Supplementary Information

Chirality dependent spin polarization of carbon nanotubes

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Part 1. The structures of the CNTs for (9,6), (9,7), (9,8) and (9,9).

Figure S1. The structures of the (9,6), (9,7), (9,8) and (9,9) CNTs.

Part 2. The relative energies of the CNTs of four different lengths.

Figure S2. The relative energies of four structural lengths of CNTs; (a) is L=2, (b) is L=3, (c) is L=4, and (d) is L=5. The energy of the closed shell is set as zero for reference.
In order to ensure the reliability of our results, we studied the relative energies of the CNTs as shown in Figure S2. Given the uniform conclusions for these four lengths, we further confirm the stability of our results and the reliability of our structures.

Part 3. The spin density of the CNTs.

![Spin density distribution of CNTs](image)

Figure S3. The spin density distribution of the \((9,m)\) CNTs for the ground state. The blue region represents the spin up and the red region the spin down. Isovalue=0.0004 a.u..

The spin density of CNTs is shown in Figure S3. It can be seen that the ground state of CNTs is antiferromagnetically coupled, which is similar to previous studies of zigzag nanotubes. The Figure also shows that the spin density of the CNTs gradually decreases with the increase of \(m\).

Part 4. The HOMO-LUMO gaps for the CNTs of four different lengths.

Table S1. HOMO-LUMO gaps for the CNTs. Data on a gray background denote CNTs whose
ground states are nonmagnetic. Unit: eV

| HOMO-LUMO gap | 2  | 3  | 4  | 5  |
|---------------|----|----|----|----|
| (9,0)         | 1.88 | 1.86 | 1.86 | 1.82 |
| (9,1)         | 1.70 | 1.54 | 1.41 | 1.20 |
| (9,2)         | 1.47 | 1.34 | 1.28 | 1.24 |
| (9,3)         | 1.11 | 1.06 | 1.06 | 1.05 |
| (9,4)         | 1.50 | 1.04 | 0.97 | 0.84 |
| (9,5)         | 1.13 | 0.73 | 0.69 | 0.63 |
| (9,6)         | 1.74 | 1.22 | 1.38 | 1.11 |
| (9,7)         | 1.25 | 0.74 | 1.18 | 1.56 |
| (9,8)         | 1.76 | 1.26 | 1.61 | 1.23 |
| (9,9)         | 1.40 | 0.73 | 1.63 | 0.71 |

From Table S1, it can be seen that the HOMO-LUMO gap gradually decreases with the spin density for the four length of CNTs. However, for the CNTs whose spin vanish, the HOMO-LUMO gap is disordered and shows no regular pattern.