Electronic Supplementary Information for

1T-CrO_2 Monolayer: A High-Temperature Dirac Half-Metal for High-Speed Spintronics

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I. SNAPSHOT OF 1T-CRO_2 AFTER PERFORMING AIMD SIMULATIONS

We perform the molecular dynamics simulation in 300 K and the snapshots are presented in the following figures. We find the 2D CrO_2 can still preserved under this temperature. We further perform the molecular dynamics simulation in 600 K and the results are presented in the following Figure S1(b)(c). We find the 2D CrO_2 can also keep well under this temperature.

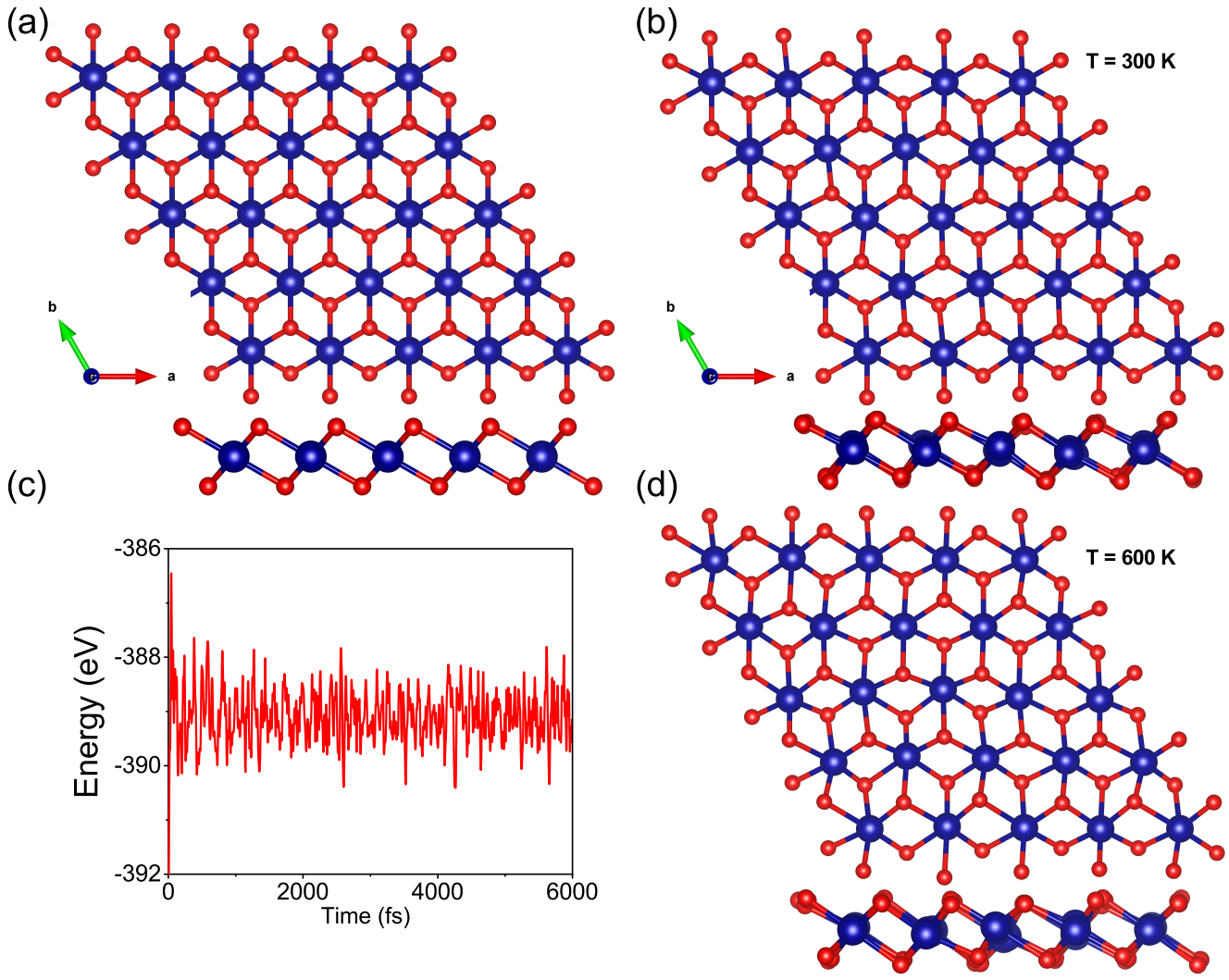

Figure S1: Snapshots of 1T-CrO_2 before and after performing AIMD Simulations and energy evolution of 600 K.

II. SYMMETRY OPERATORS OF 1T-CRO_2 AND ITS COUNTERPART IN FIRST BRILLOUIN ZONE.

For 1T-CrO_2, the point group of K or K' are C_{3v}, and the C_3 operator in this group protect the Dirac point D_1 in Figure 4(a) of main manuscript. The operator C_2 with the rotation axis Γ-K or Γ-K' protect the Dirac point D_2.

