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

Supplementary Material

Alkali metal doped two dimensional Janus $Cr_2Br_3I_3$ monolayers with quantum anomalous Hall effect

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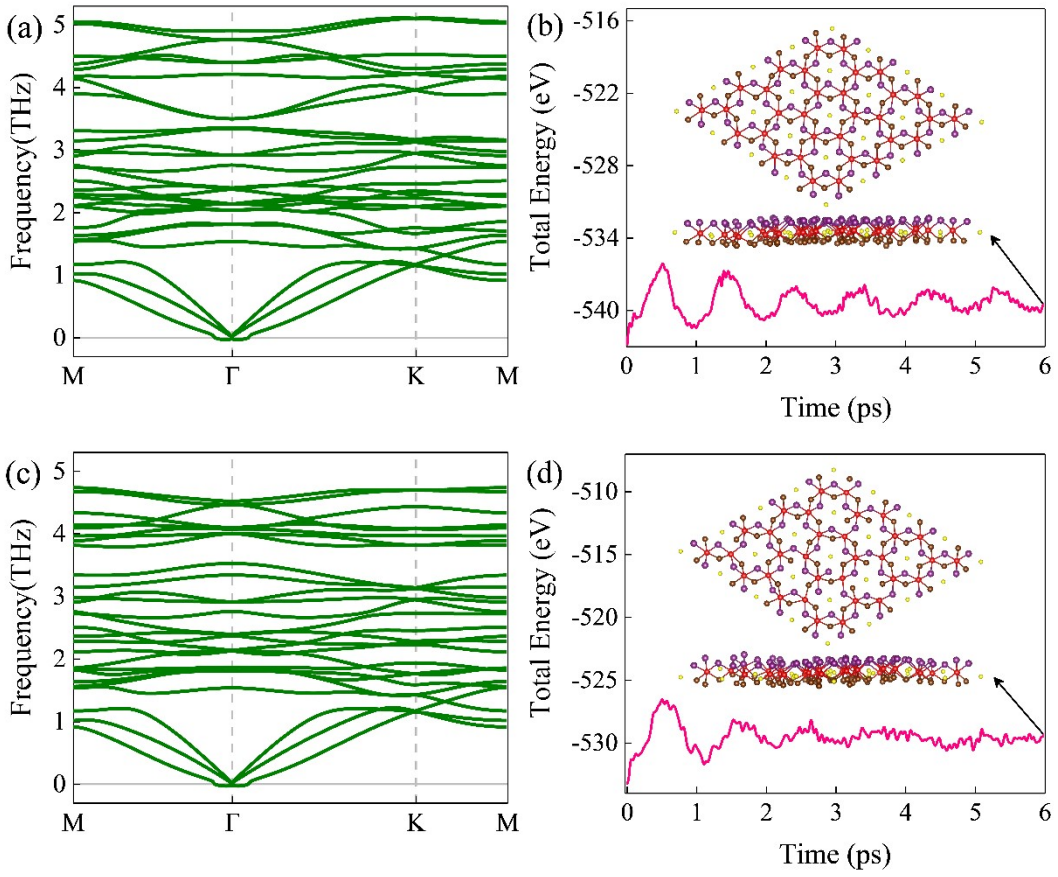

Fig. S1 The phonon dispersion spectra of the (a) Li- and (c) K doped ML $Cr_2Br_3I_3$. Total energy fluctuation at AIMD simulations of the (b) Li- and (d) K doped ML $Cr_2Br_3I_3$. The insets in (b) and (d) shows snapshots of the Li- and K doped ML $Cr_2Br_3I_3$ at 6 ps.

