Supporting Information

Significant tunneling magnetoresistance and excellent spin filtering effect in CrI_3-based van der Waals magnetic tunnel junctions

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Supplementary Figures

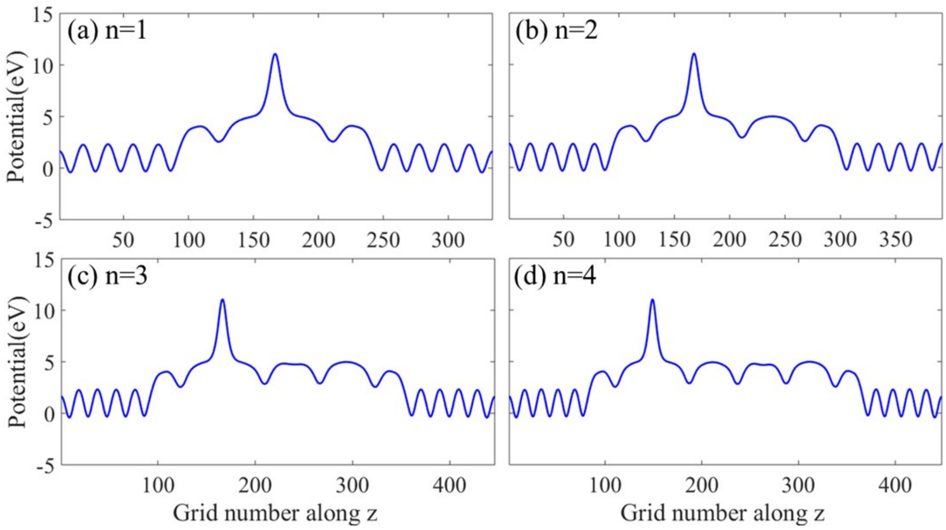

Fig. S1 (a-c) Hartree potential of Cu(111)/CrI_3/*h*-BN/n·CrI_3/Cu(111) junctions along z axis. (a) n=1; (b) n=2; (c) n=3; (d) n=4.

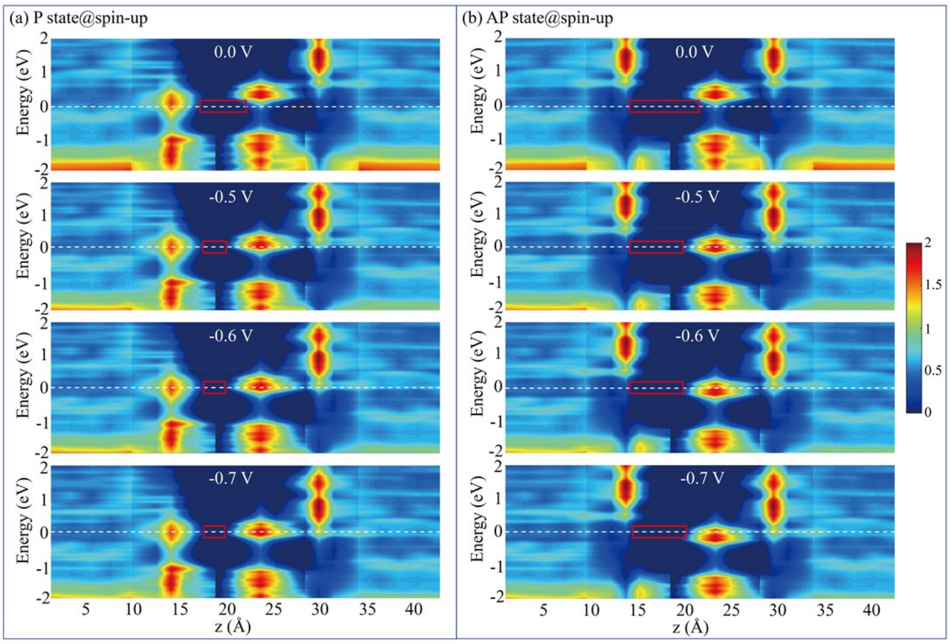

Fig. S2. Spin-up project density of states (PDOS) along the transport direction (*z* axis) of the Cu(111)/CrI_3/h-BN/2·CrI_3/Cu(111) devices in different bias voltages. (a) P state; (b) AP state. The white dashed lines indicate the Fermi level. The length of the red rectangle represents the thickness of the barrier layer at the Fermi level.

