Electronic Supplementary Material (ESI) for Nanoscale.
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Supporting Information:

Nonvolatile electrical control of 2D $Cr_2Ge_2Te_6$ and intrinsic half metallicity in multiferroic hetero-structures

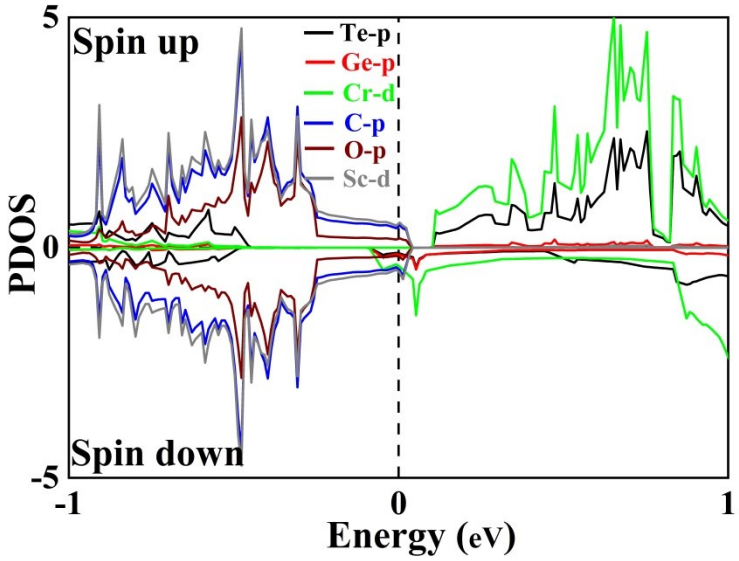

Fig. S1. (Color online) The PDOS of monolayer CGT/SCO P↓ hetero-structures with respect to Fermi level E_f is depicted. The contribution of the different components are shown with different colors.

We calculate the band structure using HSE06 functional[31] which opens up the band gaps (**see Fig. S2**). But we believe that the intrinsic half metallic character present in the CGT/ SCO P↓ is still valid, after doing the following analysis. The HSE06 hybrid functional takes into account all nonlocal exchange interactions regarding p orbital, in addition to the localized d orbital. But some time in real situation this may not work. Because in experiment the non-local correlation associated with the p orbital may suppress significantly due to many factors. In such cases the experimental band gap for a material highly deviates from that predicted by HSE calculations. For example, the experimentally reported band gap for the freestanding CGT is about 0.5 eV[41]. But this gap increases to 0.93 eV, if calculated with HSE06 hybrid functional which is far higher than the experimental value. Interestingly, the value of the band gap (0.29 eV for free-standing CGT) we calculated at PBE level is more close to the experimentally reported value. Therefore the band gaps predicted by PBE+U calculations are more reliable in our case. The deviation between PBE and HSE06 hybrid functional happens only in the determining the

electronic properties of CGT/SCO P↓, where the former leads to half metal while the later leads to semiconductor with a band gap of 0.15 eV (**see Fig. S2c**). The states of the majority spin channel in VB regarding CGT/SCO P↓ marginally miss (by 0.08 eV) to cross the Fermi level as shown in the **Fig S2c**. If the above analysis regarding the band gap of free-standing CGT is considered, then it is more likely for the majority spin channel to cross the Fermi level in order to preserve its half metallicity. However it is a test for experimentalist to confirm and resolve this issue.

