure. S4 (a) Structures along the zigzag direction. The red rectangular dashed line indicates the changing unit structure of 7 to 12. (b) Energy bands of different structures from 7-12. The gray dashed line represents the Fermi energy level.

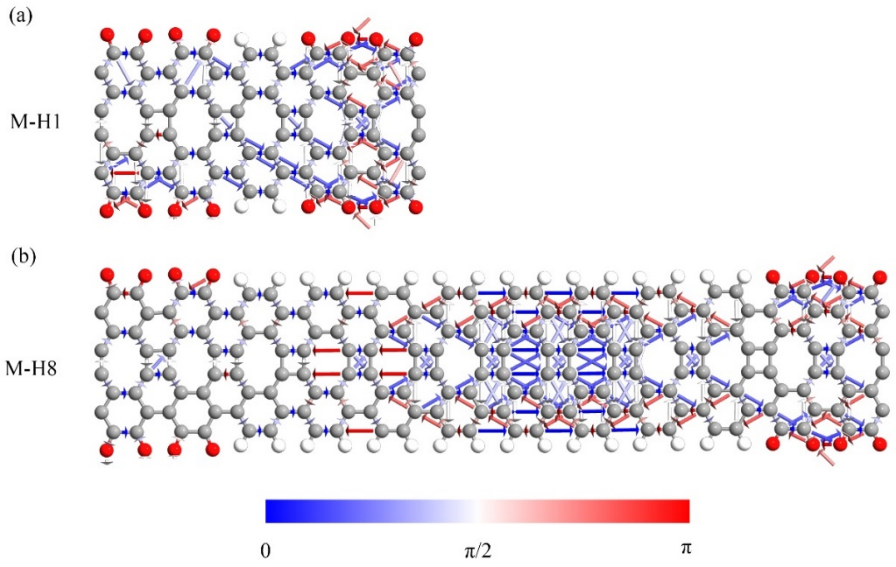

Figure. S5: Transmission pathway of G-BPN-G heterojunction devices M-H1 (a) and M-H8 (b). The bias voltage is set to 0.8 V. The color bar shows the data from 0 (blue) to π (red).

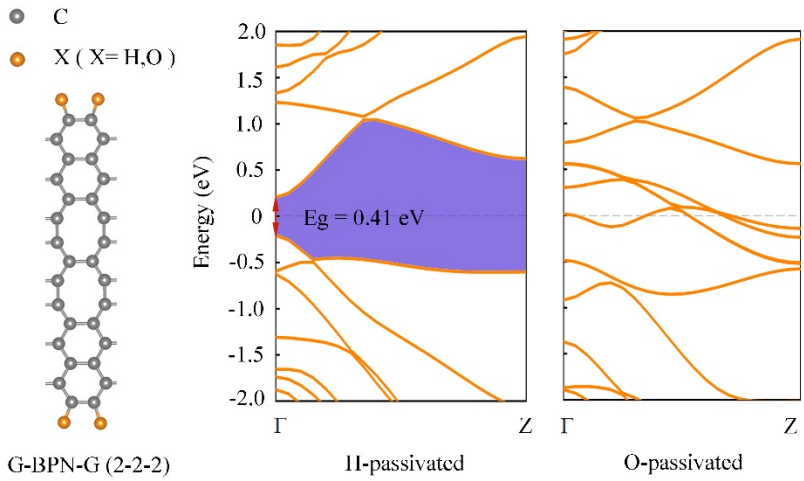

Figure. S6: H-passivated (a) and O-passivated (b) G-BPN-G (2-2-2) nanoribbon structures and energy bands.

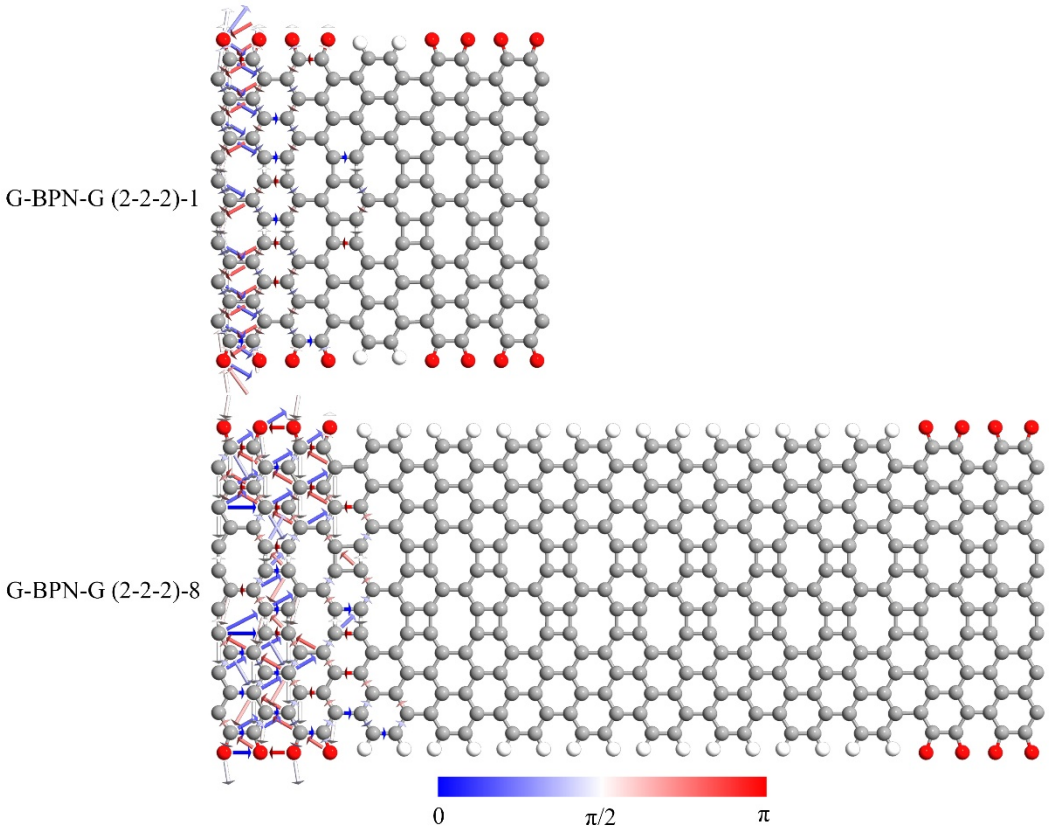

Figure. S7: Transport paths of G-BPN-G (2-2-2) nanoribbon O-passivated devices M-H1 (a) and M-H8 (b). The bias voltage is set to 0.8 V. The color bar shows the data from 0 (blue) to π (red).