Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Materials for Mn_2C Monolayer: A 2D Antiferromagnetic Metal with High Néel Temperature and Large Spin-Orbit Coupling

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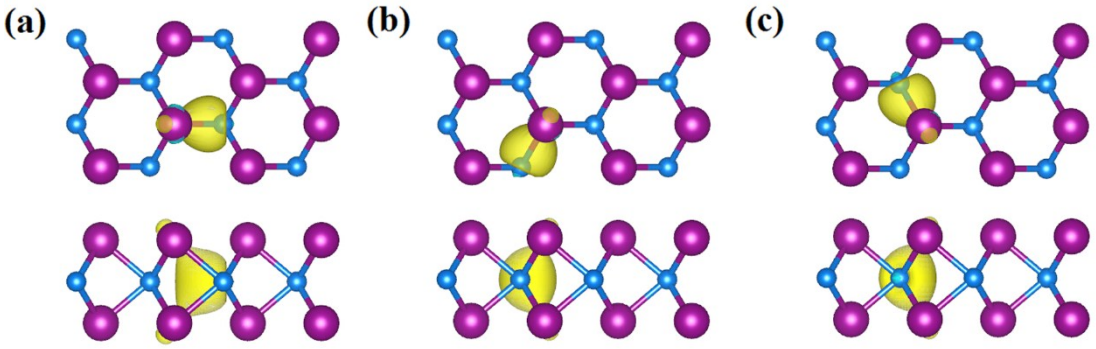

Figure S1. Bonding structure of the Mn2C monolayer. (a-c) Individual 3c-2e σ bonds of both top view (top) and side view (bottom). Mn atom is purple, and C atom is gray, respectively.

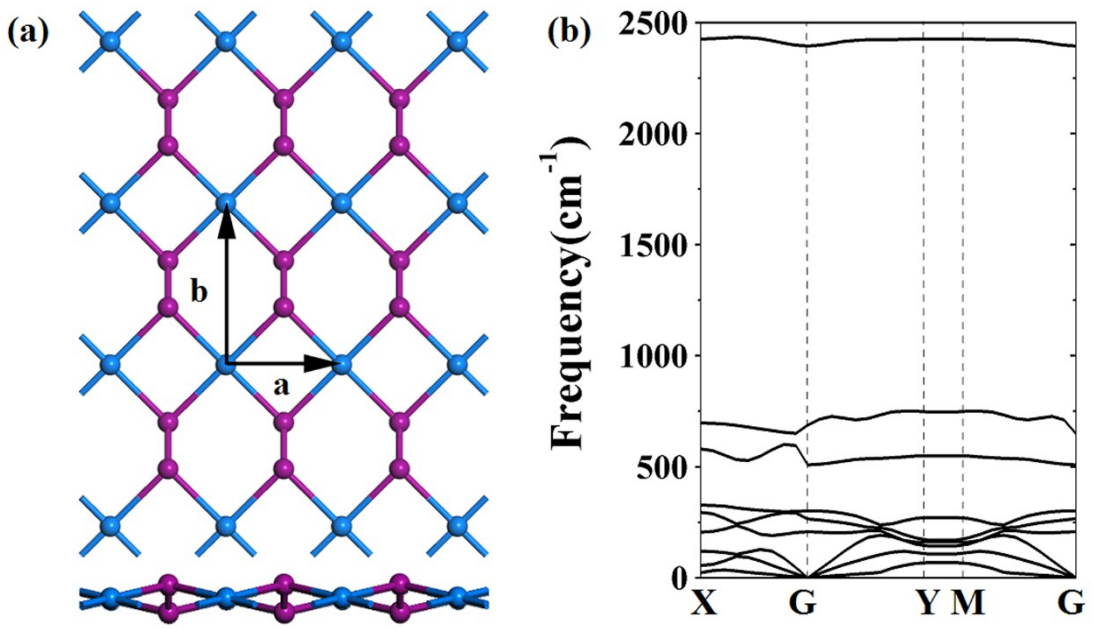

Figure S2. (a) Geometric structure of Mn_2C-II monolayer of top view (top) and side view (bottom). Mn atom is purple, and C atom is blue, respectively. (b) Phonon spectrum of Mn_2C-II monolayer. X (1/2, 0.0, 0.0), G (0.0, 0.0, 0.0), Y (0.0, 1/2, 0.0), M (1/2, 1/2, 0.0) refer to the special points in the first Brillouin zone.

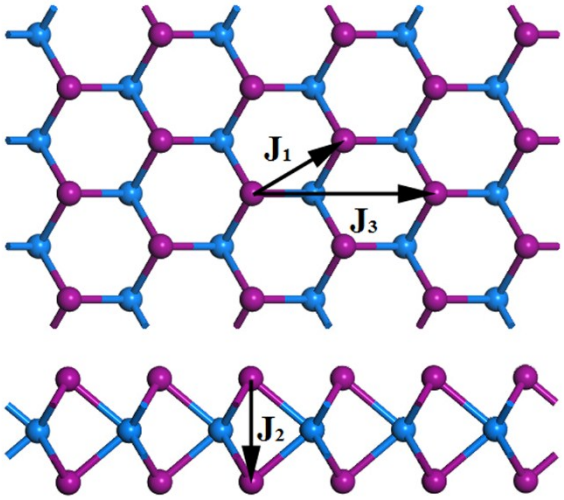

Figure S3. Nearest(J_1,$J_{i,j}$), next-nearest(J_2) and next-next-nearest(J_3) exchange interactions of the Ising model.

$E(FM)=(6J_1+3J_3+J_2)M^2$,

$E(AFM\text{-}a)=(-2J_1+2J_3+J_2)M^2$,

$E(\text{AFM-b})=(2J_1-2J_3+J_2)M^2$,

$E(\text{AFM-c})=(6J_1+2J_3-J_2)M^2$.

So, $J_1=J_{i,j}=3$meV, $J_2=0.56$ meV, $J_3=0.86$ meV.