Supplementary Material:

Nonvolatile switchable half metallicity and magnetism in MXenes $Hf_2MnC_2O_2/Sc_2CO_2$ multiferroelectric heterostructure

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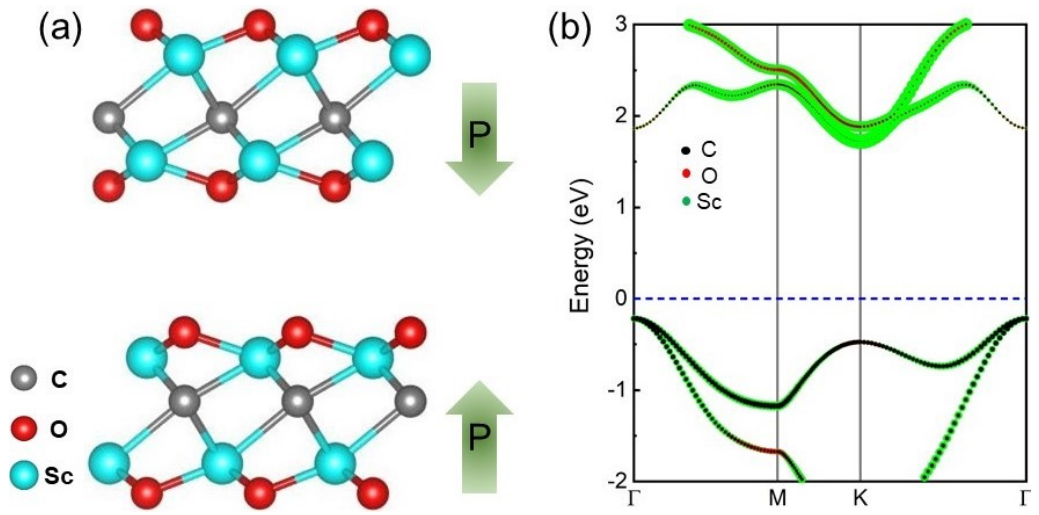

Figure S1. (a) The atom structural diagrams of Sc_2CO_2 monolayer with different polarization orientations. (b) Band structure of Sc_2CO_2 monolayer. The gray, red and cyan balls represent C, O and Sc atoms, respectively. The green arrow represents the direction of polarization.

