Supplementary Information for

Zr_2Si: An antiferromagnetic Dirac MXene

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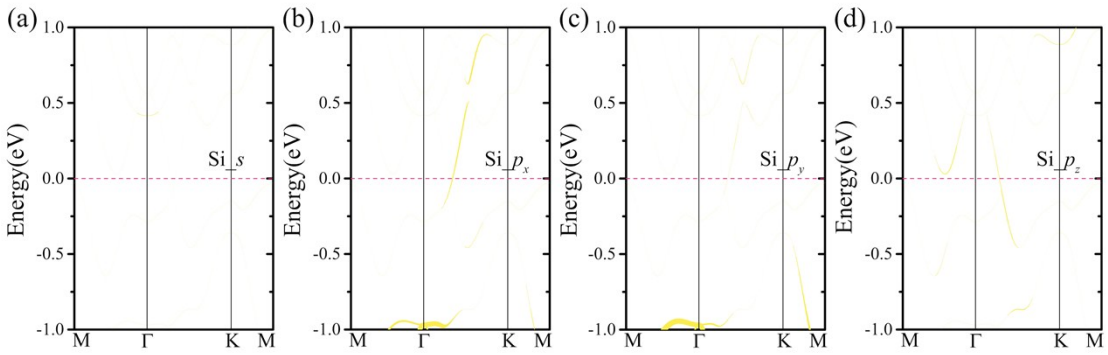

Figure S1. The orbital-resolved electronic band structures projected onto the Si of the middle plane.

