Supporting information for: Electron Transport Properties of Atomic Carbon Nanowires between Graphene Electrodes

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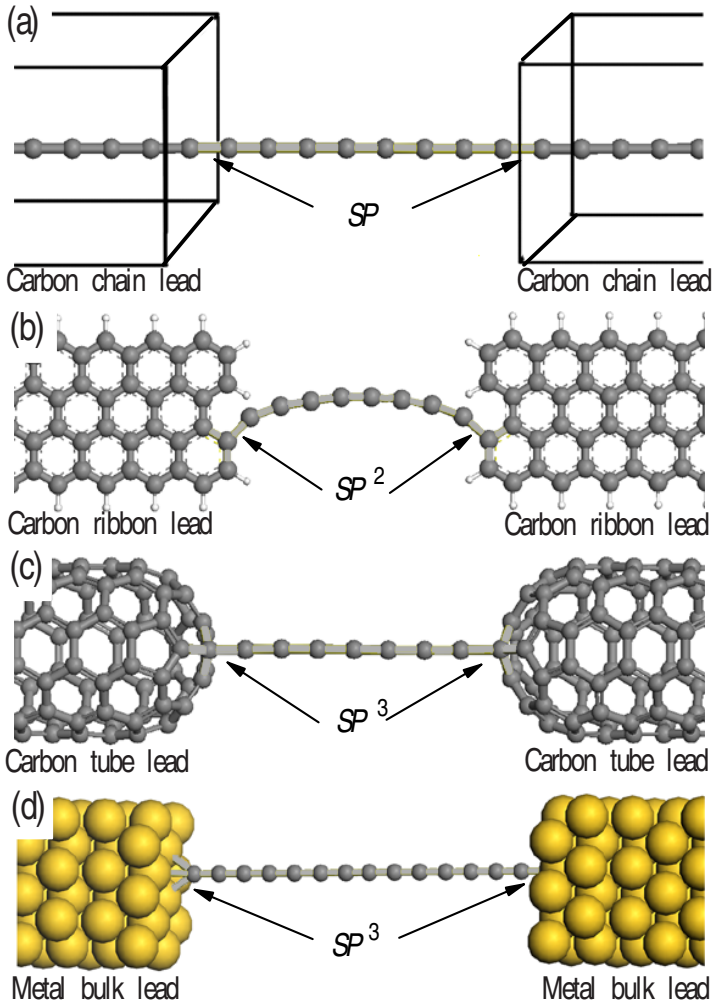

Figure S 1: (Color online) Schematic diagrams of different configurations of carbon wires and electrodes. A linear atomic carbon wire has (a) sp connection with carbon wire leads; (b) sp^2 connection with carbon ribbon leads (optimized); (c) sp^3 connection with capped carbon tube leads; (d) sp^3 connection with metal leads.

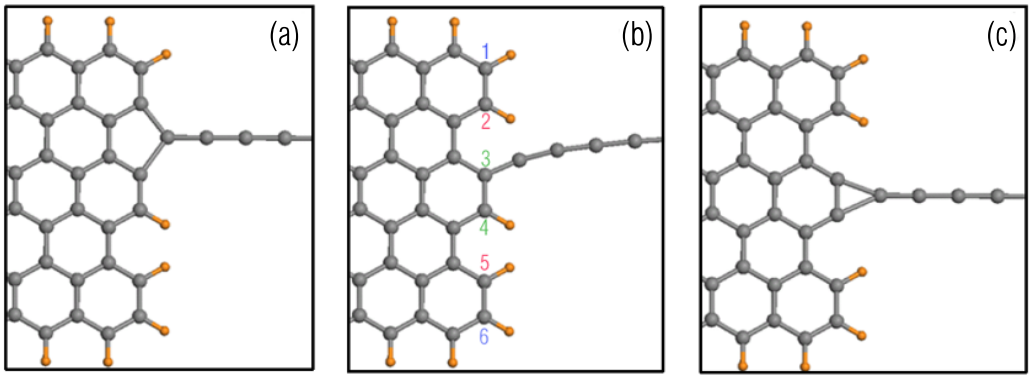

Figure S 2: (Color online) Three optimized structural configurations of carbon wire-graphene junctions. (a) five-membered carbon ring (b) six-membered carbon ring (c) three-membered carbon ring. The six-membered ring connection structure is the most energetical favor than the other two. Three different connection-points are labeled as (1,6), (2,5) and (3,4). (orange: H; grey: C)

