

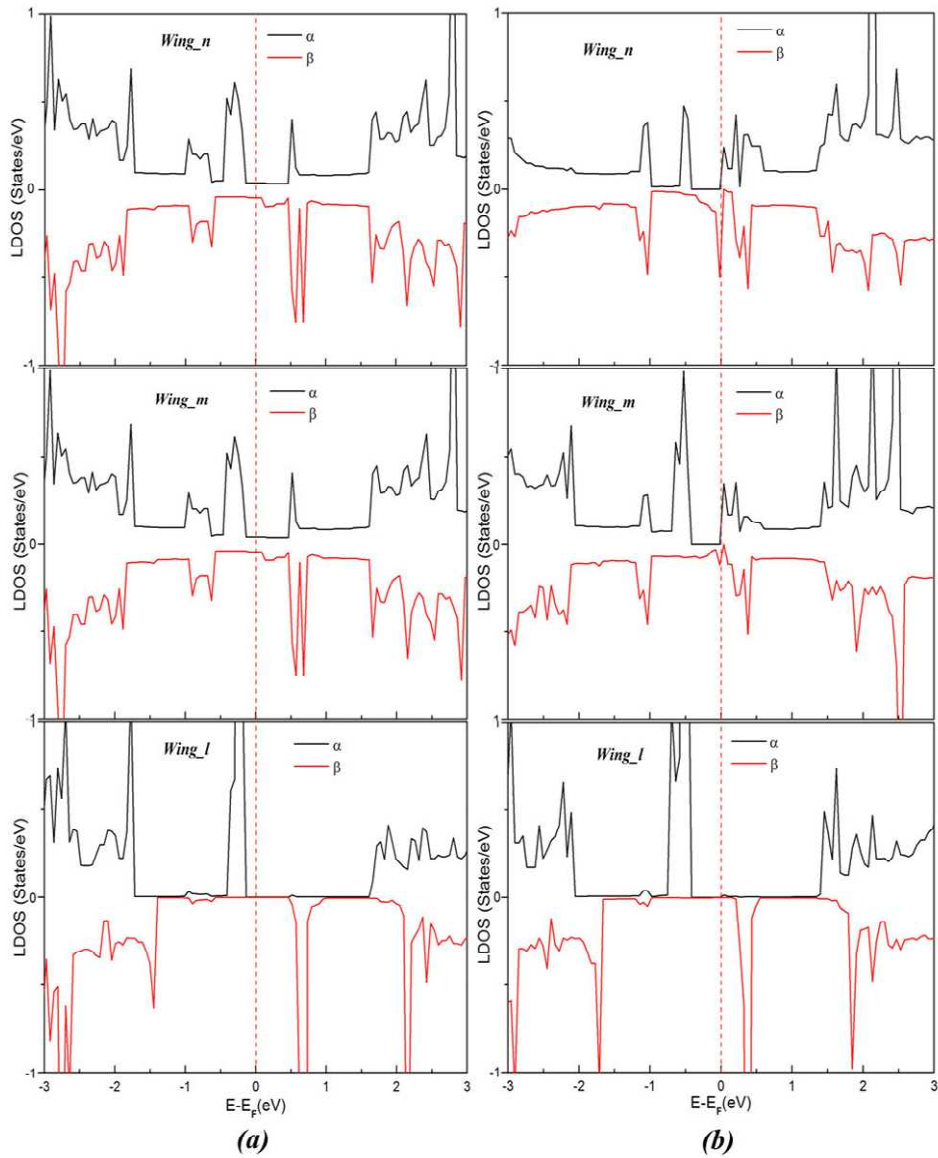
# Boron and Nitrogen Doping Induced Half-Metallicity in Zigzag Tri-wing Graphene Nanoribbons

Liang Ma<sup>1</sup>, Hong Hu<sup>2</sup>, Liyan Zhu<sup>1</sup>, and Jinlan Wang<sup>1</sup>

