Supporting Information of

Carbon nanowires made by the insertion-and-fusion method toward carbon-hydrogen nanoelectronics

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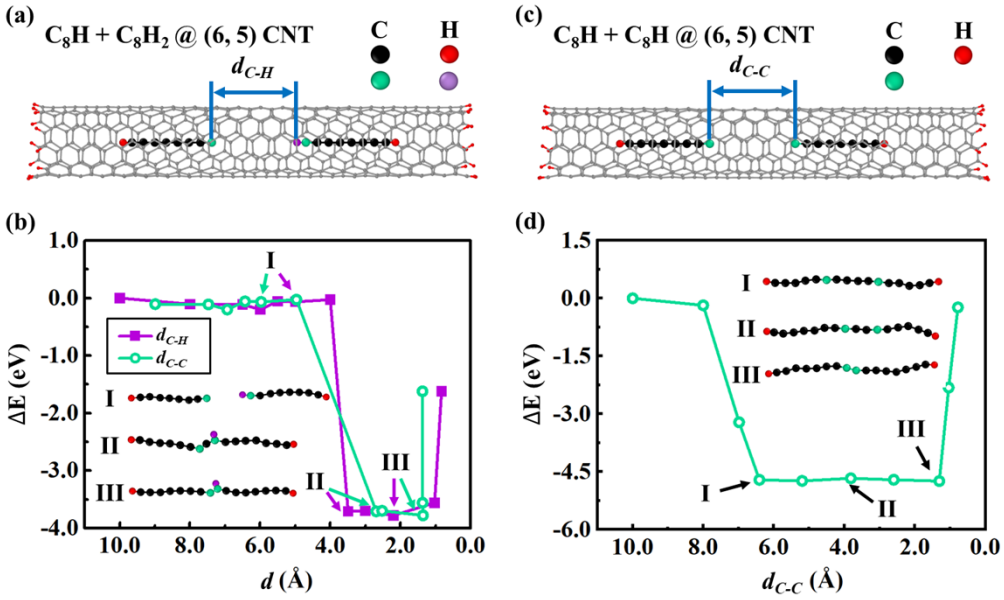

Figure S1. (a) Schematic model of the fusion process of C_8H chain and C_8H_2 chain inside (6, 5) CNT. The distance ($d_{C\text{-}H}$) was constrained between the end C atom (in green) of the C_8H chain and the end H atom (in purple) of the C_8H_2 chain. (b) Relative energies as functions of $d_{C\text{-}H}$ and $d_{C\text{-}C}$ at 973 K. (c) Schematic model of the fusion process of two C_8H chains inside (6, 5) CNT. The distance ($d_{C\text{-}C}$) was constrained between the two end C atoms (in green) of the C_8H chains. (d) Relative energies as functions of $d_{C\text{-}C}$ at 973 K. The insets in (b) and (d) are typical configurations during the fusion process and the CNTs were hidden for clear visual inspection.

To examine the effects of end-capped H atoms in the fusion reactions, we performed constrained MD simulations using an unsaturated C_8H chain where one of end C atoms was not saturated by H. As shown in Figure S1(a), the distance ($d_{C\text{-}H}$) was constrained between the end C atom of the C_8H chain and the end H atom of the C_8H_2 chain, respectively. The energy remained unchanged when $d_{C\text{-}H}$ = 10.0 - 4.0 Å [Figure S1(b)]. The C-C fusion occurred when

the energy dropped suddenly to -3.71 eV as the constrained $d_{C\text{-}H}$ decreased to 3.5 Å. Meanwhile, the distance ($d_{C\text{-}C}$) between two end C atoms of the chains decreased from 5.0 Å to 2.7 Å, ~two times length of a common single C-C bond. In fact, an unconstrained C atom jumped over the constrained end-capped C atom and inserted between the two end C atoms as a bridge, leading to the formation of $C_{16}H_3$ chain inside (6, 5) CNT [Figure S1(b)]. As $d_{C\text{-}H}$ decreased further to the equilibrium distance 1.4 Å, the two end C atoms of two chains form a bond with the minimum energy of -3.78 eV. The fusion energy of the unsaturated $C_{16}H_3$ chain was higher than -3.26 eV of saturated $C_{16}H_4$ chain [Figure 2(b)] due to the absence of H-H repulsion at the joint position.

