Supplementary Information

Stacking induced symmetry broken and gap opening in Dirac half-metal MnF_3

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Table. S1 Calculated formation energies of MnF_3, MnF_4 and Mn_2F_5 along with this work and QOMD data.

System	This work (E_f)	OQMD data[1]
MnF_3	–1.93 eV	–2.74 eV
MnF_4	–1.78 eV	–2.49 eV
Mn_2F_5	–2.13 eV	–2.69 eV

1 S. Kirklin, J. E Saal, B. Meredig, A. Thompson, J. W Doak, M. Aykol, S. Rühl and C. Wolverton, *npj Computational Materials*, 2015, 1, 15010.

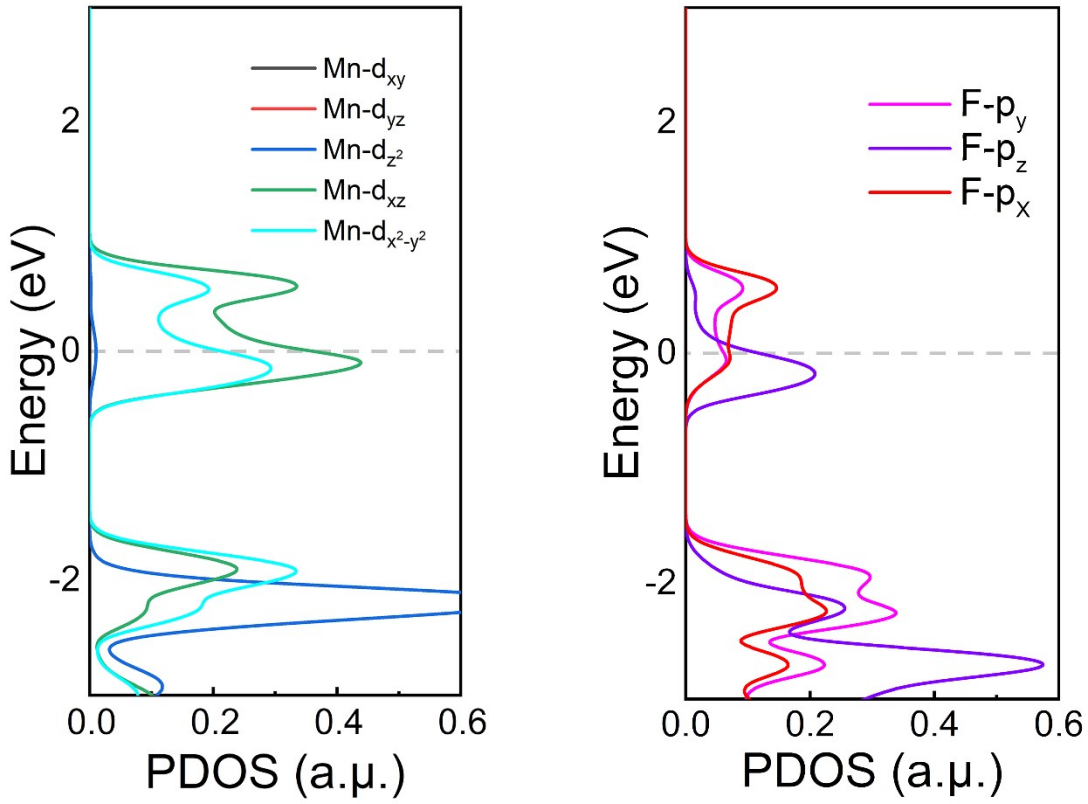

Fig. S1. PDOS of the spin-up channel in monolayer MnF_3.

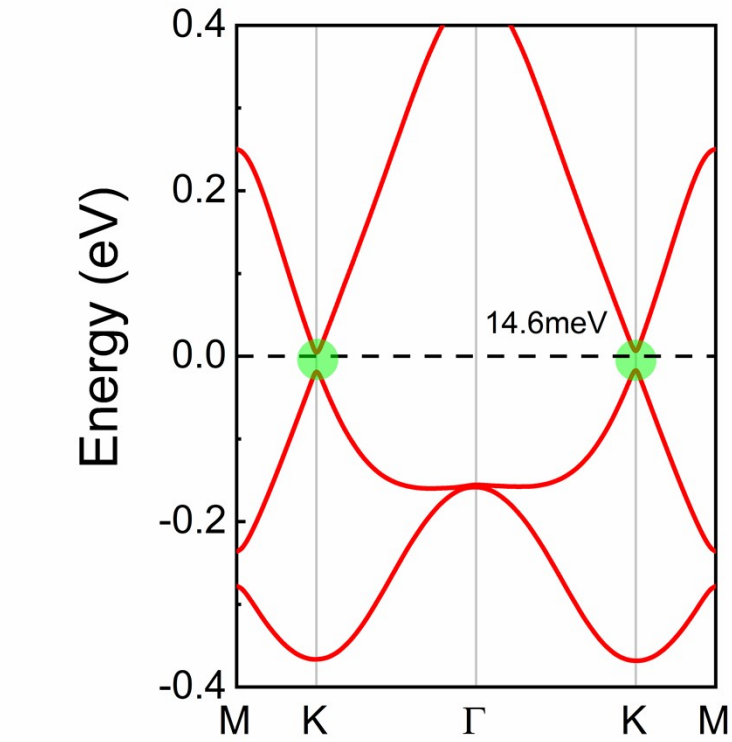

Fig. S2 Band structure of the spin-up channel in monolayer MnF_3 with considering SOC.

