Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supporting Information

$CrXTe_3$ (X= Si, Ge) nanosheets: two dimensional intrinsic ferromagnetic semiconductors

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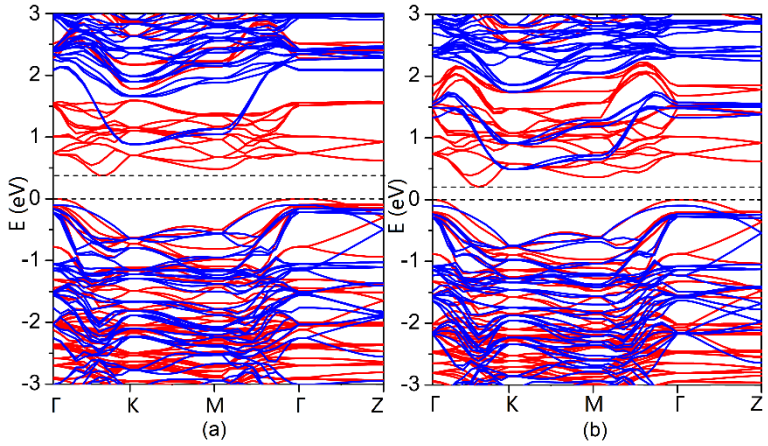

Fig. S1. Band structure for bulk (a) $CrSiTe_3$ and (b) $CrGeTe_3$ with PBE+U+VDW functional. Fermi levels are all set to zero.

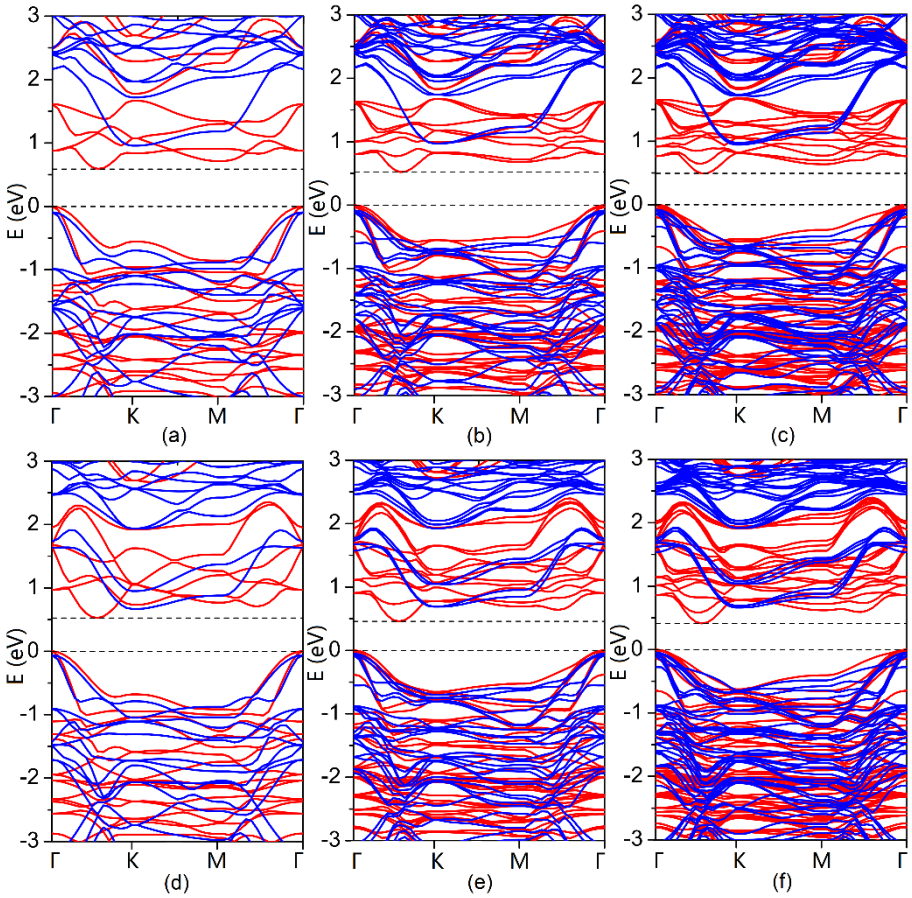

Fig. S2. Band structure for (a) monolayer, (b) bilayer and (c) trilayer $CrSiTe_3$ nanosheets with PBE+U+VDW functional. (d), (e), (f) are for $CrGeTe_3$ nanosheets.

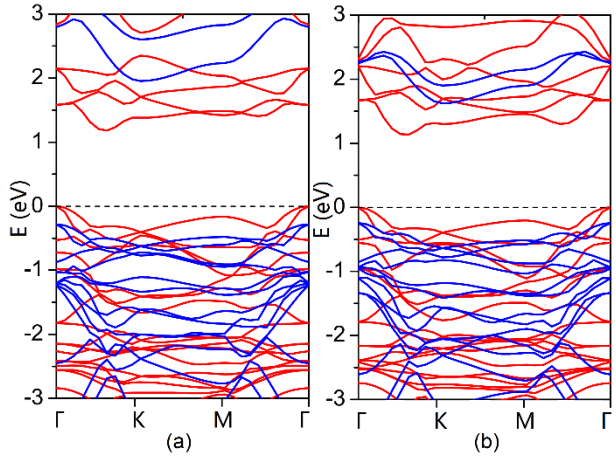

Fig. S3. Band structure for 2D (a) $CrSiTe_3$ and (b) $CrGeTe_3$ under 5% tensile strain calculated with HSE06 functional.