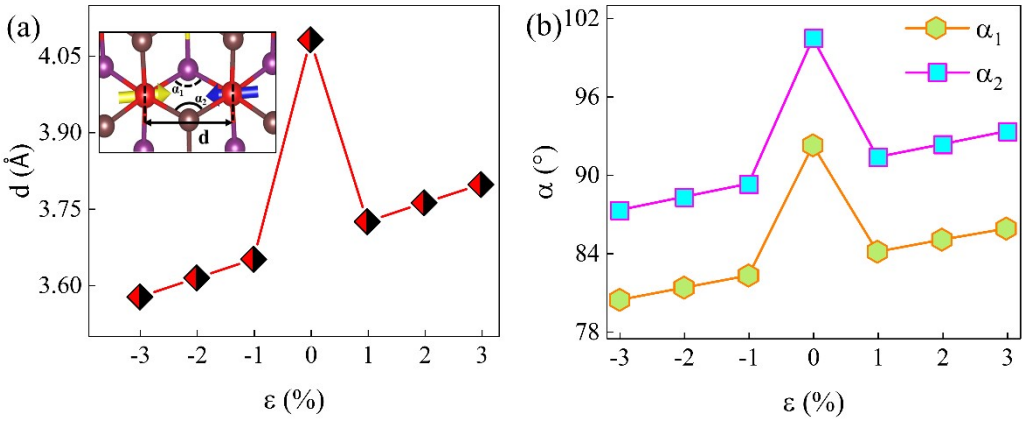

Fig. S2 (a) The strain dependence of the distance between two Cr atoms. (b) The strain dependences of α_1 angle for Cr-I-Cr and α_2 angle for Cr-Br-Cr. The insert shows the d, α_1, and α_2.

The strain dependence of the distance (d) between two Cr atoms is drawn in Fig. S2(a). The d significantly enlarges when ε is from -1% to 0%. As shown in Fig. S2(b), both the angles of α_1 and α_2 also suddenly increase from -1% to 0%. The results clearly prove the enhancement of FM superexchange interaction. Therefore, the change of d, α_1, and α_2 under various strains likely induces a sharp change of energy difference at ε = 0 through affecting the magnetic interactions in Figs. 2(a) through 2(c).