For the CrI_3/h-BN/2·CrI_3 MTJ, when the bias voltage is greater than |-0.5| V, whether it is P or AP state, the SIE reaches 100% (the currents of spin-down are zero in this bias window). Therefore, we only plot spin-up PDOSs of these bias voltages (0.0 V, -0.5 V, -0.6 V, -0.7 V) for P and AP states to explain this anomalous phenomenon, which mentioned above in the CrI_3/h-BN/2·CrI_3 MTJ. It can be seen from Fig. S2 that as the negative bias increases, the Fermi level moves relatively upward. As a result, the width of the barrier layer at the Fermi level is changed. Fig. S2(a) shows that the length of the red rectangle decreases with increasing negative bias, which means that the probability of electron tunneling at the Fermi level increases with increasing bias. For the AP state, with the increase of the negative bias, the length of the red rectangle remains basically unchanged after the bias is greater than 0 V, and the length is much larger than the length of the P state. For the AP state, with the increase of the negative bias, the length of the red rectangle remains basically unchanged after the bias is greater than 0V, and the length is much larger than the length of the P state. Therefore, in the AP state, the tunneling probability of electrons is small. The above results are consistent with the evolution of current in this bias range. So in the CrI_3/h-BN/2·CrI_3 MTJ, there will be an abnormal TMR effect under negative bias.

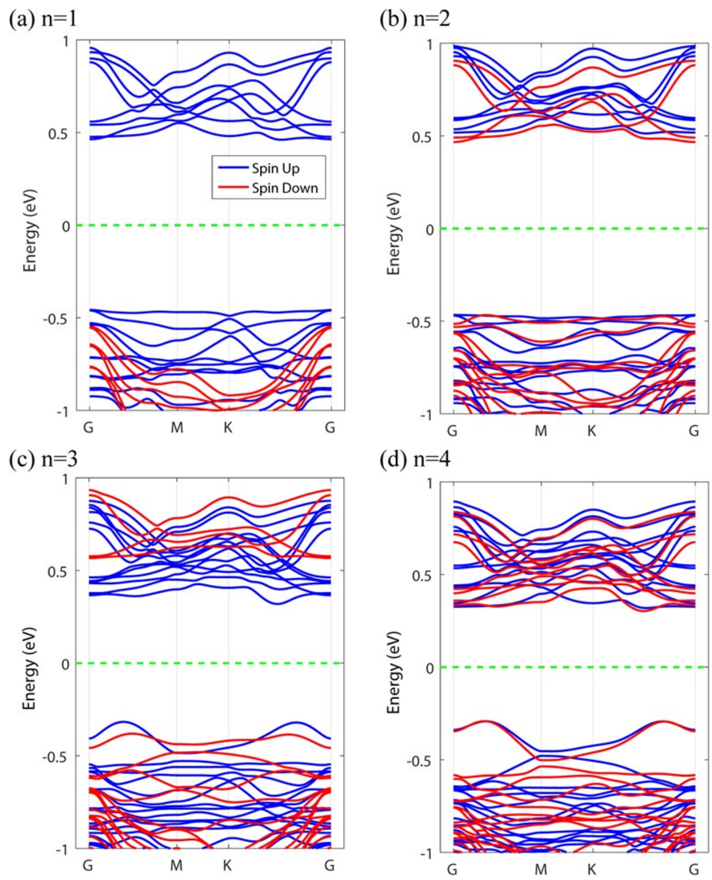

Fig. S3 The band structure of CrI_3/*h*-BN/n·CrI_3. (a) n=1; (b) n=2; (c) n=3; (d) n=4. The Fermi level is set to zero. The blue and red lines represent spin-up and spin-down, respectively, and the dashed green line represents the Fermi level.

