Supplementary Information

Magnetic properties in all-carbon graphene-fullerene nanobuds

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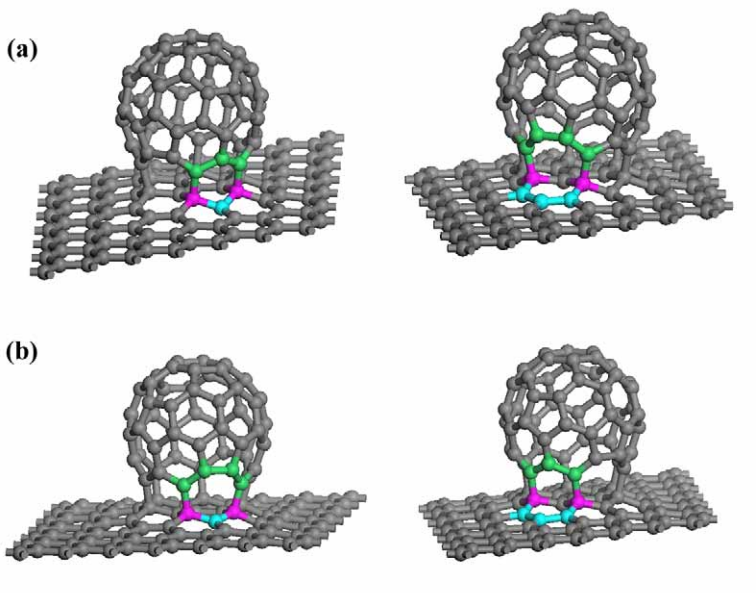

Fig. S 1 Geometric structures of (a) Case A and (b) Case B. The green colored atoms of fullerene, pink associated atoms and cyan atoms of graphene exhibit (a) six- and nine- membered rings for Case A; and (b) seven- and eight- membered rings for Case B.

Table S. 1 The energy data of four kinds of nanobuds : NM, AFM, FM and the related formation reactions. The binding energy E_b is defined as $E_{nanobuds}$-E_{C54}-$E_{graphene}$, where $E_{nanobuds}$, E_{C54}, and $E_{graphene}$ are the energies of nanobud, **isolated open cage C_{54}**, and graphene, respectively. The energy differences of AFM and FM states are compared with corresponding NM ones.

Case	E_{NM} (meV/per atom)	E_{AFM} (meV/ per atom)	E_{FM} (meV/per atom)	E_b (meV /per atom)
A	0.0 (-154969.8)	-2.2 (-154972.0)	-4.0 (-154973.8)	-67.2
B	0.0 (-154974.1)	-0.6 (-154974.7)	-2.5 (-154976.6)	-70.0
C	0.0 (-154997.1)	0.7 (-154996.4)	0.7 (-154996.4)	-90.5
D	0.0 (-155003.5)	0.3 (-155003.2)	0.3 (-155003.2)	-96.8

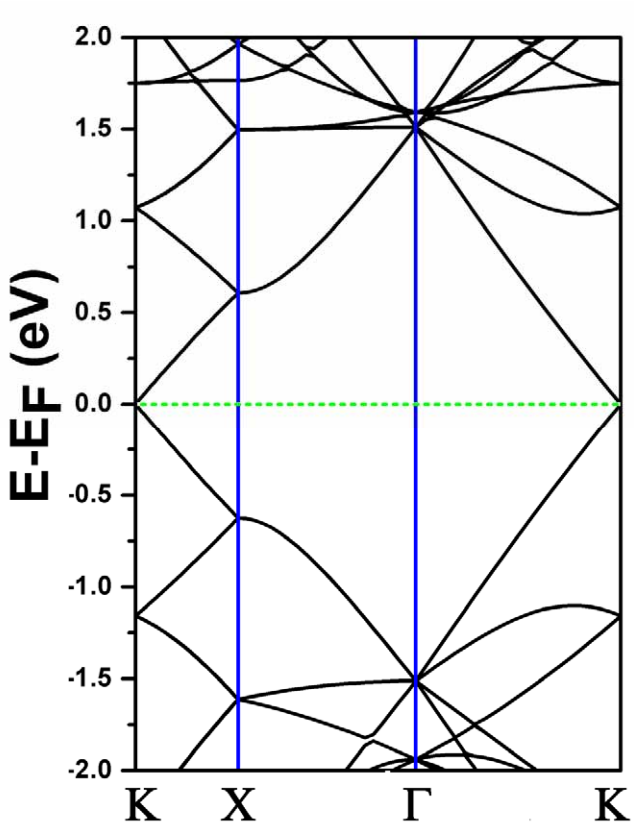

Fig. S 2 Non spin-polarized band structure in 49-unit-cell graphene. The Fermi energy is set to zero.

