Electronic Supplementary Material (ESI) for Nanoscale.

Supporting information for

"Spin filtering effect, thermal spin diode effect and high tunneling magnetoresistance in the Au/GdI_2/Au van der Waals junction"

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1. Electronic structure of bulk and 4-layer GdI_2

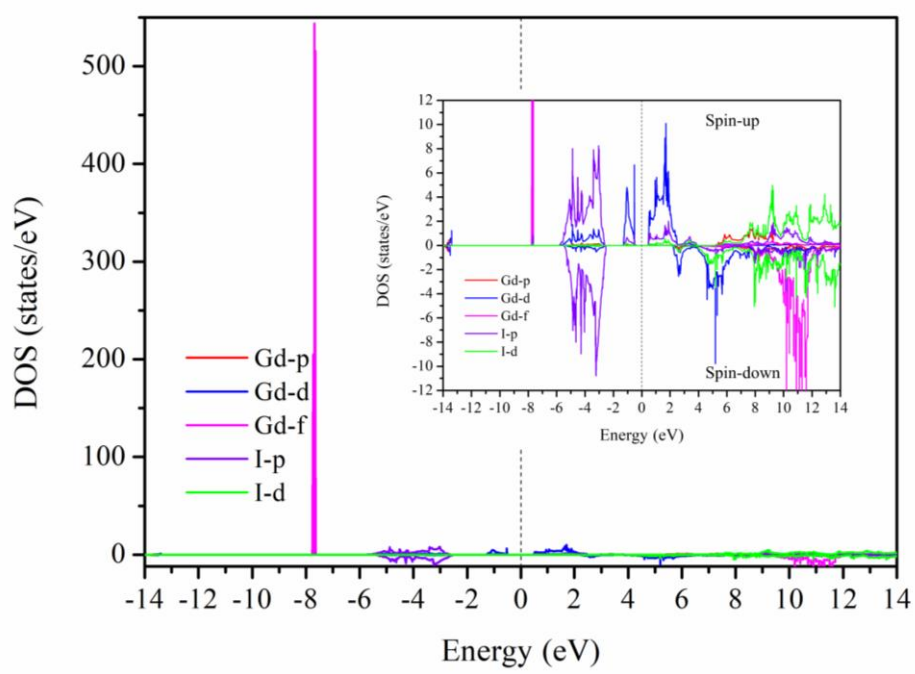

Fig. S1 The spin-dependent density of states (DOS) for ferromagnetic bulk GdI_2 within GGA-PBE. The inset shows a zoomed-in view near the Fermi level. The Fermi level is at zero eV.

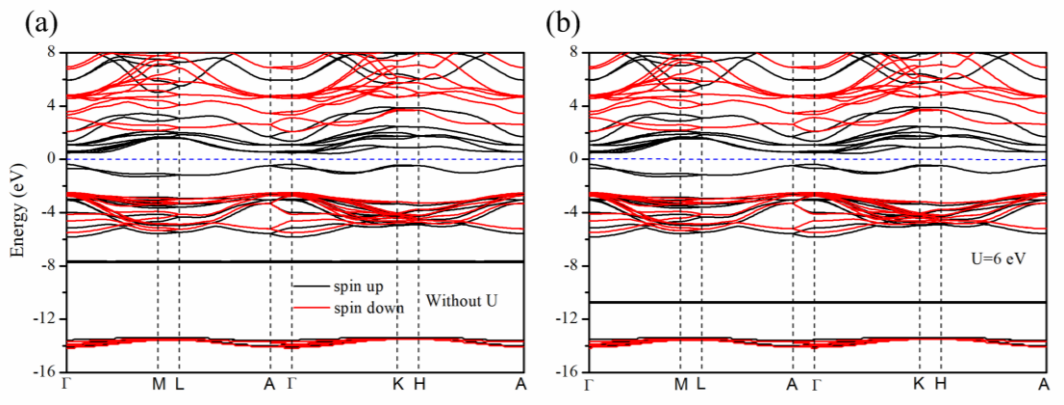

Fig. S2 The spin-dependent band structure of bulk GdI_2 without U and with U=6 eV.