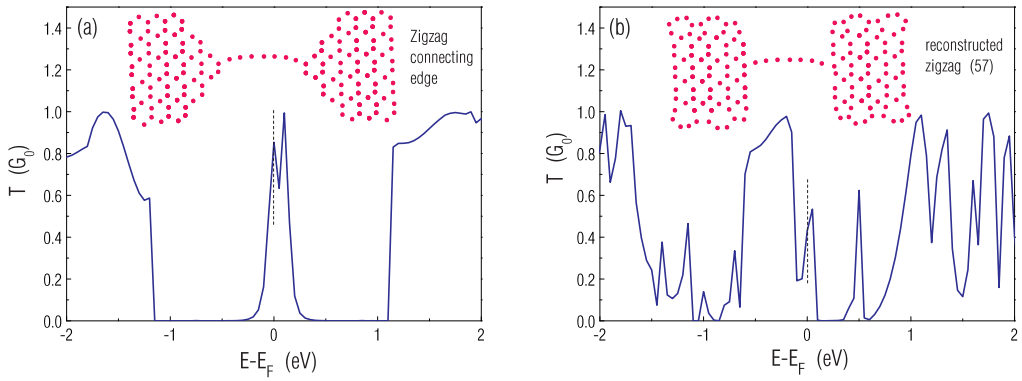

Figure S 3: (Color online) (a) The transmission spectrum of C_7 with the zigzag connecting edge. (b) The transmission spectrum of C_7 with the reconstructed (57) zigzag edge. As can be seen, the connecting edge (zigzag or armchair) does not obviously affect the transport property near the Fermi level. But the edge reconstruction does a strong suppression of transmission ($\sim$50%) due to the disruption of edge states.

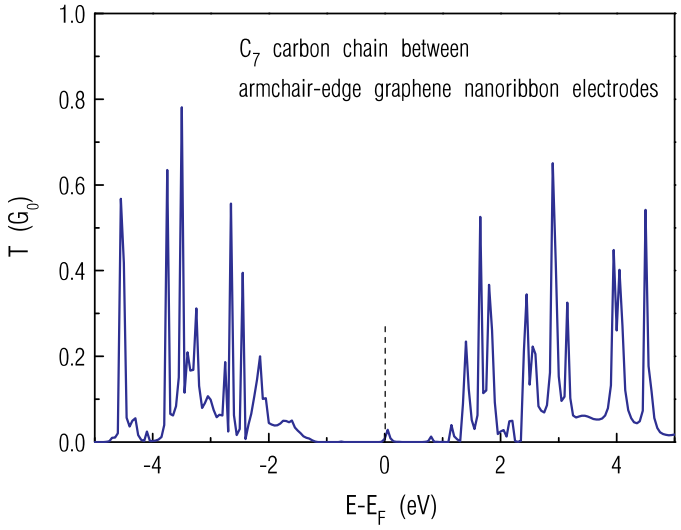

Figure S 4: (Color online) The transmission of a C_7 carbon chain between armchair-edge graphene nanoribbon electrodes ($i = 7$). There is a poor conductance near the Fermi level due the semiconducting property of armchair-edge GNR electrodes.