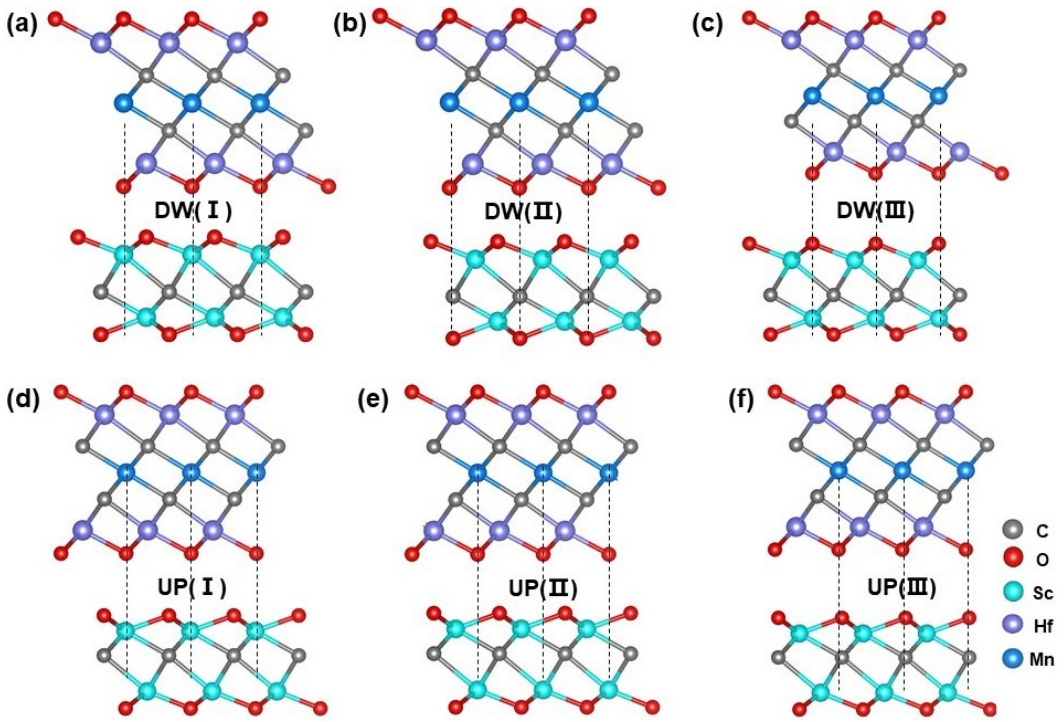

Figure S2. (a) The different stacking configurations of $Hf_2MnC_2O_2/Sc_2CO_2$ heterostructures. (a) DW-(I), (b) DW-(II), (c) DW-(III) are for $Hf_2MnC_2O_2/Sc_2CO_2\downarrow$. (d) UP-(I), (e) UP-(II), (f) UP-(III) are for $Hf_2MnC_2O_2/Sc_2CO_2\uparrow$. C, O, Sc, Mn and Hf are represented by gray, red, cyan, blue and purple balls, respectively.

Table S1. Calculated parameters of $Hf_2MnC_2O_2/Sc_2CO_2$ heterostructures. d is the interlayer distance. $d_{o\text{-}o}$ is the minimum distance between O atom in $Hf_2MnC_2O_2$ and O atom in Sc_2CO_2. $d_{o\text{-}Sc}$ is the minimum distance between O atom in $Hf_2MnC_2O_2$ and Sc atom in Sc_2CO_2. E_{tot} is the total energy.

Stacking Configurations	DW-(I)	DW-(II)	DW-(III)	UP-(I)	UP-(II)	UP-(III)
d (Å)	2.168	2.763	3.121	2.156	2.523	3.011
$d_{O\text{-}O}$ (Å)	2.839	3.271	3.121	2.825	3.139	3.011
$d_{O\text{-}Sc}$ (Å)	2.815	3.932	4.294	2.775	3.698	4.072
E_{tot} (eV)	-104.200	-104.079	-104.028	-104.227	-104.151	-104.060