To examine the fusion of C chains without end-capped H atoms where only C-C contact exists, two C_8H chains were inserted and the distance ($d_{C\text{-}C}$) of two unsaturated end C atoms was constrained [Figure S1(c)]. As $d_{C\text{-}C}$ decreased to 6.4 Å, thermal vibrations caused more unconstrained C atoms in the middle of the C_8H chains jumping into the fixed gap between the two chains, forming a $C_{16}H_2$ chain with a fusion energy of 4.7 eV [Figure S1(d)]. Further decrease of the constraint $d_{C\text{-}C}$ could eventually bring the two end C atoms together to form a bond while the fusion energies had little changes. The C chains with unsaturated end C atoms fused more early at farther distances with much larger energy drop compared with the C chains with the H saturated ends.

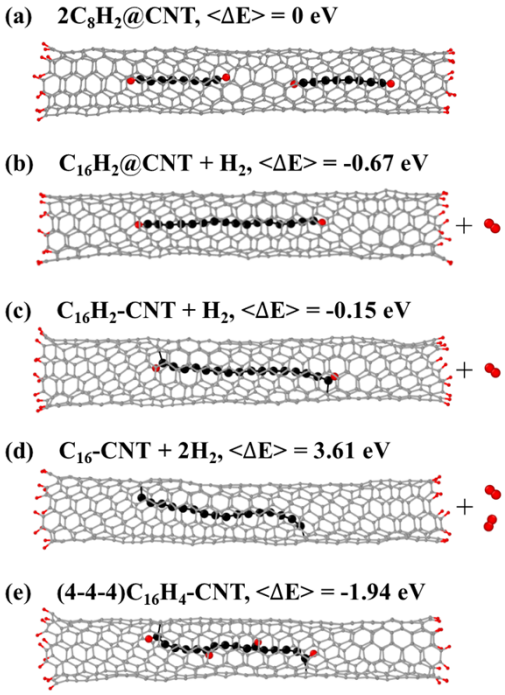

Figure S2. Configurations of carbon chains inside a finite (6, 5) CNT. (a) $2C_8H_2$@CNT and (b) $C_{16}H_2$@CNT + H_2. Configurations of carbon chains fused with the inner wall of a finite (6, 5) CNT. (c) $C_{16}H_2$-CNT + H_2, (d) C_{16}-CNT + $2H_2$, and (e) (4-4-4) $C_{16}H_4$-CNT.

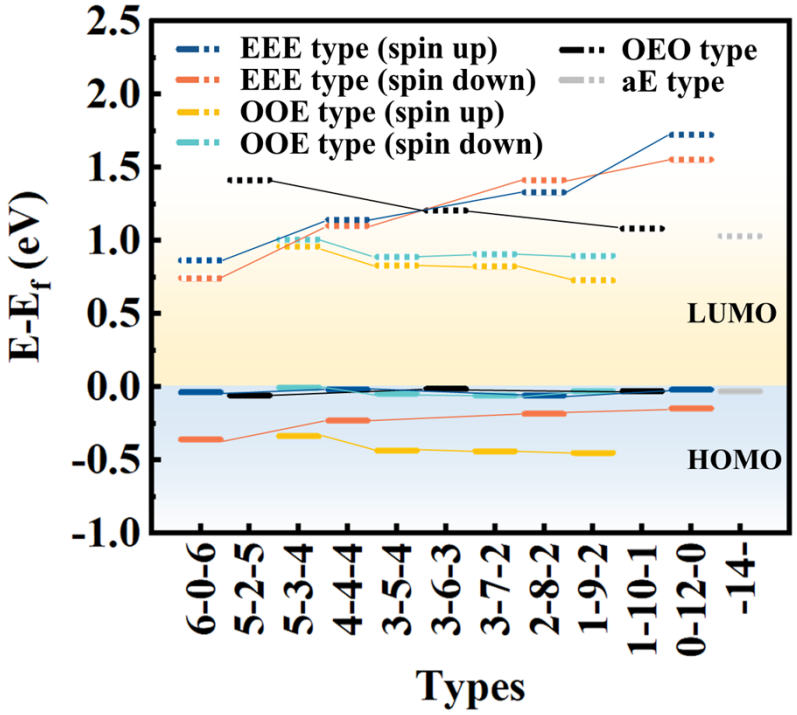

Figure S3. Energy level diagrams of the $C_{16}H_4$ chains with the typical types of H adatom configurations, including OEO, EEE, OOE, and aE types.