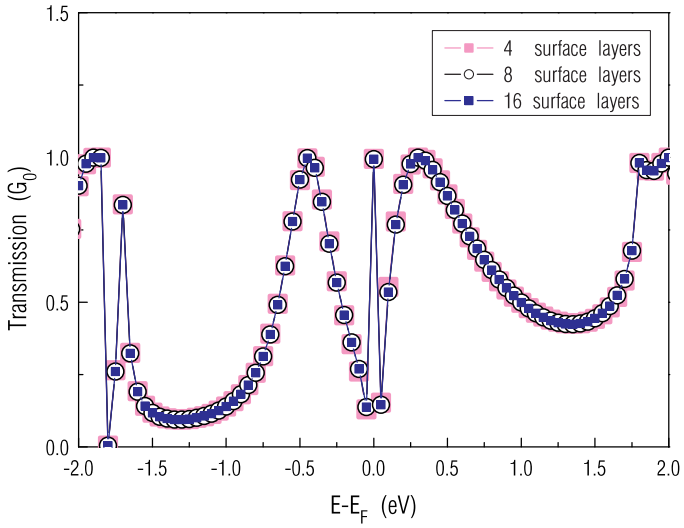

Figure S 5: (Color online) Different width surface layers of seven carbon chains are tested in order to investigate the effect of distance between the two electrodes. This is because enough surface layers are essential in order to properly screen the induced electric field between two close electrodes. As can be seen, the transport property of the carbon chains does not change appreciably when the surface layers are four or more.

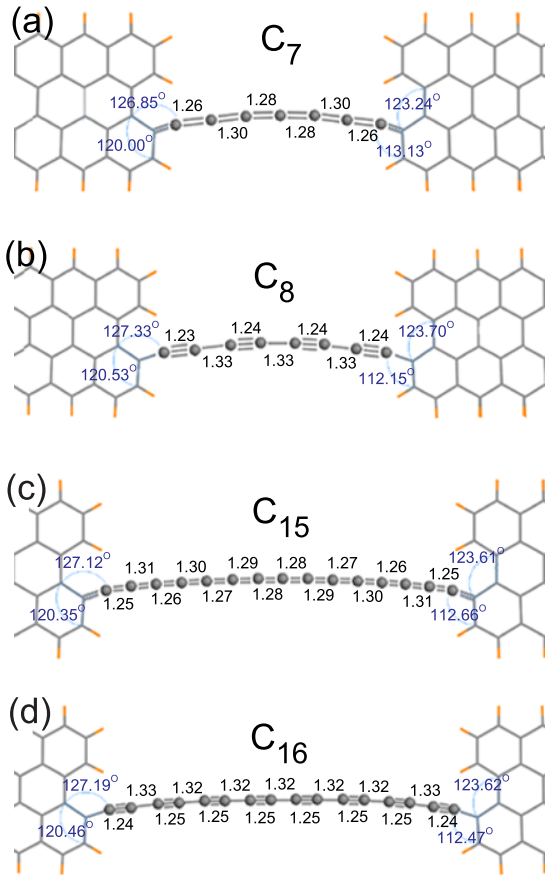

Figure S 6: (Color online) (a)-(d) The optimized scattering region of C_7, C_8, C_{15}, and C_{16} structures. the wires consisting of odd number of carbon atoms favor cumulene ($\cdots$C=C=C=C$\cdots$) ((a) and (c)), but those consisting of even number of carbon atoms prefer polyyne ($\cdots$C$\equiv$C$-$C$\equiv$C$\cdots$) ((b) and (d)).

