Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for Intrinsic ferromagnetism in two-dimensional 1T-MX_2 monolayers with tunable magnetocrystalline anisotropy

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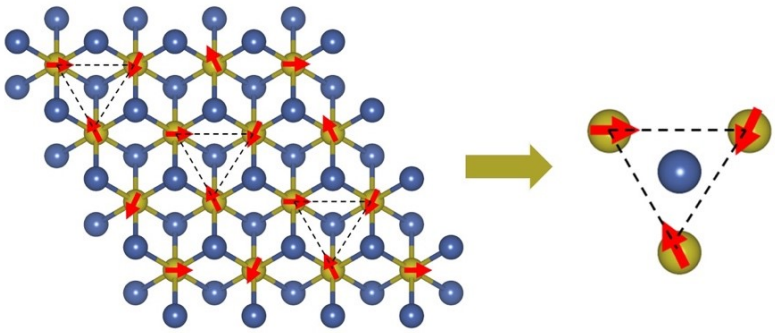

Figure S1. Noncollinear antiferromagnetic configuration of the 1T-MX_2 monolayer constructed. The yellow and blue spheres denote M and X atoms, respectively. These red arrows represent spin vectors of the three atoms and are at 120◦ to each other.

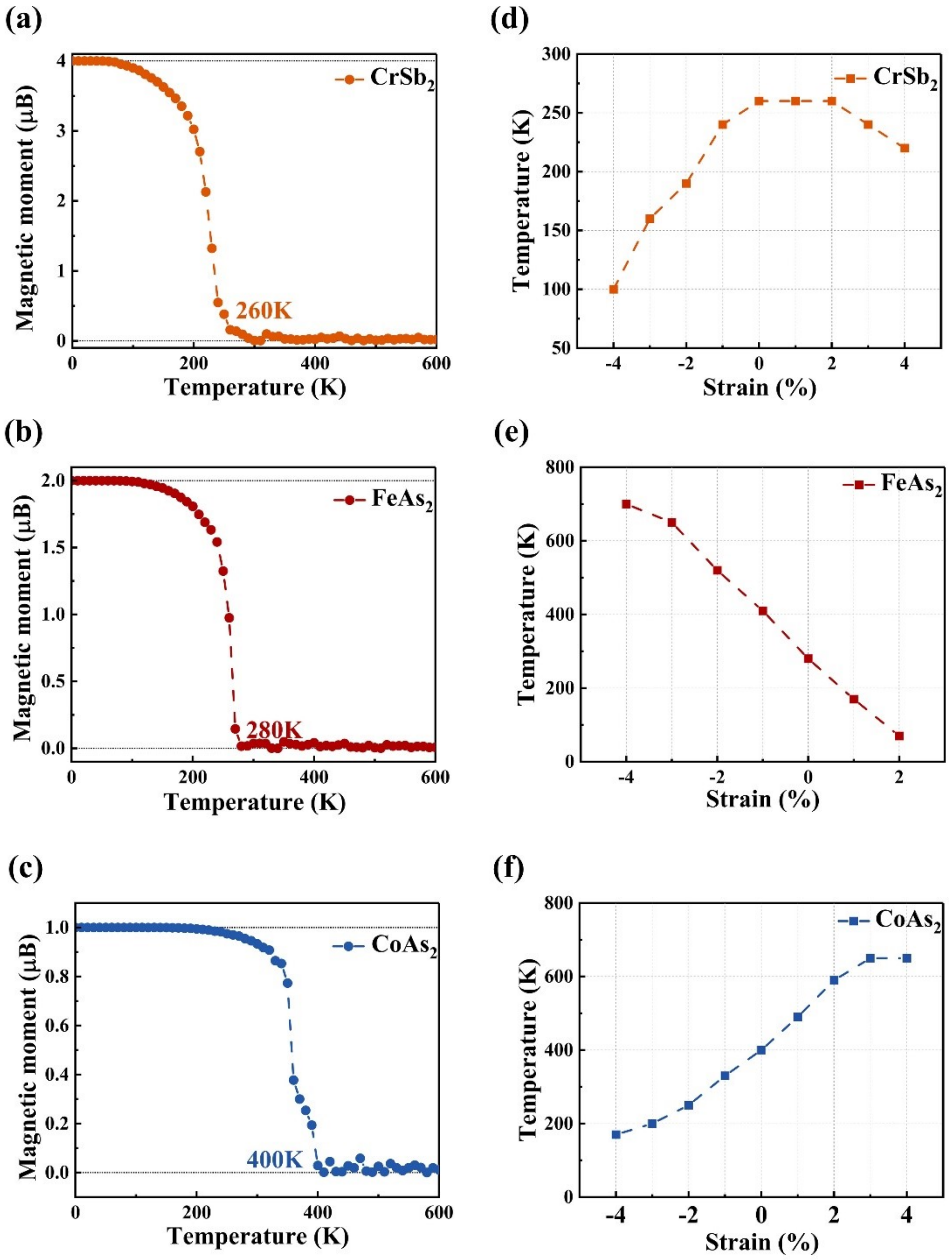

Figure S2. The magnetic moments of the (a) 1T-$CrSb_2$, (b)1T-$FeAs_2$ and (c)1T-$CoAs_2$ monolayers as a function of temperature. (d-f) The corresponding strain dependence of Curie temperature for the three FM monolayers.