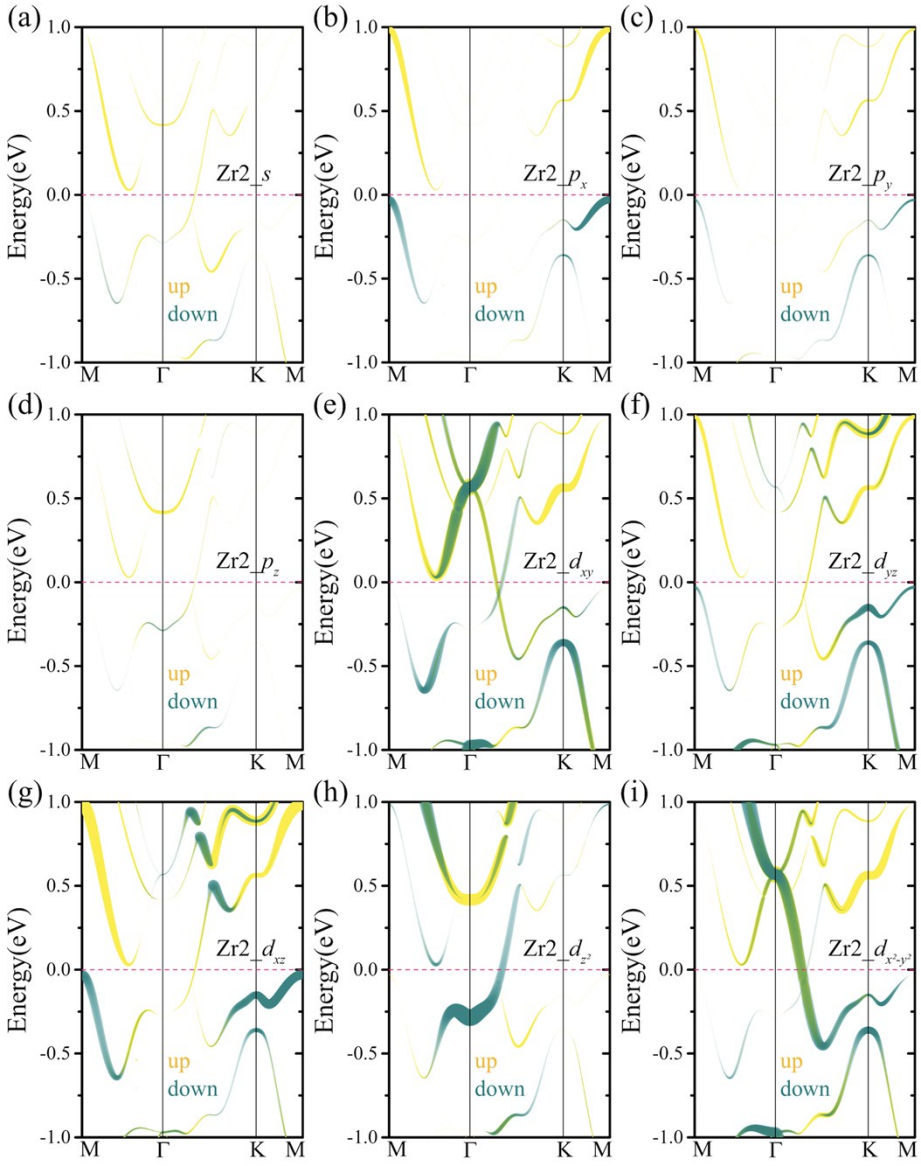

Figure S2. The orbital-resolved electronic band structures projected onto the Zr of the down plane (Zr2).

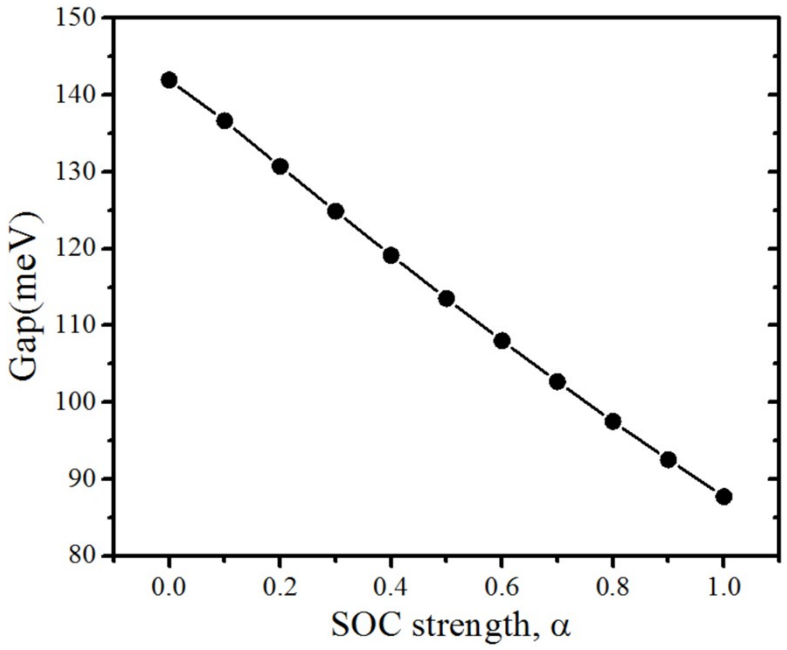

Figure S3. Variation of the band gap as a function of strength of spin-orbit coupling (SOC). The strength of SOC is tuned artificially by a factor of α ($0 \leq \alpha \leq 1$). The SOC is switched off as α =0, while α =1 corresponds to the real SOC strengh. U = 4.0 eV was used throughout the calculations.

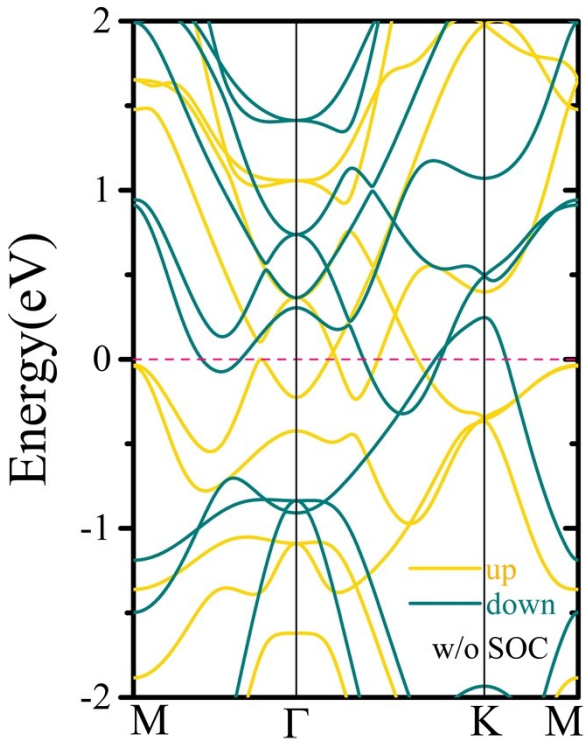

Figure S4. Band structure of the ferromagnetic (FM) Zr_2Si calculated without spin-orbit coupling (SOC). The band lines of two spin channels are indicated by yellow (spin up) and blue (spin down) lines. The energy of the Fermi level is set to zero.