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Supplementary Information: Ferromagnetic TM_2BC (TM=Cr, Mn) monolayers for spintronic devices with high Curie temperature

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1 Linear response approach

We used linear response approach formulated by Cococcioni et al.[1], as implemented in the Quantum Espresso package[2], to evaluate the U parameter in this work. In the linear-response scheme calculations, we first compute x_0 and x which represent the non-interacting (bare) and interacting density response functions of the system with respect to localized perturbations, as displayed in Fig. 6. The parameter U_{eff} is then obtained from the expression: $U_{eff} = (x_0^{-1} - x^{-1})$. The calculated U_{eff} values for t-Cr_2BC and t-Mn_2BC are 4.36 eV and 3.19 eV, respectively.

2 Magnetic configurations

Top and side views of the schematic illustration of the considered magnetic orientations are given in Fig. 7. To obtain the individual total energy of these three magnetic orientations ionic positions and cell volume are allowed to change with the suitable initial magnetic configuration. At the end of first optimization cell shape is corrected if it is destroyed, and re run for the ionic optimization.

3 Thermal stability

The thermal stability was evaluated at 300 K and 600 K using 3×3 supercell of the t-TM_2BC sheets based on AIMD simulations. There is not noticeable structural destruction (see Fig. 8), which indicates the good thermal stability of t-TM_2BC sheets above the room temperature.

4 Monte Carlo calculations

Magnetic features of the t-TM_2BC sheet have been examined by Monte Carlo (MC) simulation based on Metropolis algorithm[3,4]. We have considered a $2D$ square lattice with a lateral dimension of $L \times L$ $(L = 240)$ by applying periodic boundary conditions in x and y directions. The single-spin-tilt trials are carried out by Marsaglia algorithm[5]. MC simulations are launched with random initial configurations of magnetic moments at high temperatures. Then, temperature is gradually decreased with a temperature step of ΔT and at every temperature step, initial configuration is considered as the the final configuration of the previous temperature step. We have calculated several thermodynamic quantities such as total magnetization, magnetic susceptibility and specific heat during the simulations. One can refer to our recent paper for the definitions of these observables[6]. The thermal averages of the thermodynamic quantities are obtained by considering the 2×10^5 MC steps per site (MCSS) after discarding the first 4×10^4 MCSS for thermal equilibrium process. We have carried out 100 independent computer experiments corresponding to different initial configurations. Error bars are calculated by benefiting from by jackknife method[5].

Mermin-Wagner theorem states that isotropic two dimensional (2D) magnetic systems do not exhibit ordered phase and an effect, for instance magnetic anisotropy, is required for 2D materials to demonstrate magnetism. The Hamiltonian, which describes t-TM2BC sheets (Eq. 5 in the main text), is 2D anisotropic Heisenberg Hamiltonian and one expects an ordered phase below the Curie temperature of the system. As the reviewer stated, exchange interaction constants of both systems are much larger than magnetic anisotropy constants. We present the temperature dependence of the components of the magnetization in the Fig. 5. As one can see from the figure, x- and y-component of the magnetization (M_x and M_y) takes values close to zero even below the Curie temperature. On the other side, the contribution to the total magnetization (which is shown in the main text (manuscript) as Figure 5 (a) and Figure 5 (d)) comes from the z-component, M_z. Moreover, we have performed test MC calculations to analyze the magnetization profile when the magnetic anisotropy constant is taken as zero for t-Mn_2BC sheet in Fig. 6. It can be seen that the magnetization of the system has no preferred direction and an ordered phase cannot be observed for all the magnetization components. These findings indicate that small uniaxial anisotropy along the z direction is sufficient to favor the alignment of magnetic moments through the z direction and for the observation of ferromagnetism in the both systems.

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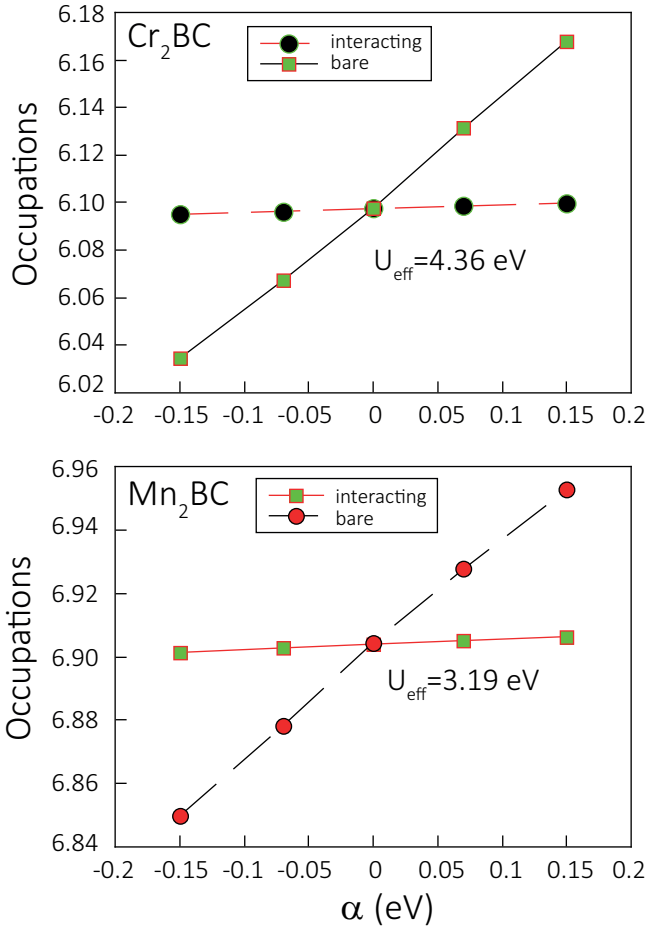

