

Electronic Supplementary Information

Adsorbing the 3d-Transition Metal Atoms to Effectively Modulate the Electronic and Magnetic Behaviors of Zigzag SiC Nanoribbons

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(I) The computational test on the modified 8-zSiCNR systems with TM atoms at the center

When adsorbing the TM atom (TM = Ti, Cr, Mn, Fe and Co) over the center of 8-zSiCNR, we consider all four possible adsorption sites including the top site of C atom (T_C), the top site of Si atom (T_{Si}), the bridge site over the Si-C bond (B) and the hollow site of the hexagon ring (H). The computed results show that the modified zSiCNR configuration with TM atom at the bridge site cannot be obtained. Therefore, for each adsorbed TM atom, we can eventually obtain three conformations ((I)~(III)) of TM-modified 8-zSiCNR at the center, as shown in Figure S1. By comparison, we can find that the most stable conformations for each series are a- II , b- I , c- I , d-III and e- I , respectively (Figure S1), which are accordingly named as $Ti(T_{Si})$ -zSiCNR-*center*, $Cr(T_C)$ -zSiCNR-*center*, $Mn(T_C)$ -zSiCNR-*center*, $Fe(H)$ -zSiCNR-*center* and $Co(T_C)$ -zSiCNR-*center* in the main text.

Similarly, all four possible adsorption sites including T_C , T_{Si} , B and H are also considered to obtain the most stable one at the Si/C edge of zSiCNR in their respective series. Finally, for each adsorbed TM atom, we can obtain three modified conformations ((I-*eC*)~(III-*eC*)) with TM at the C edge (Figure S2) and three modified conformations ((I-*eSi*)~(III-*eSi*)) with TM at the Si edge (Figure S3). By making a comparison, we can find that the most stable configurations for each series of TM-modified 8-zSiCNR at the C edge are a- II -*eC*, b-III-*eC*, c- II -*eC*, d-III-*eC* and e-III-*eC*, respectively (Figure S2), which are correspondingly named as $Ti(T_{Si})$ -zSiCNR-*eC*, $Cr(H)$ -zSiCNR-*eC*, $Mn(T_{Si})$ -zSiCNR-*eC*, $Fe(H)$ -zSiCNR-*eC* and $Co(H)$ -zSiCNR-*eC* in the main text. However, the most stable configurations for each series of TM-modified 8-zSiCNR at the Si edge are a- I -*eSi*, b- I -*eSi*, c- I -*eSi*, d- I -*eSi* and e- I -*eSi*, respectively (Figure S3), which are accordingly named as $Ti(T_C)$ -zSiCNR-*eSi*, $Cr(T_C)$ -zSiCNR-*eSi*, $Mn(T_C)$ -zSiCNR-*eSi*, $Fe(T_C)$ -zSiCNR-*eSi* and $Co(T_C)$ -zSiCNR-*eSi* in the main text.