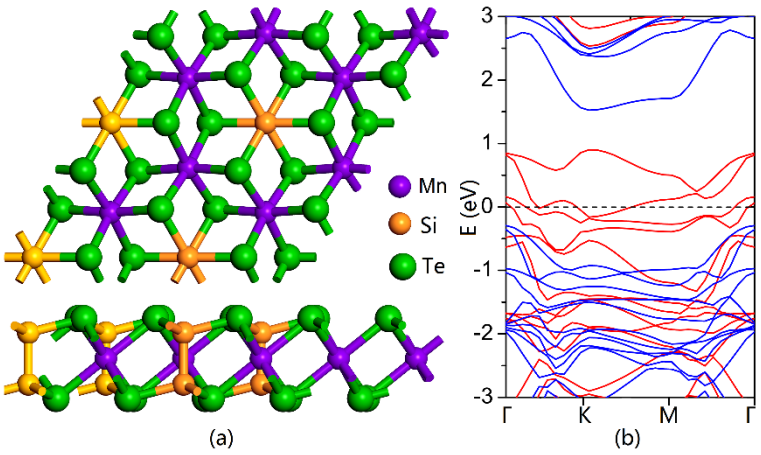

Fig. S4. (a) Optimized structure and (b) band structure for 2D $MnSiTe_3$ with HSE06 functional.

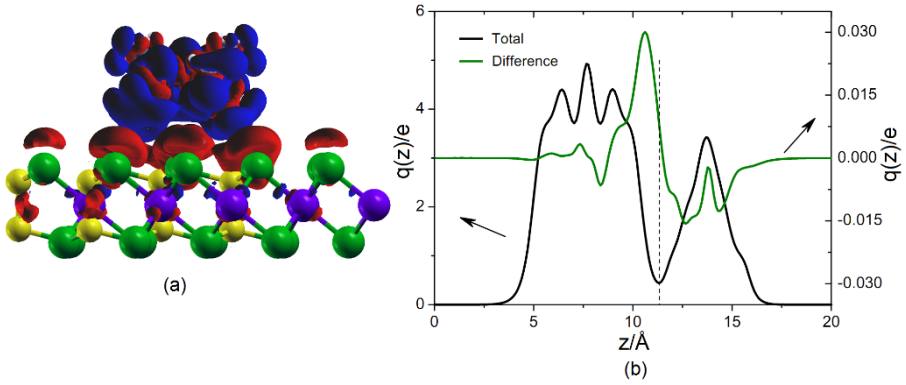

Fig. S5. (a) The spatial distribution of difference charge density defined as $\rho_{diff} = \rho_{CrSiTe_3+TDAE} - \rho_{CrSiTe_3} - \rho_{TDAE}$ plotted with an isovalue of 0.002e/Å^3. Red and blue indicate positive and negative values, respectively. (b) The charge averaged along Z direction q (z) for the total charge (black line) and difference charge (green line) of TDAE-$CrSiTe_3$ adsorption system. The vertical dotted line shows a spatial partitioning of TDAE and $CrSiTe_3$, to which integration of difference charge q_{diff} (z) from z= 0 gives an amount of 0.38e.

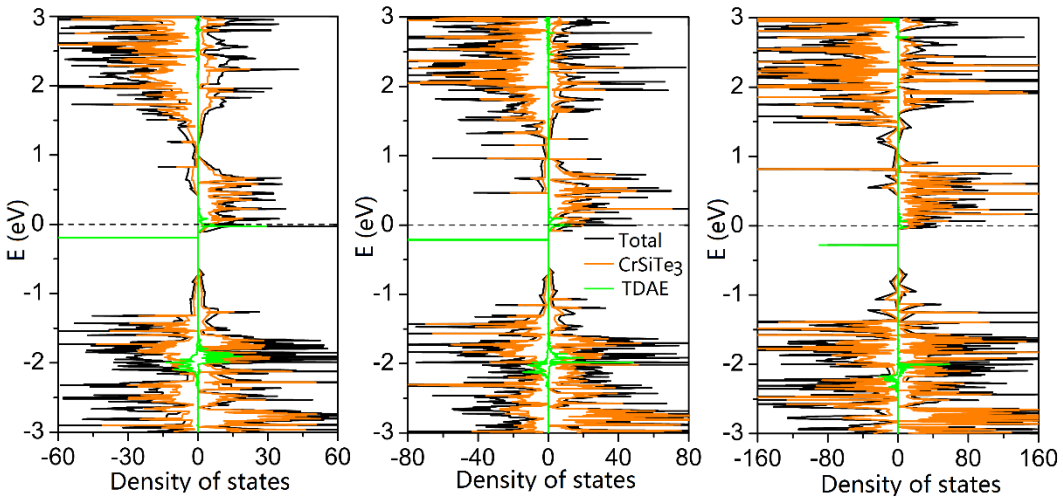

Fig. S6. Density of states for 2D $CrSiTe_3$ adsorbed by (a) 1/3, (b) 1/4 and (c) 1/9 monolayer of TDAE molecules. Half-metallicity is robust under different adsorption concentrations.