Fig. 1 Linear response of d orbital occupations as a function of potential shift α. The curves depicted by the squares and circles lines are labeled bare and interacting. The inverse response functions are deduced numerically by calculating the slope of the curves. x_0 follows from the slope of curve bare, whereas x from the slope of curve interacting.

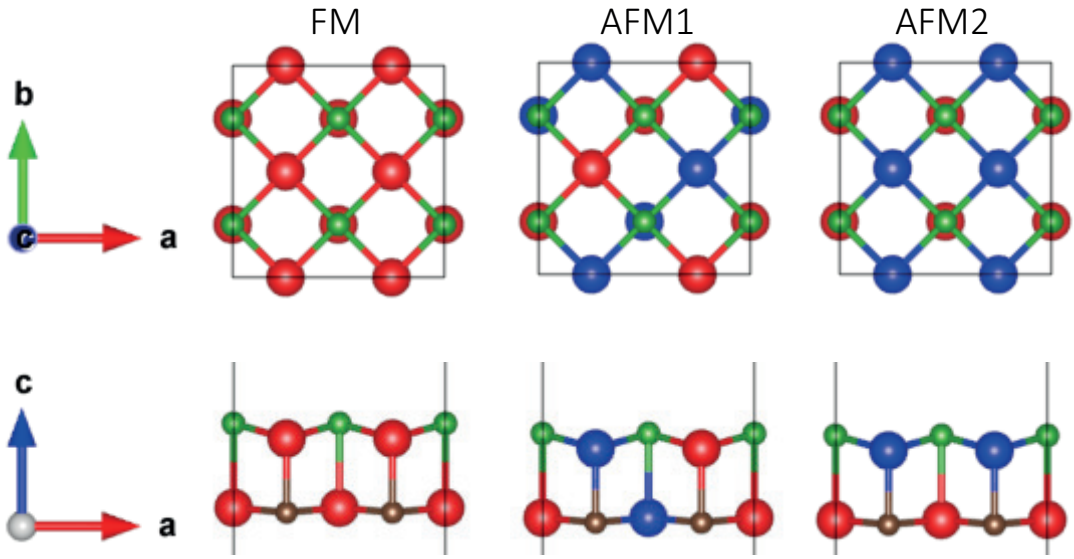

Fig. 2 Top and side views of geometric structures of an FM and two different AFM1 AFM2 states for both t-Cr_2BC, and t-Mn_2BC sheets. Red and blue color denote the spin-up and spin-down, respectively.