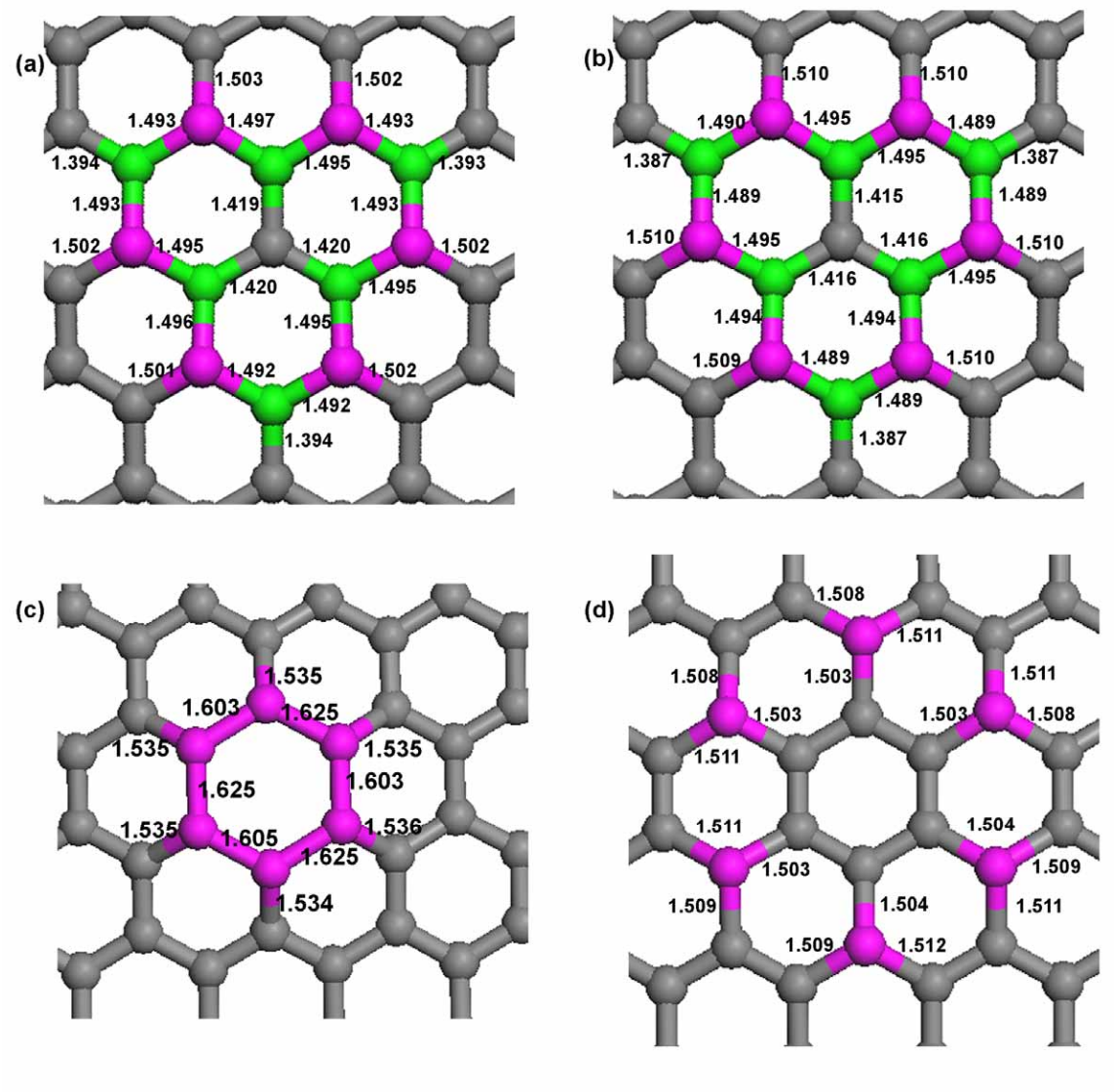

Fig. S 3 The bond lengths (Å) in Case A-D are marked in (a)-(d), respectively. The pink carbon atoms are denoted as associated positions. The green carbon atoms in (a) and (b) are presented the spin positions.