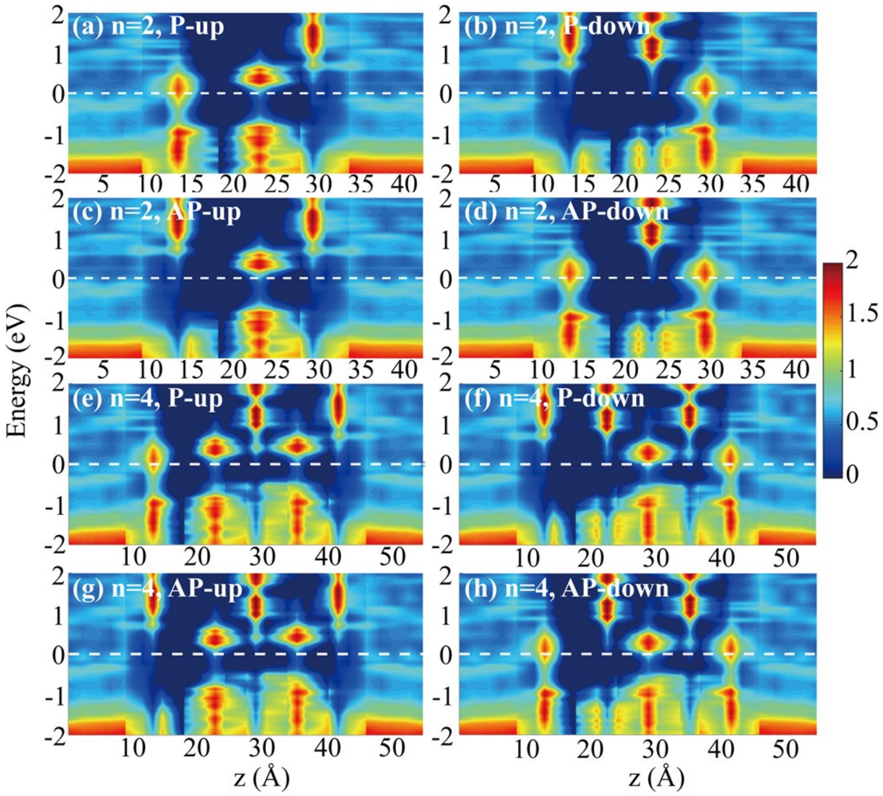

Fig. S4. Project density of states (PDOS) along the transport direction (z axis) of the Cu(111)/CrI_3/h-BN/n·CrI_3/Cu(111) devices at equilibrium. (a-d) n=2: (a) spin-up and (b) spin-down electronic states in the P state, and (c) spin-up and (d) spin-down electronic states in the AP state. (e-h) n=4: (e) spin-up and (f) spin-down electronic states in the P state, and (g) spin-up and (h) spin-down electronic states in the AP state. The white dashed lines indicate the Fermi level.

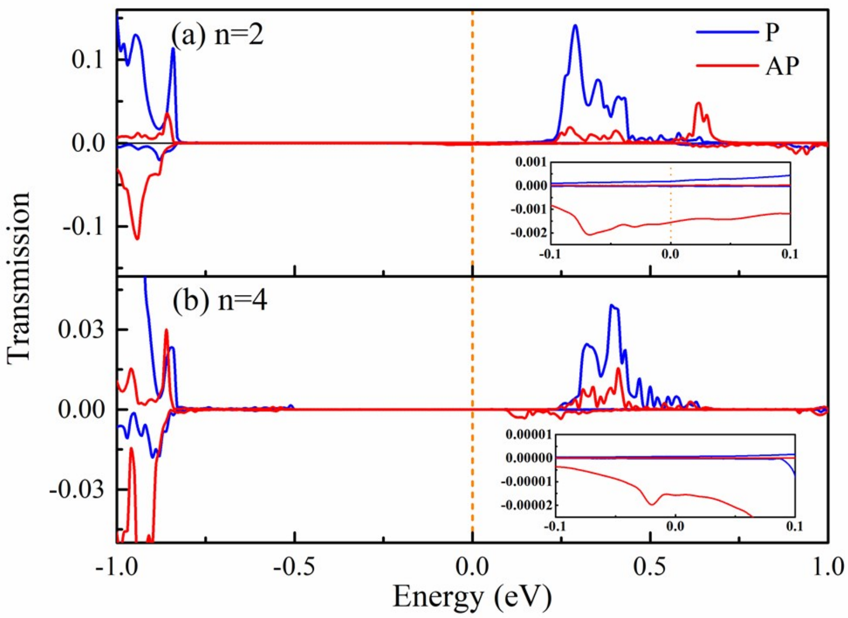

Fig. S5 Zero bias voltage transmission coefficient versus electron energy in P and AP states of Cu(111)/CrI_3/*h*-BN/n·CrI_3/Cu(111) junctions: (a) n=2 and (b) n=4. The Fermi level is set to zero. The sign of transmission indicates the spin direction ("-" represents spin down state.).