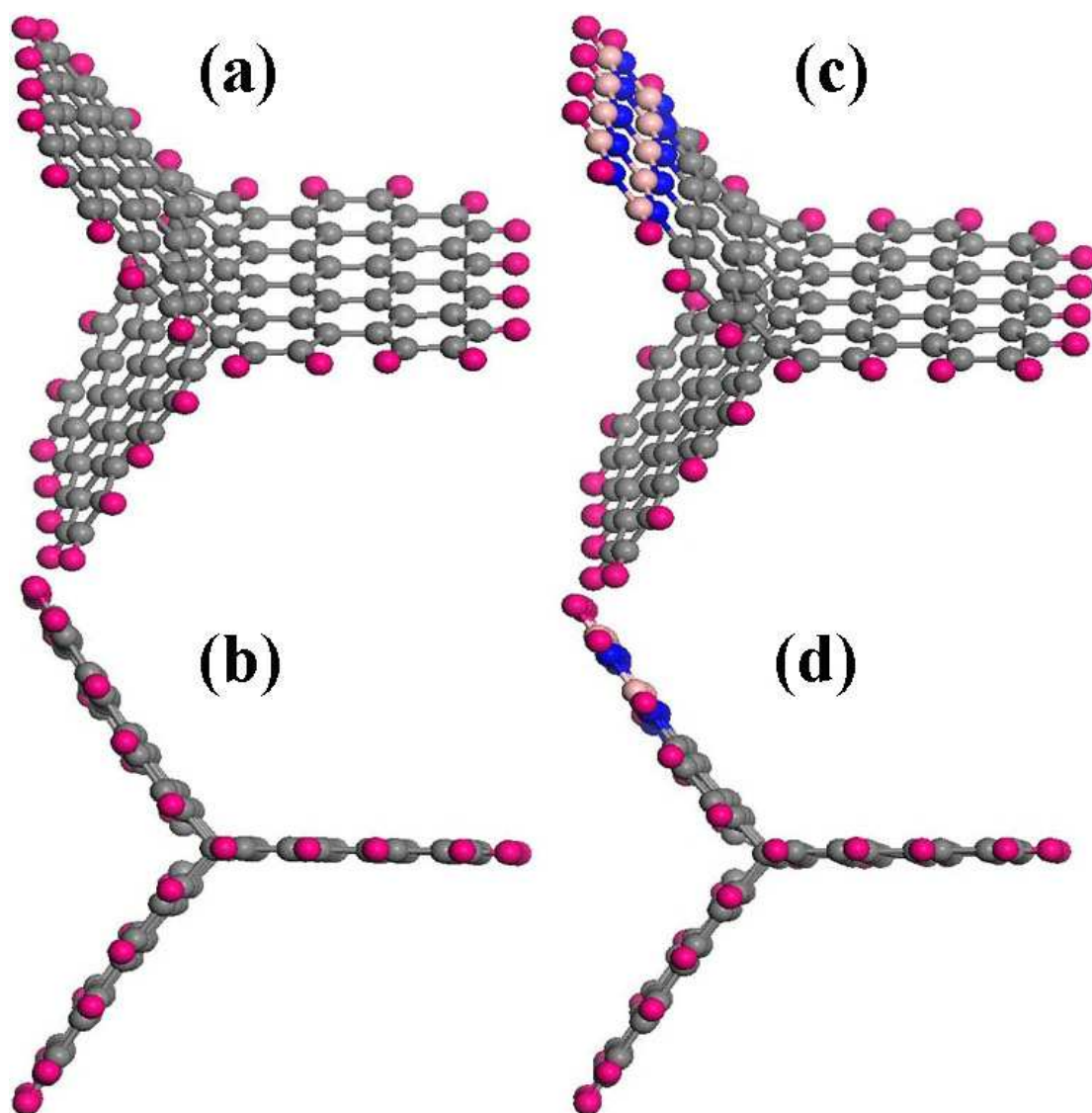
<sup>1</sup>Department of Physics, Southeast University, Nanjing, 211189, China

<sup>2</sup>Institute of Textiles and Clothing, Hong Kong Polytechnic University, Kowloon, Hong Kong, China

## Supporting Information



**Figure S1.** Local densities of state (LDOS) of each wing of undoped ZZ-TWG (**4, 4**, **4**) (a) and BN doped ZZ-TWG (**4-2**, **4**, **4**) (b). The label  $\alpha$  and  $\beta$  represent spin up and spin down channels respectively.



**Figure S2.** Optimized structures of undoped ZZ-TWG (4, 4, 4) (a) and (b); BN doped ZZ-TWG (4-2, 4, 4) (c) and (d) with finite length.