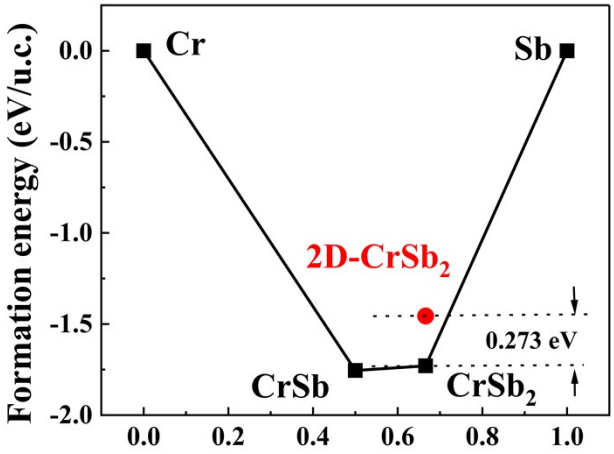

Figure S3. Calculated formation energy convex hull for Cr-Sb systems. The elemental reference states are taken from its bulk (bcc-Cr, trigonal-Sb). The stable intermediate phases of Cr-X systems are selected from the databases of Materials Project[1] (https://materialsproject.org/materials).

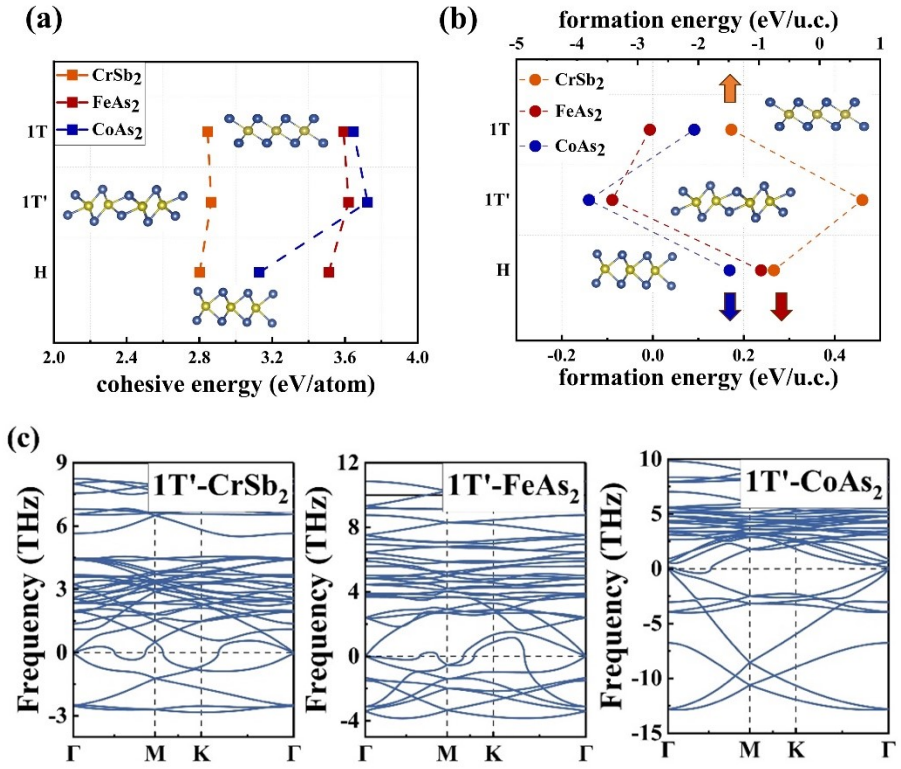

Figure S4. The calculated cohesive energy (a) and formation energy (b) of three representative 2D MX_2 crystals where the insets show their corresponding crystal

structures. The arrows indicate the energy range of the three materials. (c) The phonon spectrum of three 2D materials with 1T' phase.

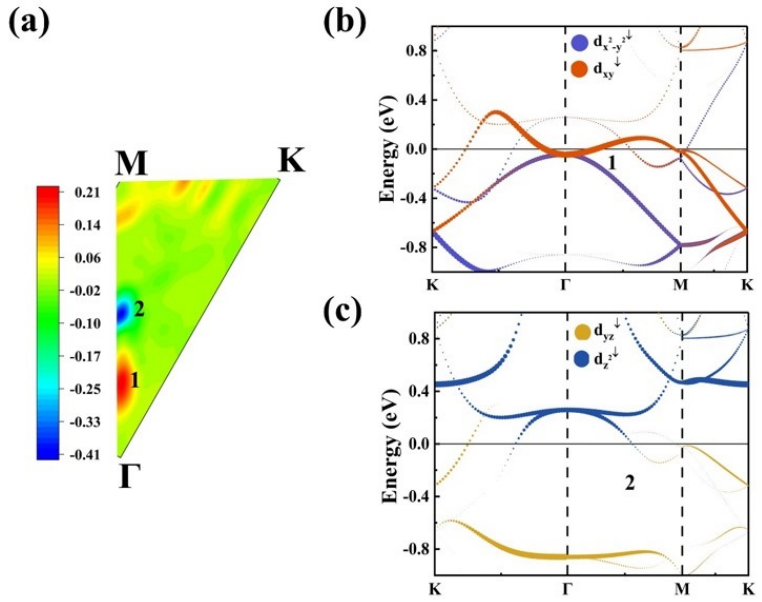

Figure S5. (a) The k-resolved MCA (in erg/cm^2) in the 2D BZ for 1T-$CoAs_2$. Energy- and k-resolved distributions of (b) d_{xy} *and* $d_{x^2-y^2}$ orbitals and (c) d_{yz} and d_{z^2} of the minority-spin bands along the symmetry directions for Co atom. The numerals represent the k-points where the MCA has large positive or negative contributions.

1. A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, K. A. Persson, Commentary: The Materials Project: a materials genome approach to accelerating materials innovation. APL Mater. 2013, **1**, 011002.