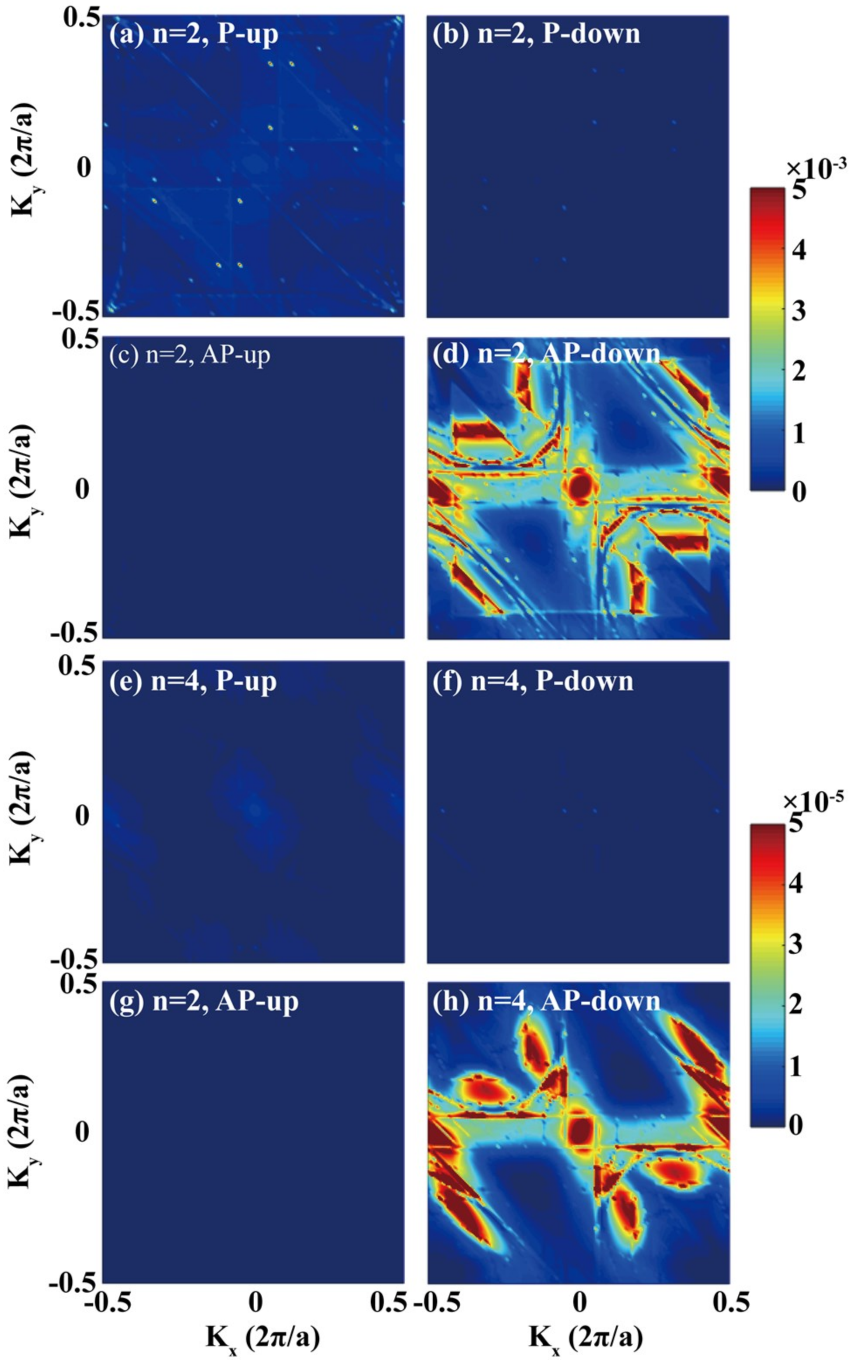

Fig. S6 Transmission coefficients in the two dimensional Brillouin zone (2D-BZ) for the Cu(111)/CrI_3/*h*-BN/n·CrI_3/Cu(111) junctions (n=2, 4) at the Fermi level. (a-d) n=2: (a) spin-up and (b) spin-down in P state; (c) spin-up and (d) spin-down in AP state. (e-h) n=4: (e) spin-up and (f) spin-down in P state; (g) spin-up and (h) spin-down in AP state.