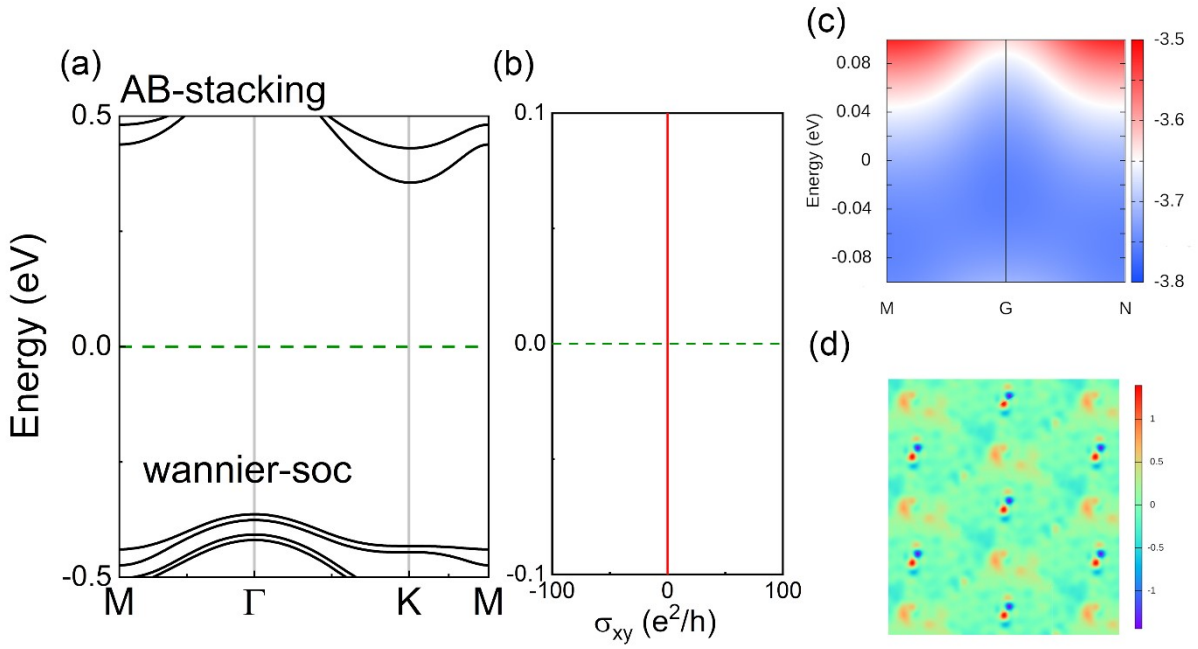

Fig. S3 (a) Band structure of AB-stacking MnF_3 bilayer calculated using the MLWFs method with SOC. (b) The corresponding anomalous Hall conductivity (σ_{xy}), (c) edge state of a semi-infinite sheet, and (d) the Berry curvature with SOC.

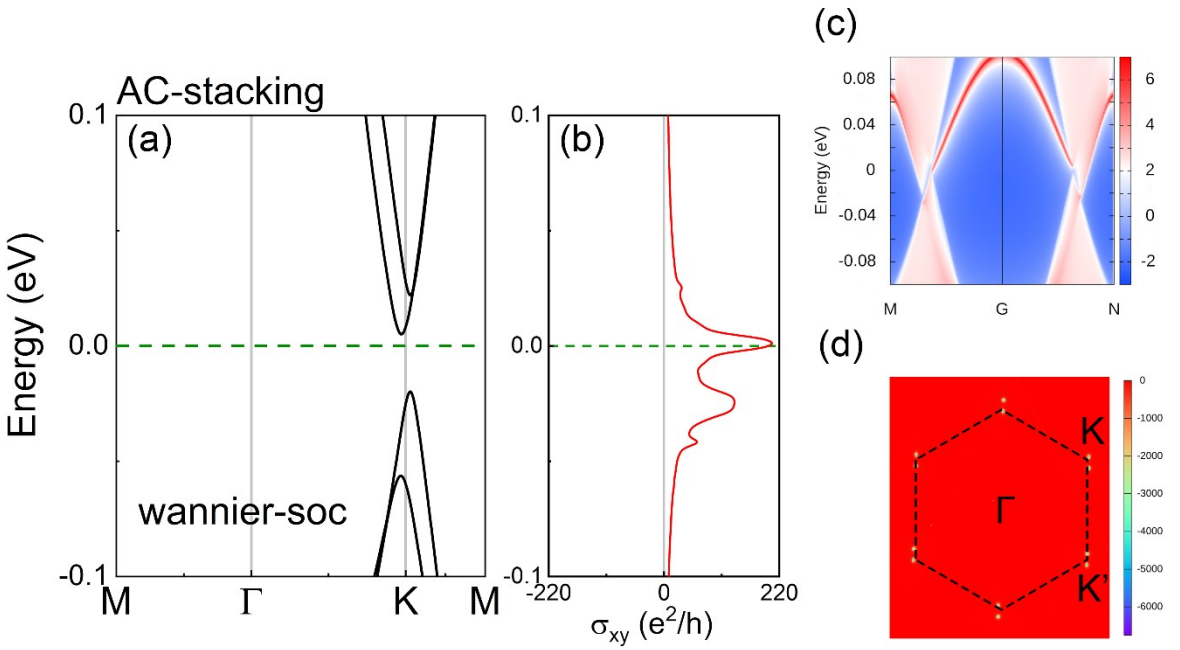

Fig. S4 (a) Band structure of AC-stacking MnF_3 bilayer calculated using the MLWFs method with SOC. (b) The corresponding anomalous Hall conductivity (σ_{xy}), (c) edge state of a semi-infinite sheet, and (d) the Berry curvature with SOC.