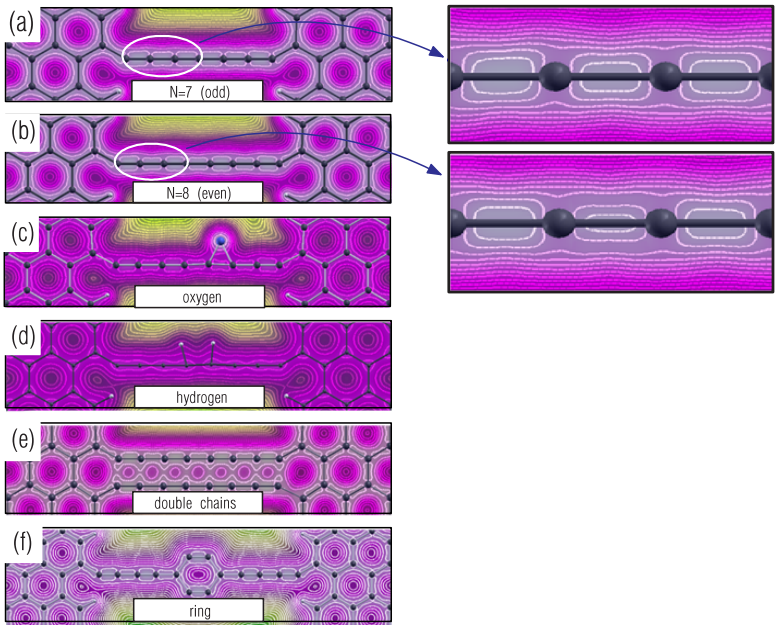

Figure S 7: (Color online) (a)-(f) Electron density of carbon wire-graphene junctions. The different bonding configurations of odd-numbered carbon wires (a) and even-numbered carbon wires (b) can be seen from their electron density distribution. The adsorbed oxygen atom (c), apt to epoxy, which can block the electrical current due to the electron trap property of oxygen atoms. The calculated conductance of double wires is less than twice of a singe wire. This is due to the spatial overlapping of electron cloud between two wires as shown in (e).

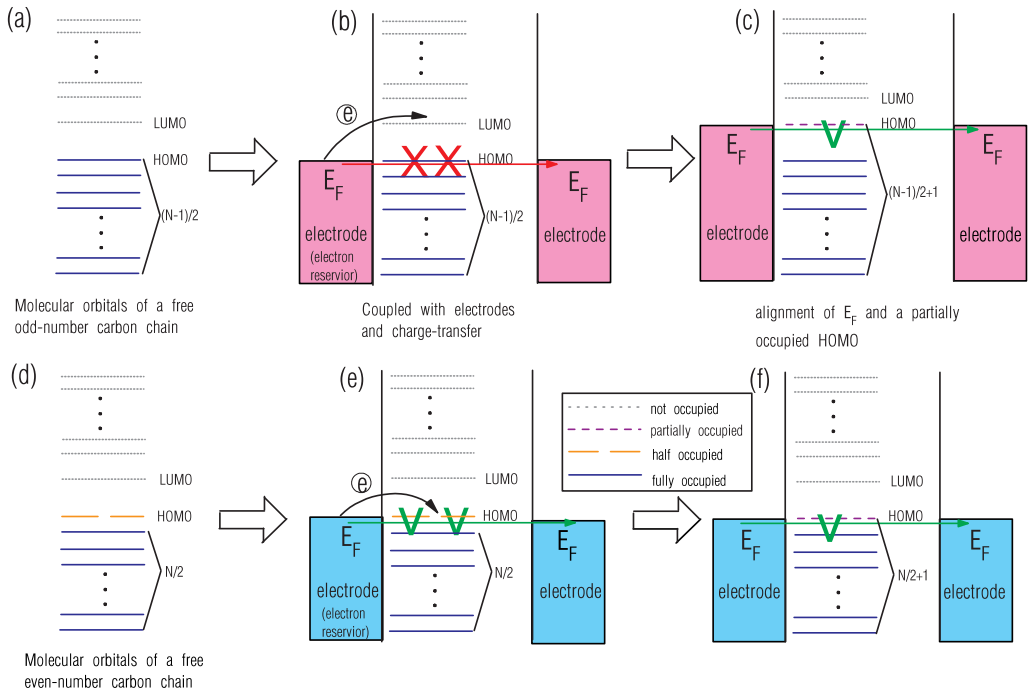

Figure S 8: (Color online) (a) Molecular orbitals of a free odd-numbered carbon wire (molecule) with $(N-1)/2$ fully occupied HOMO. (b) A free carbon wire is coupled with electrodes and charge-transfer occurs which make empty LUMO of the free carbon wire becoming partially occupied. (c) Alignment of the Fermi level of electrodes and a partially occupied HOMO, resulting in electron transport from left electrode to right electrode. (d)Molecular orbitals of a free even-numbered carbon wire with $N/2$ fully occupied HOMO and one half-occupied HOMO. (e) A free carbon wire is coupled with electrodes and charge-transfer occurs which make the half-occupied HOMO becoming partially occupied. (f) Alignment of the Fermi level of electrodes and a partially occupied HOMO. Therefore, both odd- and even-numbered carbon wire are conductible when they are coupled with electrodes.