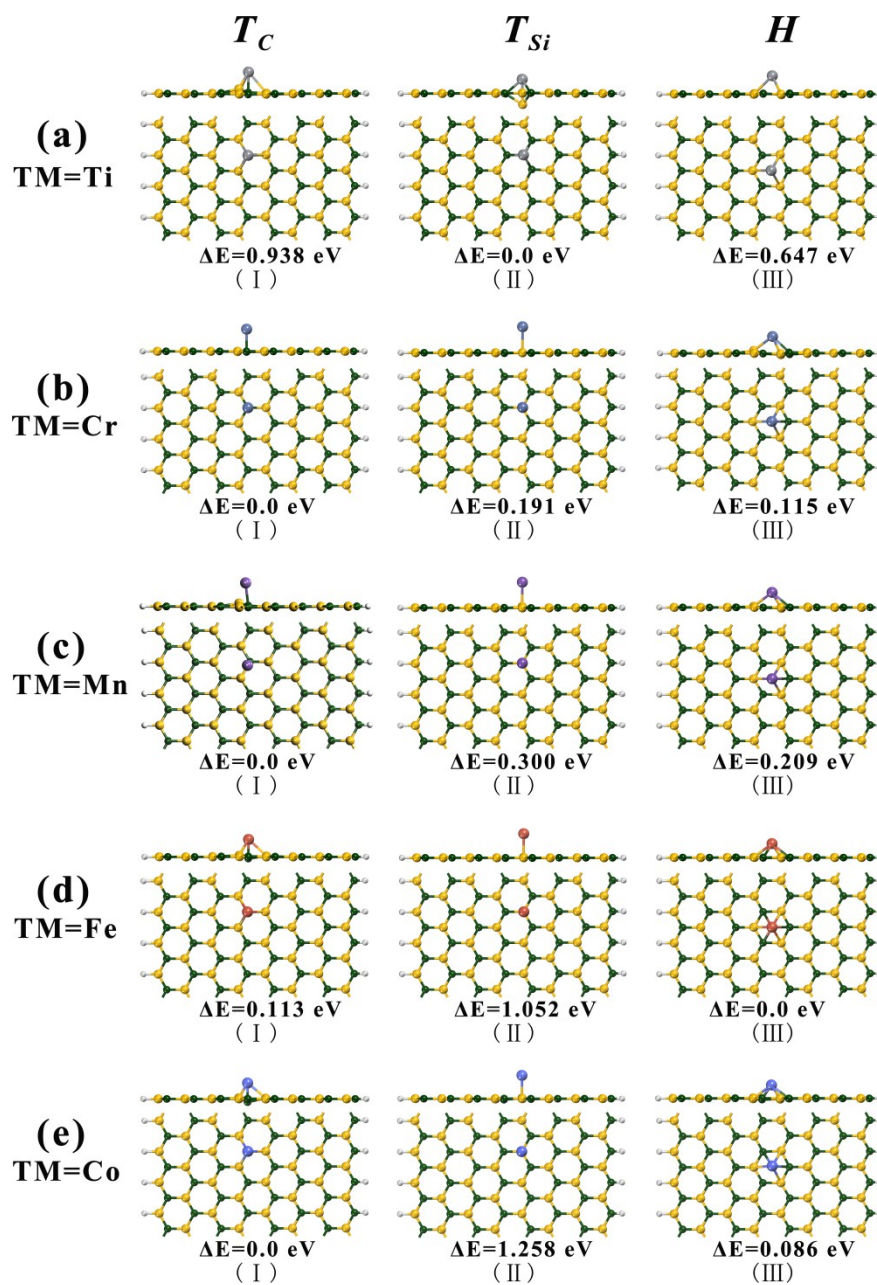


Figure S1 The side view and top view of modified 8-zSiCNR with the TM atom at the center: (a) Ti, (b) Cr, (c) Mn, (d) Fe, (e) Co, and the relative energy ΔE (eV) between the TM-modified conformations at three different adsorption sites including (I) T_C , (II) T_{Si} and (III) H .

