Supplementary material:

Computational mining of Janus Sc$_2$C-based MXene for spintronic, photocatalytic, and solar cell applications

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Fig. S1 Phonon dispersion curves for (a) Sc$_2$COHF, (b) Sc$_2$COHCl, (c) Sc$_2$COHO, (d) Sc$_2$COHH, (e) Sc$_2$COF, (f) Sc$_2$COCl, (g) Sc$_2$CHF, (h) Sc$_2$CHCl, (i) Sc$_2$CFCl.
**Fig. S2** The HSE06 band structures of Janus (a) Sc$_2$COHF, (b) Sc$_2$COHCl, (c) Sc$_2$COHH, (d) Sc$_2$CHF, (e) Sc$_2$HCl, (f) Sc$_2$CFCl.
Fig. S3 Various possible magnetic configurations of Sc$_2$CTT$^\prime$ including (a) one ferromagnetic state and (b-d) three antiferromagnetic states with up-spins (↑) and down-spins (↓) on the Sc atom.
**Fig. S4** The band structure of Sc$_2$COF with (a) spin-up and (c) spin-down states, and (b) the spin-resolved density of states. The Fermi level is set at 0 eV as indicated by a dashed line.
Fig. S5 The band structure of Sc₂COH with (a) spin-up and (c) spin-down states, and (b) the spin-resolved density of states. The Fermi level is set at 0 eV as indicated by a dashed line.
**Fig. S6** The band structure of Sc$_2$COOH with (a) spin-up and (c) spin-down states, and (b) the spin-resolved density of states. The Fermi level is set at 0 eV as indicated by a dashed line.
Fig. S7 (a) The energy differences between FM, AFM and NM states of Sc$_2$COF as a function of tensile strain. The spin-resolved density of states of Sc$_2$COF under (b) 5% tensile strain for FM states and (c) 6% tensile strain for AFM states, respectively.
Fig. S8 (a) The energy differences between FM, AFM and NM states of Sc$_2$COOH as a function of tensile strain. The spin-resolved density of states of Sc$_2$COOH under (b) 5\% tensile strain for FM states and (c) 6\% tensile strain for AFM states, respectively.
Fig. S9 (a) The energy differences between FM, AFM and NM states of Sc$_2$COH as a function of tensile strain. The spin-resolved density of states of Sc$_2$COH under (b) 5\% and (c) 10\% tensile strain for FM states, respectively.
Fig. S10 Band alignment of (a) Sc$_2$COHF, (b) Sc$_2$COHH and (c) Sc$_2$CHF with respect to the redox potentials of water.
Fig. S11 The density of states of $\text{Sc}_2\text{COHH/InS}$ heterostructure.