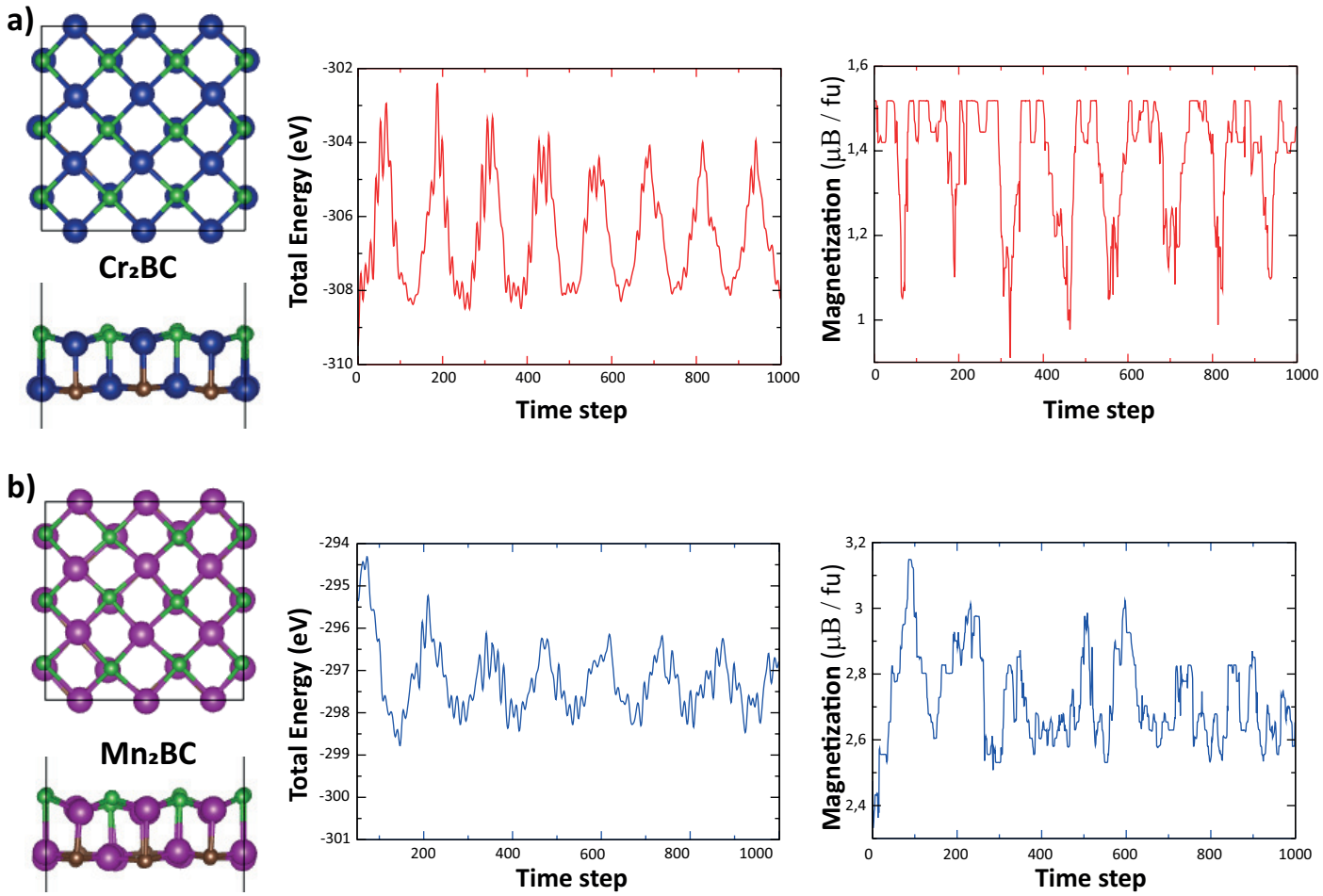

Fig. 3 Top and side view 3×3×1 supercell structures of a) t-Cr_2BC and b) t-Mn_2BC sheets under a Nose-Hoover thermostat at 600 K. In addition, total energy versus time step and magnetic moment per formula unit (fu) versus time step also illustrated.

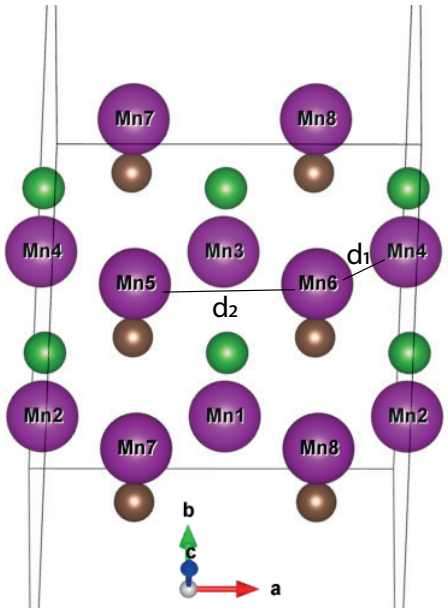

Fig. 4 A typical example of slanted top view spin configuration for estimating the exchange-interaction constants for t-Mn_2BC sheets. d_1 and d_2 denote the first and second nearest neighbor respectively.