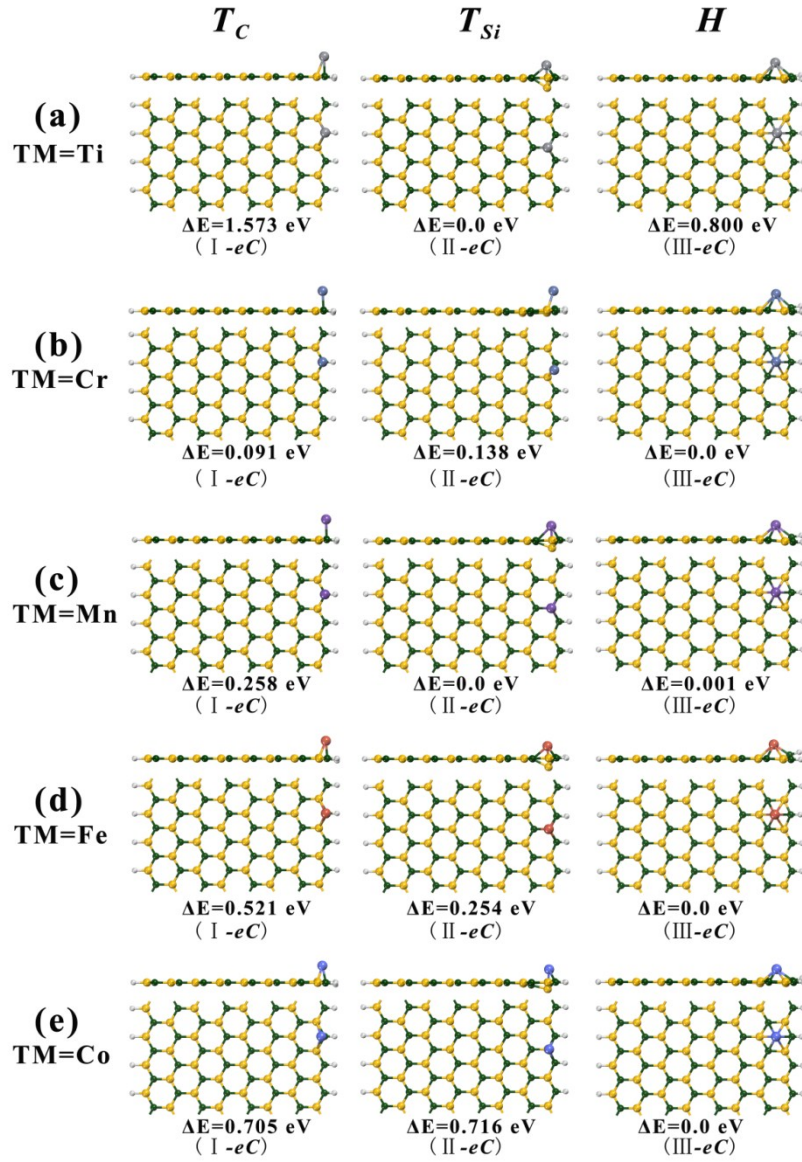


Figure S2 The side view and top view of modified 8-zSiCNR with the TM atom at the C edge: (a) Ti, (b) Cr, (c) Mn, (d) Fe, (e) Co, and the relative energy ΔE (eV) between the TM-modified conformations at three different adsorption sites including (I -eC) T_C , (II -eC) T_{Si} and (III -eC) H .

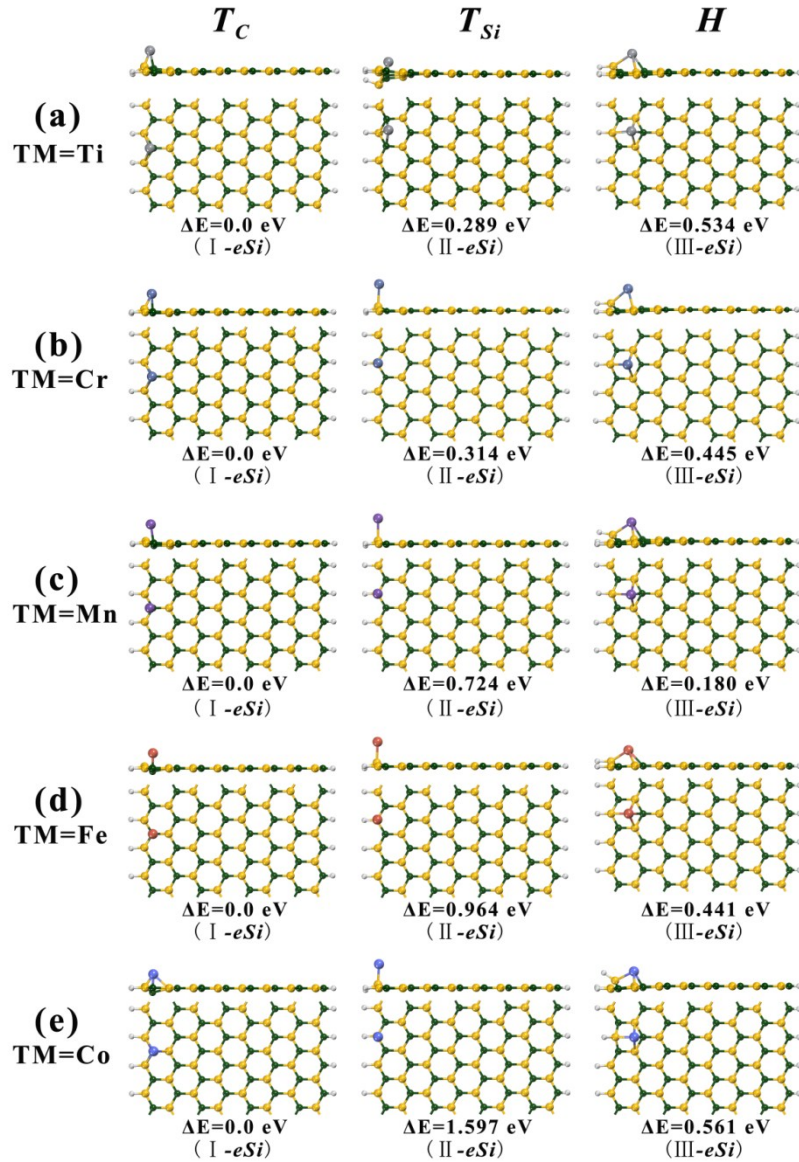


Figure S3 The side view and top view of modified 8-zSiCNR with the TM atom at the Si edge: (a) Ti, (b) Cr, (c) Mn, (d) Fe, (e) Co, and the relative energy ΔE (eV) between the TM-modified conformations at three different adsorption sites including (I -eSi) T_C , (II -eSi) T_{Si} and (III -eSi) H .