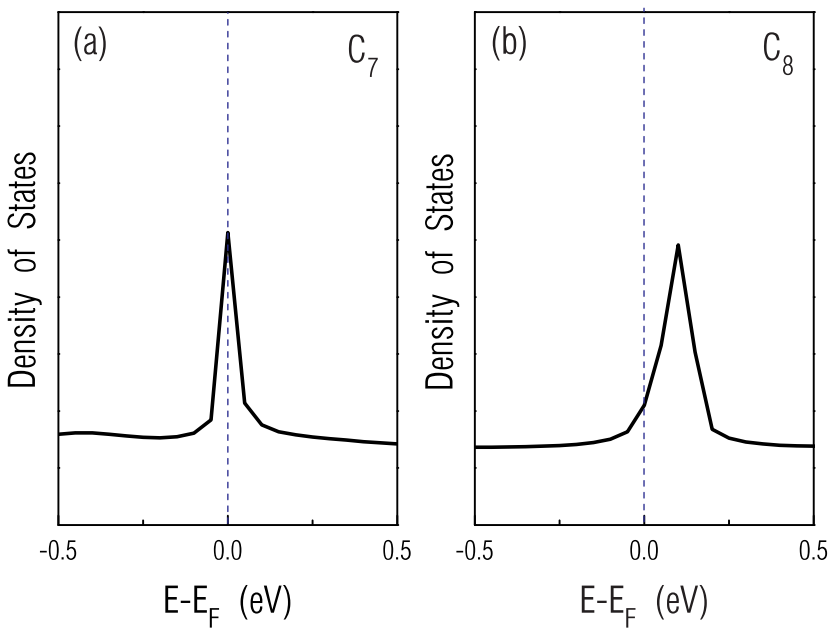

Figure S 9: (Color online) (a)Density of states of C_7 at the Fermi level; (b)Density of states of C_8 at the Fermi level. Higher density of states at the Fermi level, higher transmission at the Fermi level.

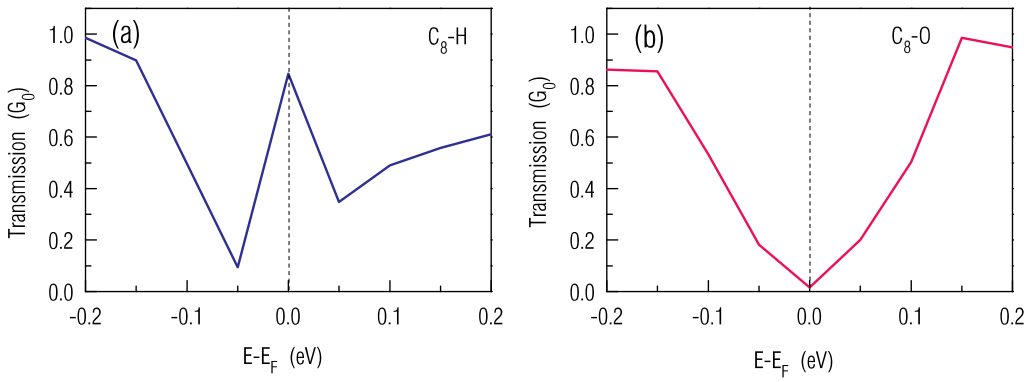

Figure S 10: (Color online) (a) The enlarged view of the transmission spectrum of hydrogen adsorbed C_8 near the Fermi level. (b) The enlarged view of the transmission spectrum of oxygen adsorbed C_8 near the Fermi level.