Electronic Supplementary Information:

Dihalogen Edge-Modification: An Effective Approach to Realize the Half-Metallicity and Metallicity in Zigzag Silicon Carbon Nanoribbons

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A computational test on the determination of ground state by considering different antiferromagnetic configurations of the sampled 2F-zSiCNR-1F system

It is known that, to determine the ground state of the studied dihalogen-edge-modified zSiCNRs systems, we have performed the spin-unpolarized and spin-polarized computations, where the nonmagnetic (NM), ferromagnetic (FM) and antiferromagnetic (AFM) states are considered, and the involved AFM configuration possesses the same spin orientation at each edge yet opposite between two edges. Here, to show that the involved AFM state is the lowest-lying in energy among the possible AFM arrangements, we have made a computational test by sampling the 2F-zSiCNR-1F system, where a supercell with four repeated units is employed (Figure S1).

The computed results show that eight AFM configurations can be obtained (Figure S1), which are denoted as AFM-n (n = 1 ~ 8). Among them, the lowest-lying in energy is the AFM-1 configuration with the same spin aligned at each edge yet opposite spin between two edges (Table S1), which is corresponding to the AFM state involved in the present work. It is worth mentioning that the AFM-1 configuration has been extensively employed to make a comparison with the corresponding NM and FM states, in order to determine the ground state of zSiCNR-related systems reported previously, e.g., the pristine zSiCNR,[1,2] as well as other edge-modified[1,3,4] or functionalized[5,6] zSiCNR systems. So, the lowest-lying AFM-1 arrangement is only considered to determine the ground state of the studied dihalogen-edge-modified zSiCNR systems in this work.

References:

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Figure S1. Schematic representation of ferromagnetic (FM), nonmagnetic (NM) and eight obtained antiferromagnetic (AFM-n (n = 1~8)) configurations for the sampled 2F-zSiCNR-1F system. The symbols plus and minus at the ribbon edges represent spin up and spin down, respectively.

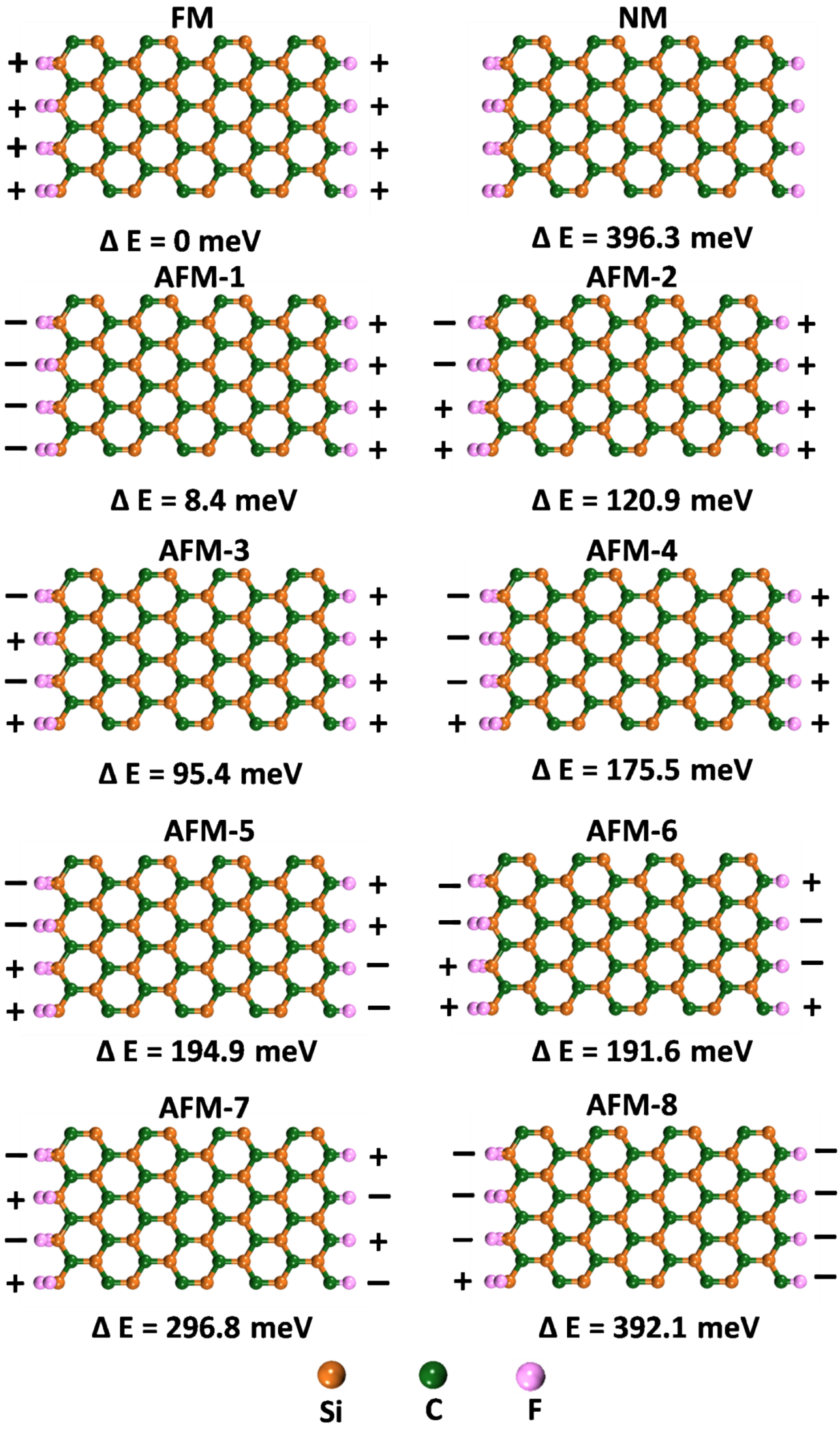

Table S1. Relative energies (meV) of the different magnetic configurations to the ground state (FM). The NM, FM and AFM-n (n = 1~8) represent nonmagnetic, ferromagnetic and different antiferromagnetic configurations, respectively.

System	ΔE (meV)									
	NM	FM	AFM-1	AFM-2	AFM-3	AFM-4	AFM-5	AFM-6	AFM-7	AFM-8
2F-zSiCNR-1F	396.3	0.0	8.4	120.9	95.4	175.5	194.9	191.6	296.8	392.1