Supporting Information for 'Novel two-dimensional ferromagnetic semiconductors: Ga-based transition-metal trichalcogenide monolayers'

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The phonon band along the Γ-Y direction of the AFM-Z configuration in $CrGaTe_3$ monolayer and the biggest imaginary mode are shown in Fig. S1. The largest instability mode is located at the K-point (0, 0.33, 0), which involves the collective vertical vibration and the relative in-plane vibration of the atoms in the two sides. Accordingly, we have optimized the 1 × 3 supercell but not found a lower energy atomic structure in AFM-Z phase, demonstrating the AFM-Z state is a local energy minimum point and the substrate may support the stability of the AFM-Z configuration.

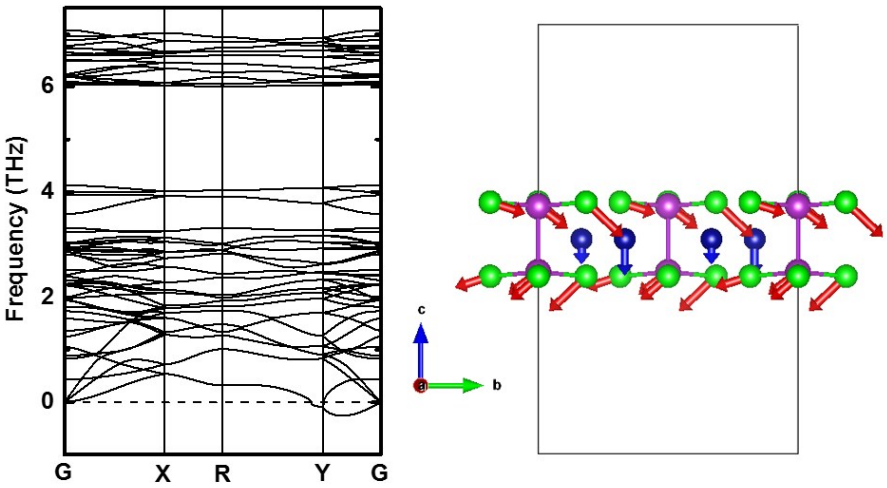

Fig. S1 (a) Phonon dispersion curve of $CrGaTe_3$ monolayer in AFM-Z configuration.

(b) Displacement vectors of the biggest imaginary mode in the K-point (0, 0.33, 0).

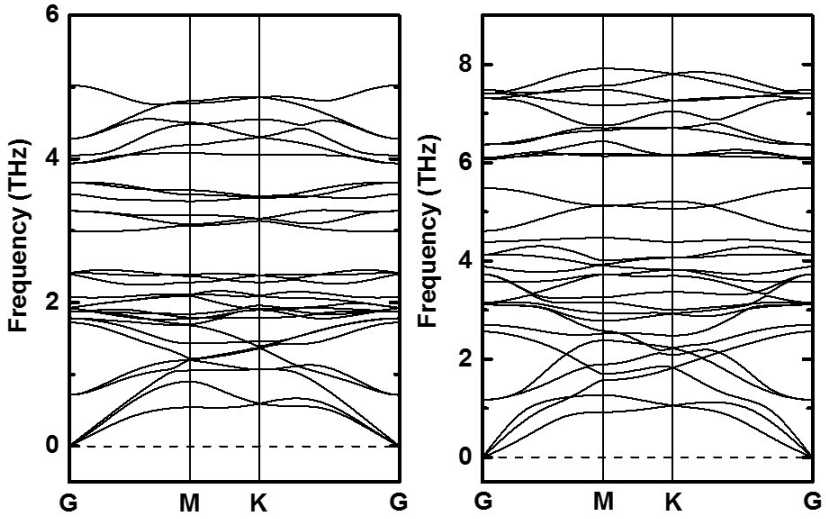

Fig. S2 Phonon band structures of ferromagnetic monolayer (a) $CrGaTe_3$ and (b) $CrGaSe_3$ under 5% tensile strain

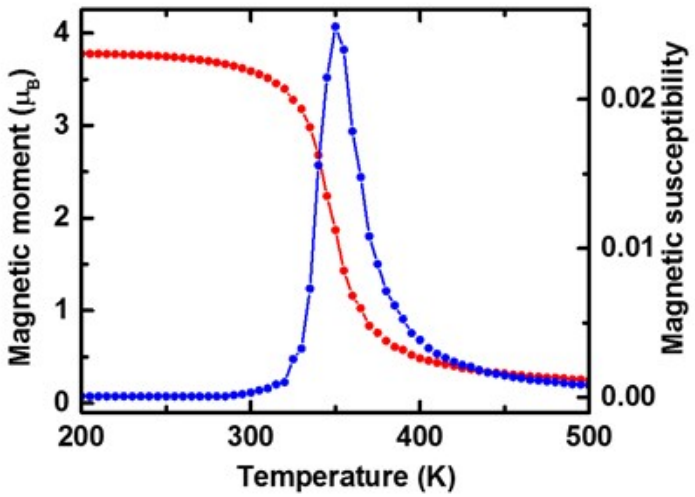

Fig. S3 The magnetic moment per Cr atom and magnetic susceptibility of $CrGaTe_3$ monolayer as a function of temperature under 8% tensile strain.