Supporting Information (SI)
Exploring room-temperature anti-ferromagnetism in newly predicted 2D MBene M_4B_6 (M: Cr, Mn, Fe) monolayer using first-principles calculations

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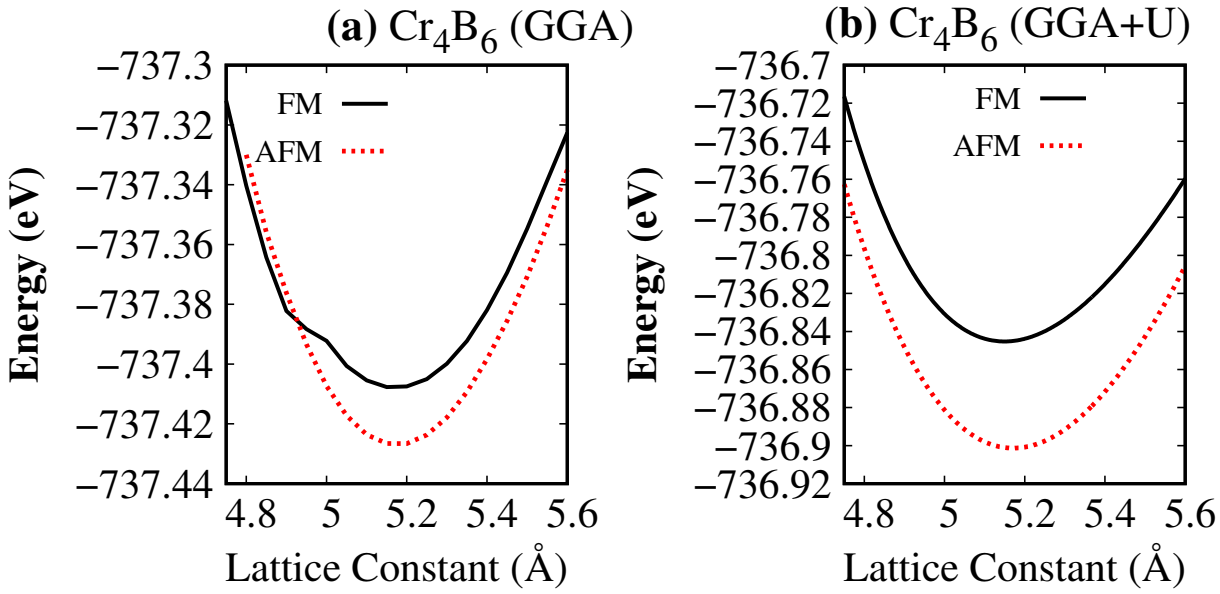

Figure SI 1: Total energy vs. lattice constant for both the FM and AFM states under each method (a) GGA and (b) GGA+U for a Cr_4B_6 monolayer. The solid black line represent the FM state, while the red-dashed line indicate the AFM state.

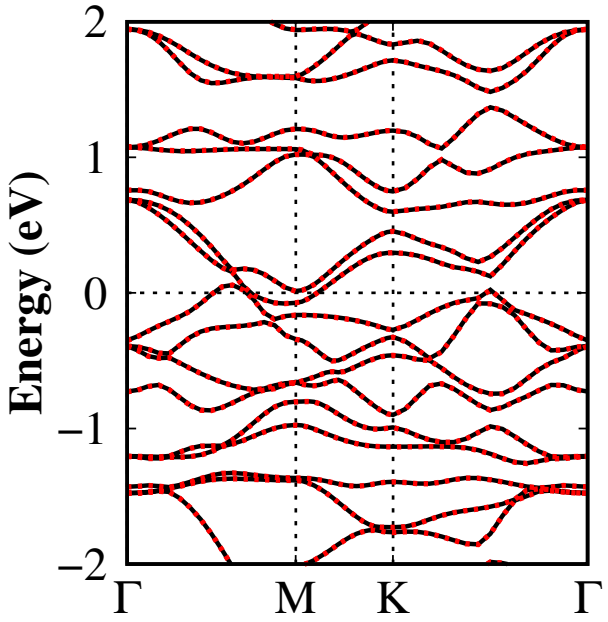

Figure SI 2: GGA+U calculated electronic band structure of Cr_4B_6 monolayer at equilibrium lattice constant in most stable AFM state. The solid black and red-dashed lines indicate the spin-up and spin-down channels, respectively. The horizontal dashed line at zero represents the Fermi-energy level.

