# Supporting Information

# Metal-semiconductor-metal transition in zigzag carbon nanoscrolls

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## 1. The calculated results of ACNSs.

Using first-principles calculations, we have also investigated electronic properties of ACNSs during their rolling processes from GNRs by bending deformation. The results are summarized in Table S1. From this table, it can be seen that all the ACNSs with different widths exhibit semiconducting behaviors during their rolling processes, which indicates that electronic properties transition (e.g., a metal-semiconductor-metal transition in ZCNSs) is not observed in the ACNSs. Thereby, the focus of our study is solely on the ZCNSs.

**Table S1** Properties of *n*-ACNSs (*n* represents dimer lines in ACNS): distance between two edges $d_{C\text{-}C}$ (Å) and band gap $E_g$ (eV) (N: non-overlapped edges, O: overlapped edges).

| ACNSs | 33-ACNS | | | | | 35-ACNS | | | | | 37-ACNS | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $d_{C\text{-}C}$ | 9.97 | 3.87 | 3.40 | 4.05 | 6.12 | 8.45 | 4.26 | 3.40 | 4.20 | 7.41 | 6.86 | 3.45 | 3.40 | 3.88 | 7.20 |
| types | N | N | O | O | O | N | N | O | O | O | N | N | O | O | O |
| $E_g$ | 0.23 | 0.23 | 0.18 | 0.18 | 0.21 | 0.07 | 0.08 | 0.05 | 0.09 | 0.10 | 0.32 | 0.32 | 0.33 | 0.34 | 0.32 |

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2. Partial density of states of the edge C atoms in ZCNSs.

Fig. S1† displays partial density of states (PDOSs) of the edge C atoms in N-ZCNSs and O-ZCNSs. It is clear to see that the Fermi level of metallic ZCNSs and the VBM and CBM of semiconducting ZCNSs are mainly contributed by the C *p* orbital of edges in spite of their two edges overlapped or non-overlapped. Thus, the electronic contributions of O-ZCNSs are similar to those of N-ZCNSs whether they are metallic or semiconducting.

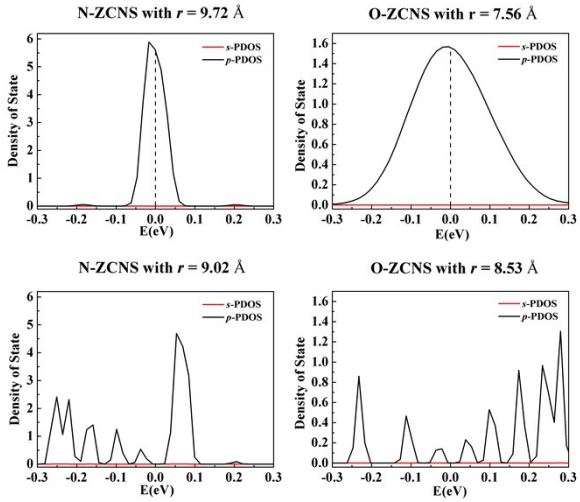


**Fig. S1†** Partial density of states (PDOSs) of the edge C atoms for: N-ZCNSs and O-ZCNSs. The Fermi level is set to zero.