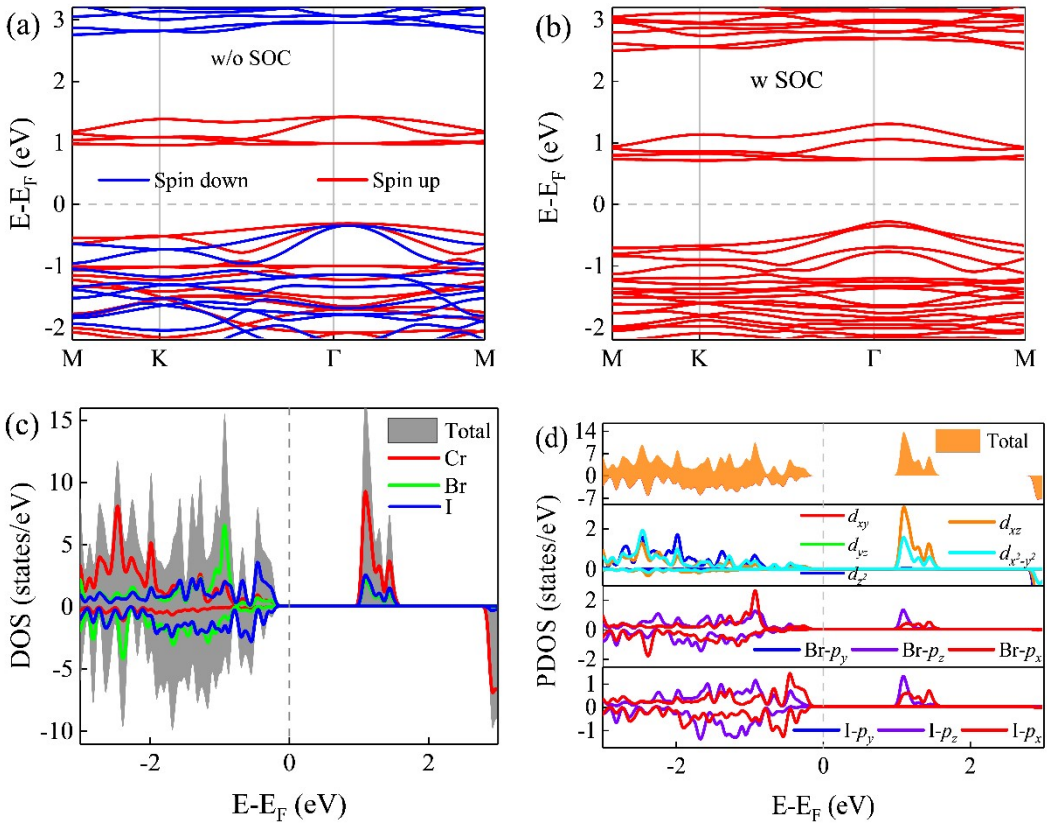

Fig. S3 Band structures of pristine ML $Cr_2Br_3I_3$. (a) without SOC. (b) with SOC. Density of states (DOS) and Projected density of states (PDOS) of pristine ML $Cr_2Br_3I_3$.