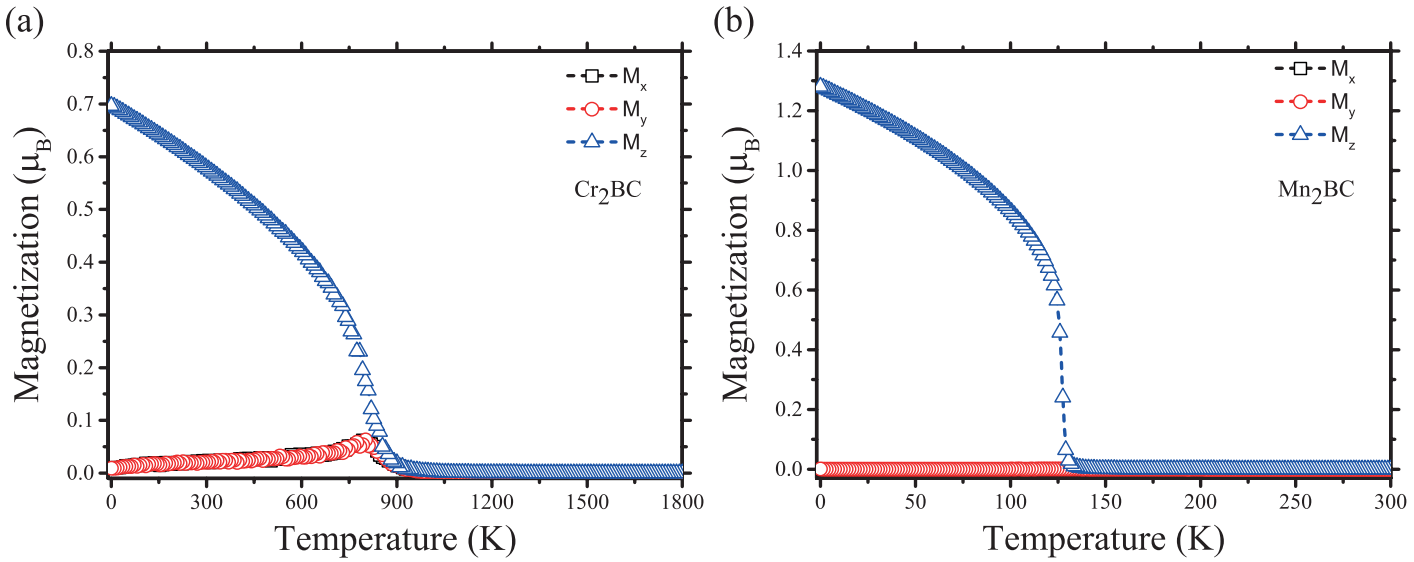

Fig. 5 Temperature dependence of components of magnetization (M_x, M_y and M_z) for (a) t-Cr_2BC and (b) t-Mn_2BC.

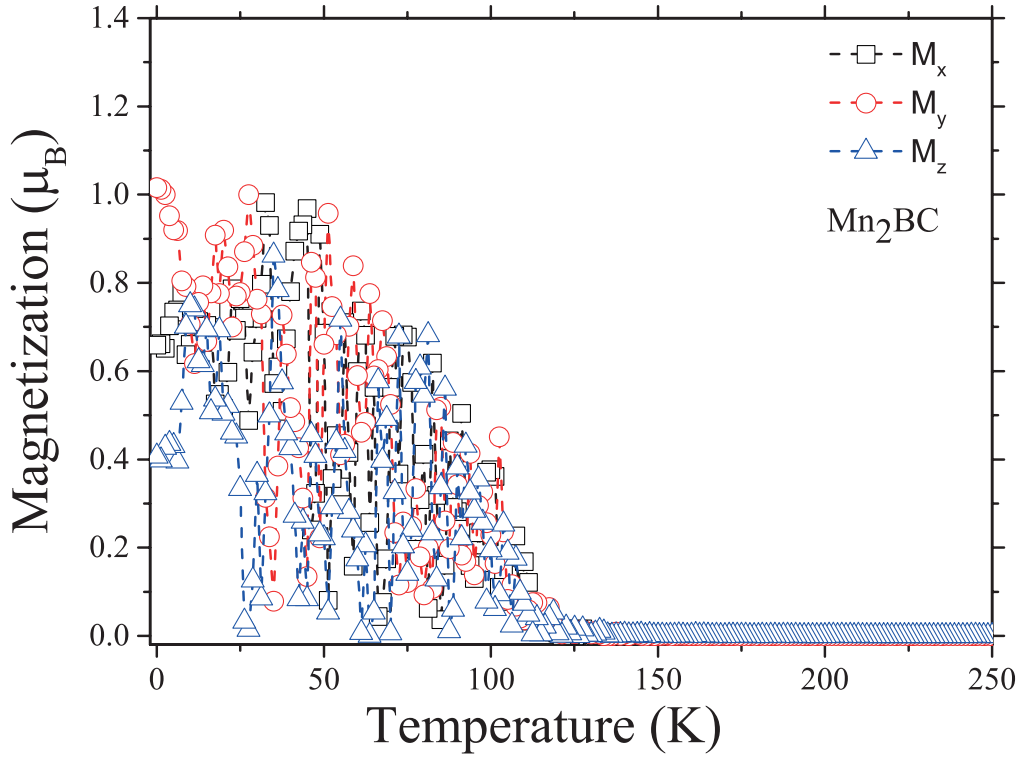

Fig. 6 Temperature dependence of components of magnetization (M_x, M_y and M_z) for t-Mn_2BC when the magnetic anisotropy constant is taken as zero.

Notes and references

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