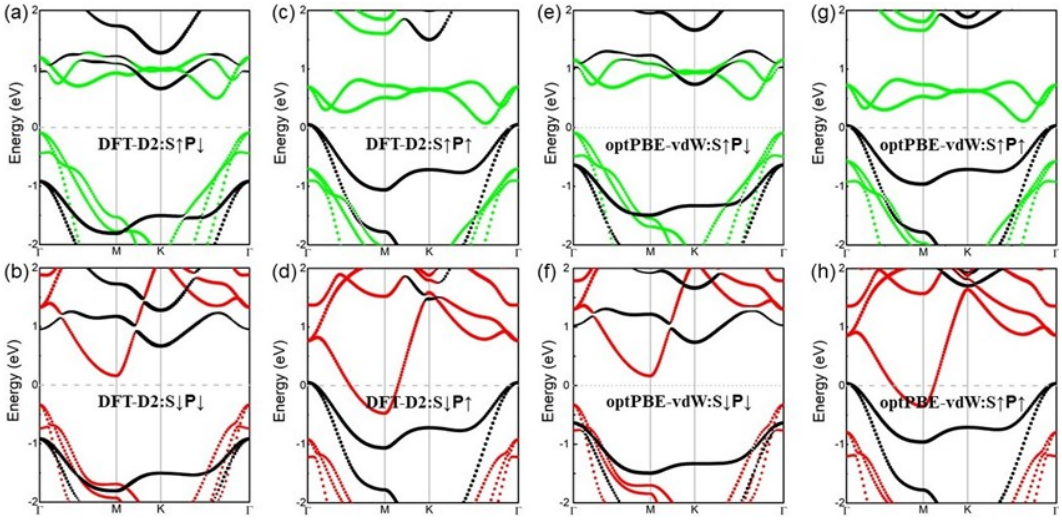

Figure S3. Electronic band structures of (a, b, e, f) $Hf_2MnC_2O_2/Sc_2CO_2$ P↓, (c, d, g, h) $Hf_2MnC_2O_2/Sc_2CO_2$ P↑ with DFT-D2 and optPBE-vdW methods, respectively. Green and red lines represent the contributions from spin-up and spin-down channels of $Hf_2MnC_2O_2$, black lines denote the contributions from Sc_2CO_2 monolayer.

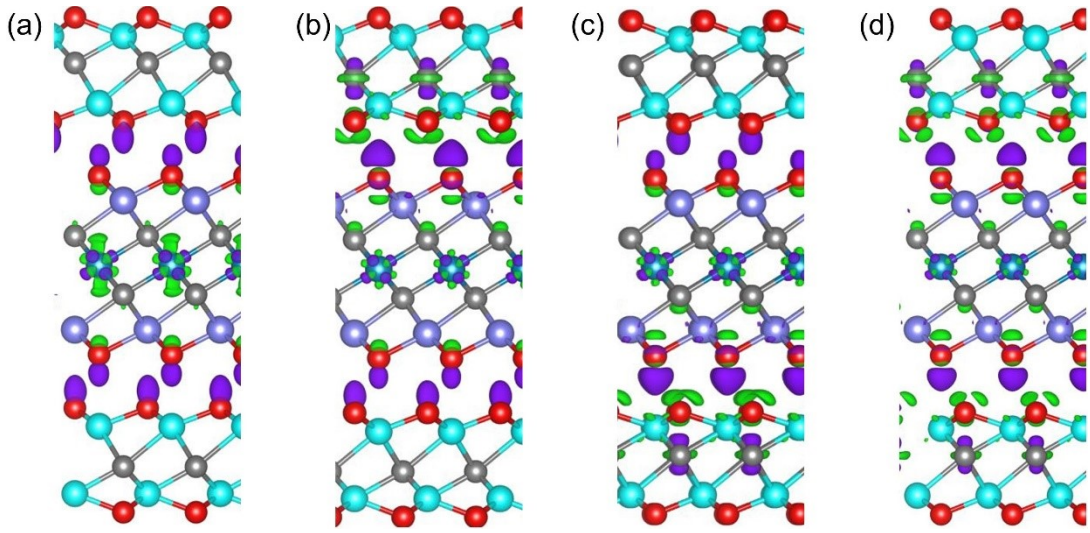

Figure S4. The differential charge density of four structural states (a) P_1, (2)P_2, (c) P_3, and (d) P_4. The green and purple colors represent charge depletion and accumulation, respectively.

Table S2. The magnetic anisotropic energy ($MAE=E_{100}-E_{001}$) of $Hf_2MnC_2O_2/Sc_2CO_2$ heterostructure with different van der Waals corrections.

		$MAE=E_{100}-E_{001}$
$Hf_2MnC_2O_2/Sc_2CO_2\downarrow$	DFT-D3	-93 μeV
	DFT-D2	-97 μeV
	optPBE-vdw	-89 μeV
$Hf_2MnC_2O_2/Sc_2CO_2\uparrow$	DFT-D3	47 μeV
	DFT-D2	64 μeV
	optPBE-vdw	30 μeV