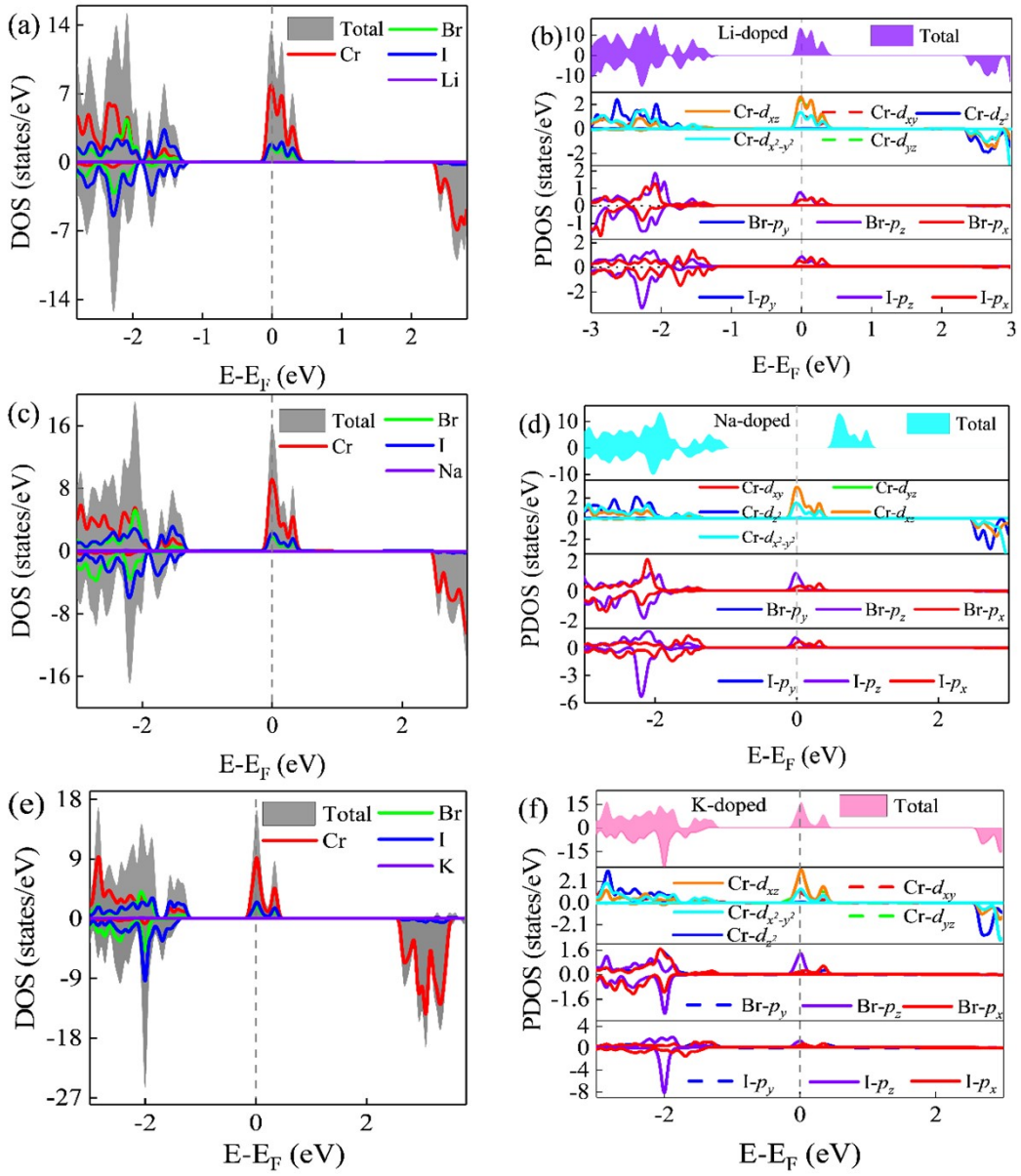

Fig. S4 DOS of (a) Li doped, (c) Na doped, and (e) K doped ML $Cr_2Br_3I_3$. PDOS of (b) Li doped, (d) Na doped, and (f) K doped ML $Cr_2Br_3I_3$.

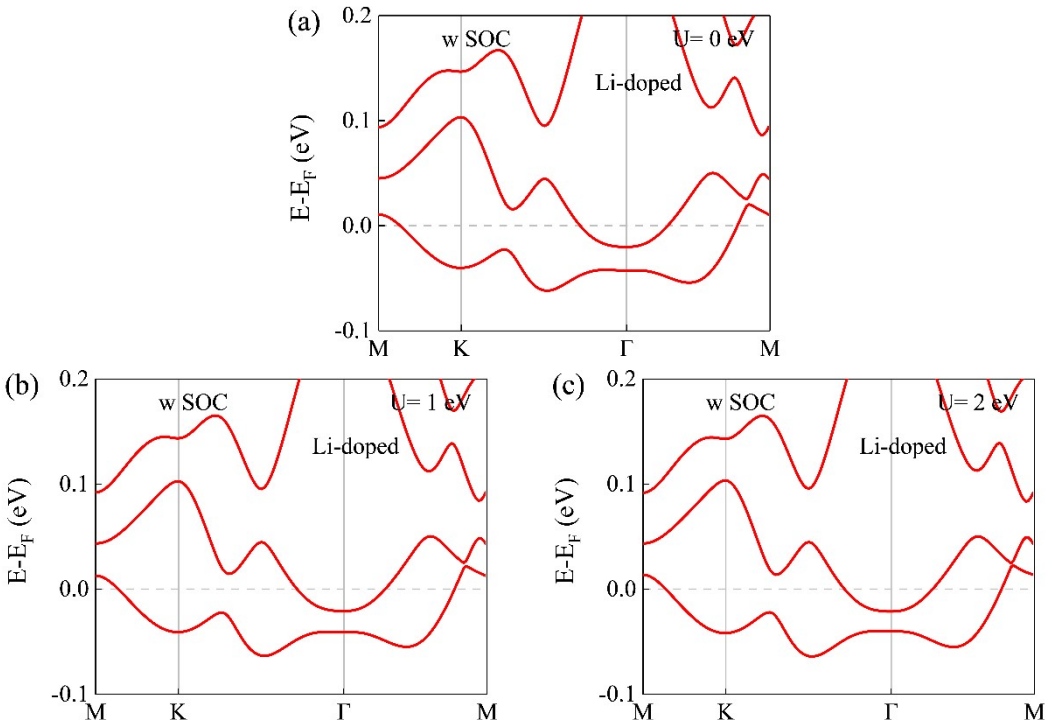

Fig. S5 Band structures of Li doped ML $Cr_2Br_3I_3$ with SOC at different U values. (a) U = 0 eV. (b) U = 1 eV. (c) U = 2 eV.