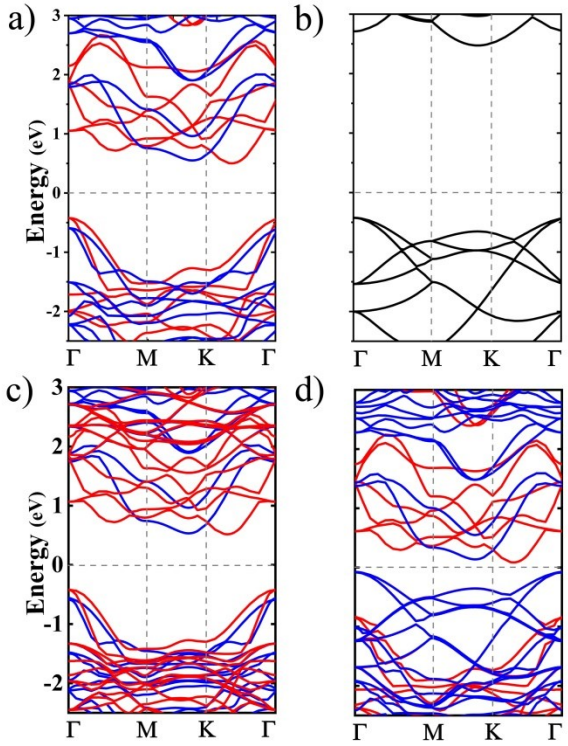

Fig. S2. (Color online) Electronic band structures of a) CGT, b) MXene SCO, c) CGT/SCO P↑ hetero-structures, and d) CGT/SCO P↓ hetero-structures. The Fermi level E_f is set at zero. Red and blue lines denote the contributions from spin-up (S↑) and spin-down (S↓) channels, while black lines represent the contributions of the MXene SCO.

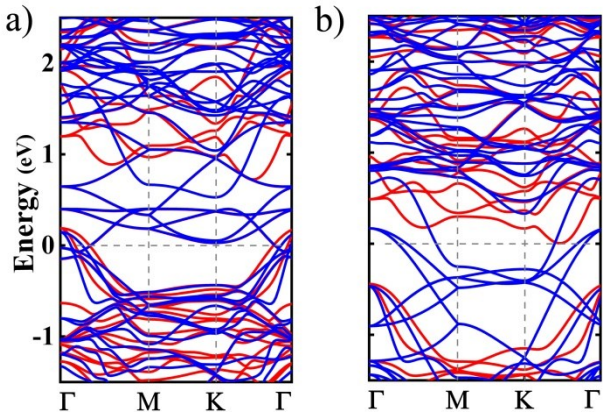

Fig. S3. (Color online) Electronic band structures of a) CGT/bilayer-SCO P↑ hetero-structures, and b) CGT/bilayer-SCO P↓ hetero-structures with respect to Fermi level E_f. Red and blue lines denote the contributions from spin-up (S↑) and spin-down (S↓).

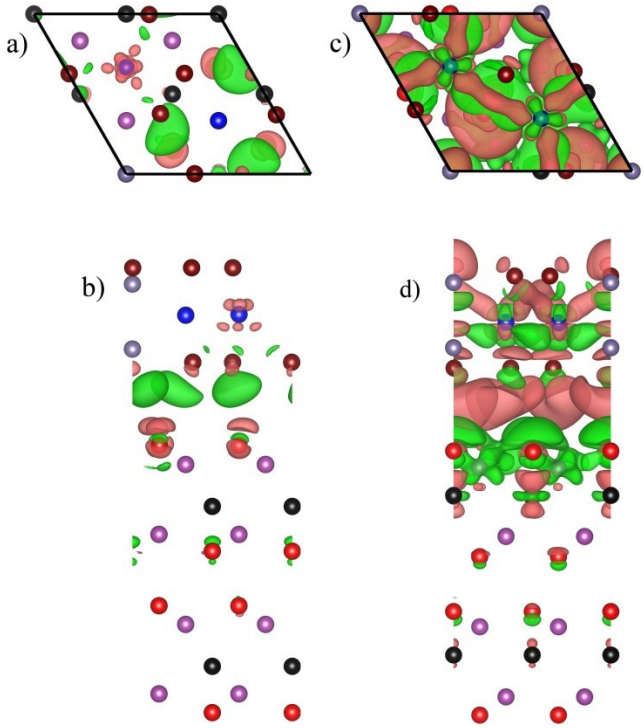

Fig. S4. (Color online) Top and side of the differential charge density of the CGT/bilayer-SCO P↑ is shown in a) and b), while that of CGT/bilayer-SCO P↓ is depicted in c) and d). The green color represents charge depletion whereas pink color represents charge accumulation. The Cr, Ge, Te, Sc, C, and O atoms are denoted by blue, silver, gray, pink, black and red balls respectively.