Electronic Supplementary Information

Adsorbing the Magnetic Superhalogen MnCl$_3$ to Realize the Intriguing Half-metallicity and Spin-Gapless-Semiconductor in Zigzag or Armchair SiC Nanoribbon

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(1) The computational test on the modified 8-zSiCNR and 13-aSiCNR systems with superhalogen MnCl$_3$ at the center

When adsorbing the superhalogen MnCl$_3$ at the ribbon center for 8-zSiCNR and 13-aSiCNR, we consider all four possible adsorption sites for the Mn atom in MnCl$_3$ including the top site of C atom ($T_C$), top site of Si atom ($T_{Si}$), bridge site over Si-C bond ($B$) and hollow site of SiC hexagon ring ($H$). The computed results reveal that the modified zSiCNR or aSiCNR configuration with the MnCl$_3$ at the bridge site of ribbon center cannot be obtained. Consequently, we can respectively obtain three conformations for the MnCl$_3$-modified 8-zSiCNR and 13-aSiCNR systems at the center (Figures S1 and S2). By comparison, we can find that adsorbing the MnCl$_3$ at the top of C atom ($T_C$) can obtain the most energetically stable configurations for the modified zSiCNR and aSiCNR systems (Figures S1 and S2), and they have been correspondingly named as MnCl$_3$-$T_C$-8-zSiCNR-center and MnCl$_3$-$T_C$-13-aSiCNR-center in the main text.

**Figure S1** The side view and top view of modified 8-zSiCNR with the superhalogen MnCl$_3$ at the ribbon center, and the relative energy $\Delta E$ (eV) between the MnCl$_3$-modified 8-zSiCNR systems at three different adsorption sites including (a) $T_C$, (b) $T_{Si}$, and (c) $H$. 

- $T_C$: $\Delta E = 0.0$ eV
- $T_{Si}$: $\Delta E = 0.967$ eV
- $H$: $\Delta E = 0.418$ eV
Figure S2 The side view and top view of modified 13-aSiCNR with the superhalogen MnCl₃ at the ribbon center, and the relative energy ΔE (eV) between the MnCl₃-modified 13-aSiCNR systems at three different adsorption sites including (a) Tₐ, (b) Tₛ, and (c) H.

(II) The computational test on the MnCl₃-modified SiCNR systems by using the double supercell

Table S1. The relative energies ΔE (meV) between the parallel and antiparallel couplings of two neighboring MnCl₃ for the modified SiCNR systems. Note that these modified SiCNR systems with two MnCl₃ in the supercell can be denoted by adding (double) into the names of corresponding ones with one MnCl₃.

| Systems                      | ΔE (meV) |
|------------------------------|----------|
|                              | Parallel | Antiparallel |
| MnCl₃-Tₐ-6-zSiCNR-eSi(double) | 0.0      | 1.5          |
| MnCl₃-Tₐ-8-zSiCNR-eSi(double) | 0.0      | 4.3          |
| MnCl₃-Tₐ-8-zSiCNR-center(double) | 0.0    | 1.4          |
| MnCl₃-Tₐ-8-zSiCNR-eC(double)   | 0.0      | 65.4         |
| MnCl₃-Tₐ-9-aSiCNR-edge(double) | 0.0      | 3.2          |
| MnCl₃-Tₐ-11-aSiCNR-edge(double) | 0.0    | 1.2          |
| MnCl₃-Tₐ-13-aSiCNR-edge(double) | 0.0      | 3.5          |
| MnCl₃-Tₐ-13-aSiCNR-center(double) | 0.0  | 3.3          |