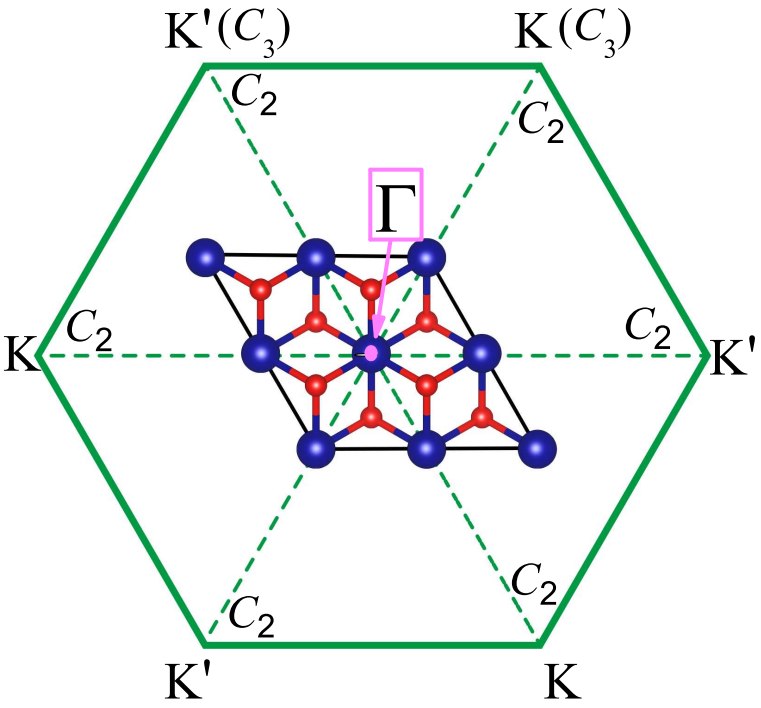

Figure S2: Symmetry operators of 1T-CrO_2 and its counterpart in first Brillouin zone.

III. ENERGY BAND STRUCTURE WITH ±4% IN-PLANE EXTERNAL STRAIN.

The energy band structures of 1T-CrO_2 with the ±4% biaxial strain are shown in Figure S3. We find the Dirac cones are still preserved near the Fermi level under external strain.

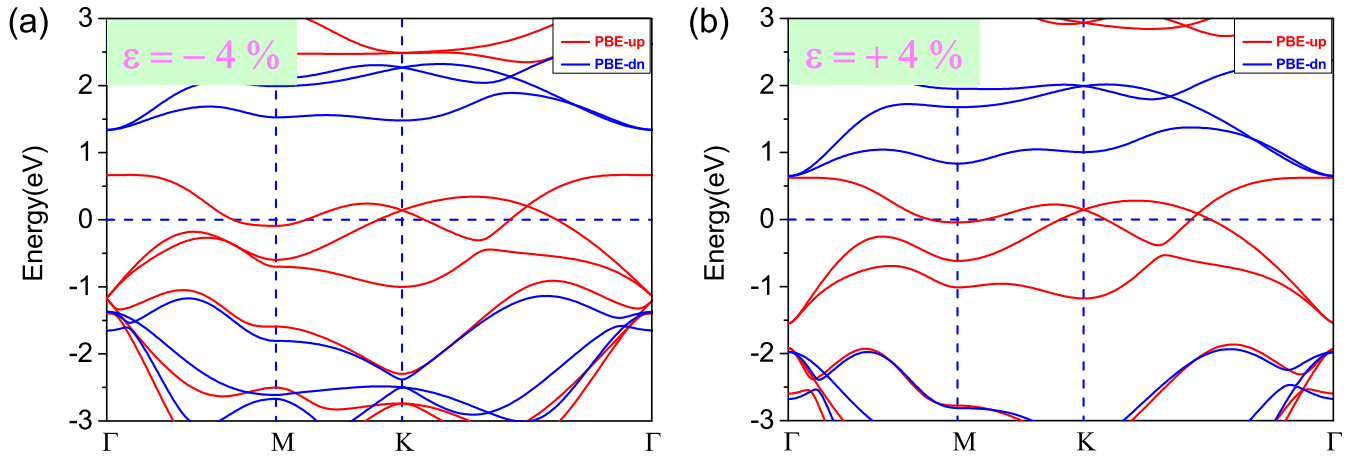

Figure S3: Band structures of 1T-CrO_2 under the biaxial strain ±4%.

IV. ENERGY BAND STRUCTURE WITH DIFFERENT HUBBARD U

To estimate the correlation effects to our electronic state, we calculate the energy band structure with GGA + U method. We chose a broad range of U_{eff} from 0 eV to 5 eV to allow a detailed examination of the correlation effects on electronic structure of this system. The results are presented in Figure S4. We find the DHM characteristics of 1T-CrO_2 monolayer is robust to the electronic correlation effect.