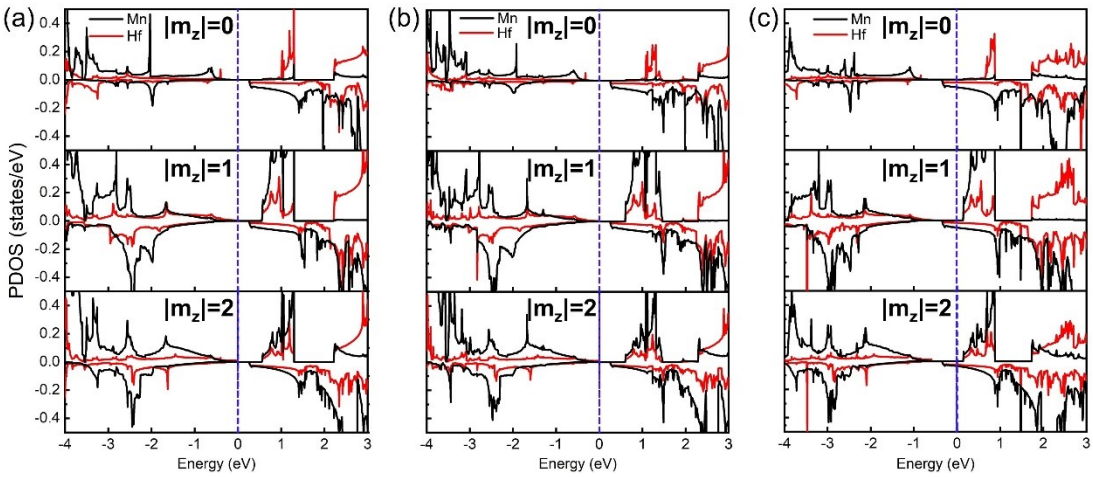

Figure S5. The d-orbital decomposed PDOS of (a) $Hf_2MnC_2O_2$, (b) $Hf_2MnC_2O_2/Sc_2CO_2$-P↓, (c) $Hf_2MnC_2O_2/Sc_2CO_2$-P↑. The Mn and Hf are represented by black and red colors, respectively.

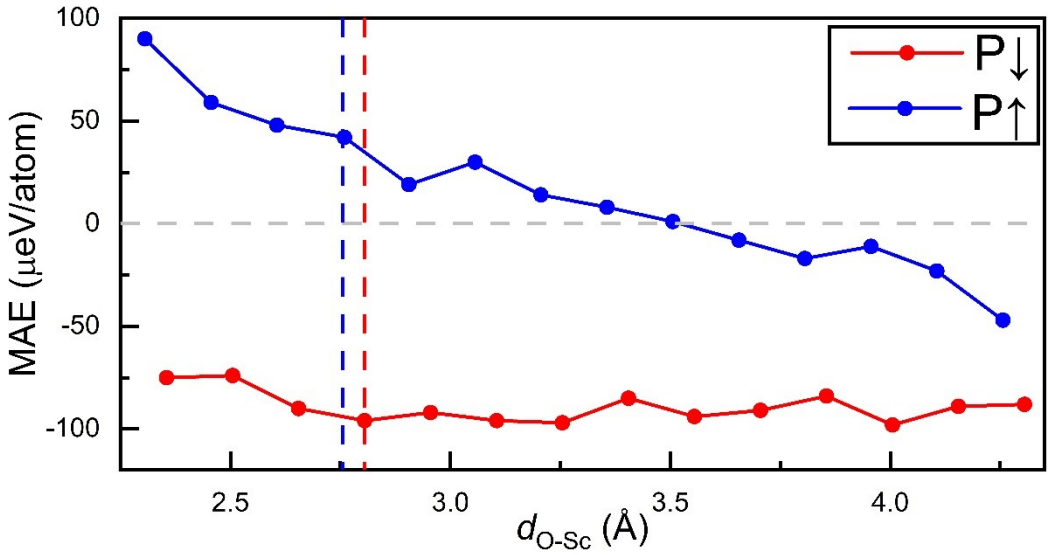

Figure S6. The MAE of $Hf_2MnC_2O_2/Sc_2CO_2$-P↓ (red dot line) and $Hf_2MnC_2O_2/Sc_2CO_2$-P↑ (blue dot line) as function of the $d_{O\text{-}Sc}$. The red and blue dash vertical lines indicate equilibrium positions of $Hf_2MnC_2O_2/Sc_2CO_2$-P↓ and $Hf_2MnC_2O_2/Sc_2CO_2$-P↑, respectively.