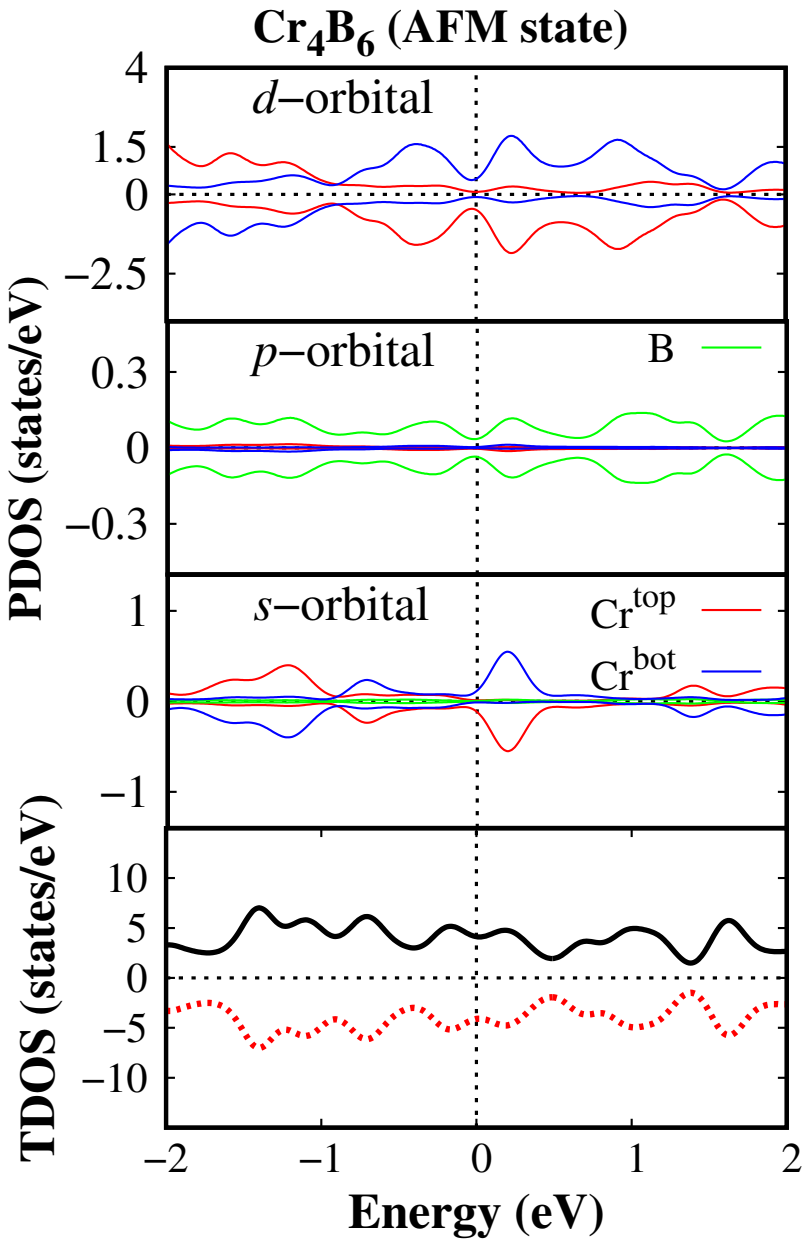

Figure SI 3: GGA+U calculated spin-polarized TDOS and PDOS for Cr_4B_6 monolayer at equilibrium lattice constant in most stable AFM state. The solid black and red-dashed lines indicate the spin-up and spin-down channels, respectively. The horizontal dashed line at zero represents the Fermi-energy level.