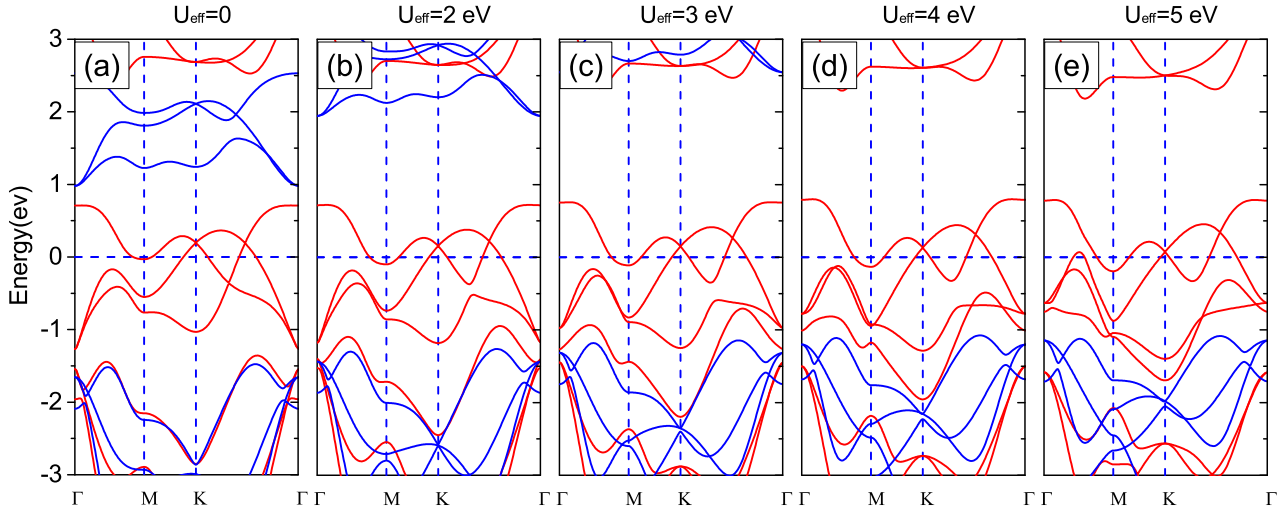

Figure S4: Band structure from DFT + U. (a)-(e) represent the spin-polarized energy bands structure with U_{eff} = 0, 2, 3, 4 and 5 eV.

V. MAGNETIC ORDER AND T_c UNDER IN-PLANE EXTERNAL STRAINS

The exchange constant J should depend on strain because it can change the interactions between different atoms. In figure S5, we present the values of J with different biaxial strains and corresponding Curie temperatures from Monte Carlo simulations. We find the magnetic ground states of 1T-CrO_2 alway keep ferromagnetic in the range -10% to 10%. No obvious change is observed for the the values of J and Curie temperature between -5% and 10%. A evident decrease happen from -5% to -10% for the values of J.

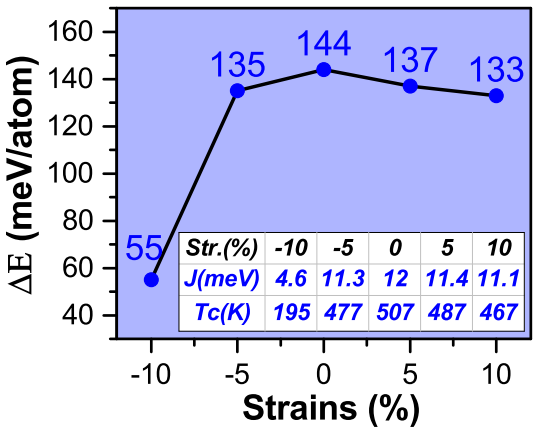

Figure S5: The $\triangle E$ under in-plane biaxial external strains and it's corresponding J and T_c of FM states.

VI. RELATIONSHIPS OF STRESS AND STRAINS

The stress-strain diagram under only tensile strains.The stress is suddenly changed at the strain of 20%. It is indicated that 20% is the elastic limit of 2D CrO_2. That is to say this material can keep its original stable structure when the strain is not beyond 20%.

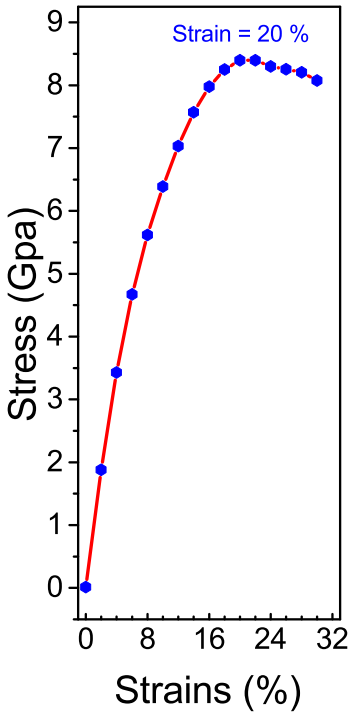

Figure S6: Stress-strain diagram of 1T-CrO_2.

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