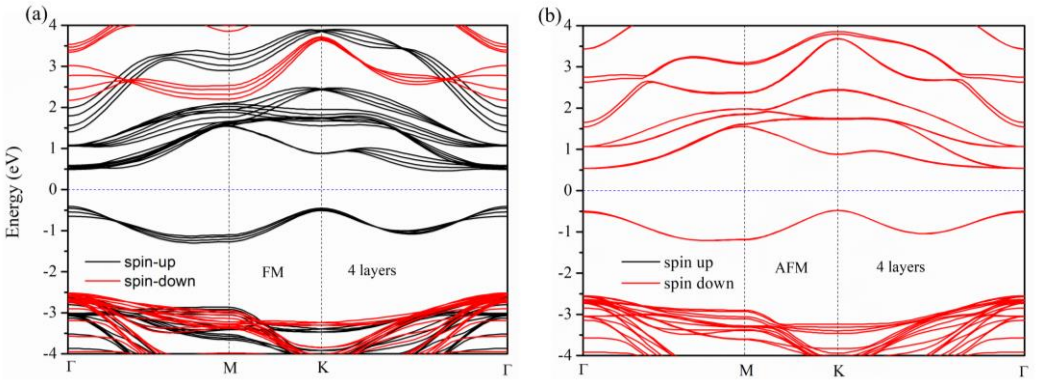

Fig. S3 Spin-dependent band structures within GGA-PBE for four-layer GdI_2 in FM (a) and AFM (b) states.

2. The effect of SOC on band structure and transport properties

We calculate the ferromagnetic and antiferromagnetic band structures of bulk GdI_2 within GGA+SOC (Fig. S4). Compared to those within GGA (Figs. 1(c,d)), it is found that the SOC effect is very slight likewise that of monolayer GdI_2 which energy gap is decreased by only 0.01 eV by SOC (Fig. S8 in Ref. 21), and there is almost no change of the shape of energy band.

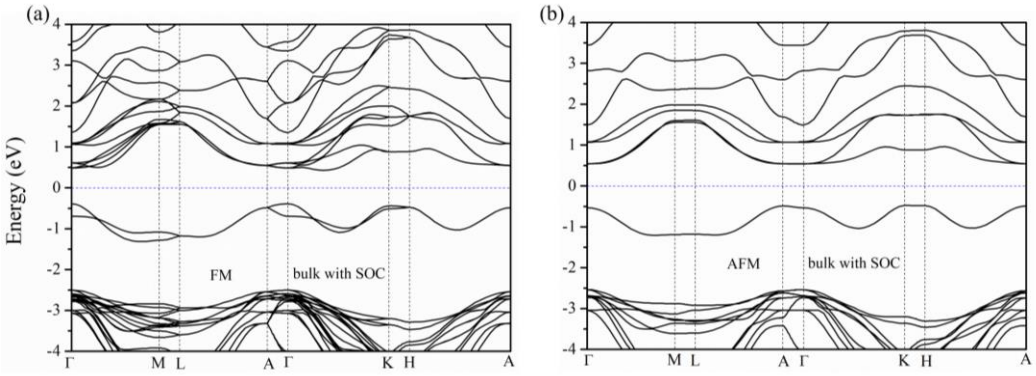

Fig. S4 The spin-dependent band structure of bulk GdI_2 with SOC in FM (a) and AFM (b).

Then, as an example, we calculate the spin-dependent conductance and TMR at zero bias voltage within SOC. As shown the following Table S1, the SOC decreases a little the conductance and the TMR value, but the TMR value is still high, 570% at zero bias voltage. Similar phenomenon at the finite bias voltage can be deduced.

Table S1 Spin-dependent conductance and TMR value at zero bias voltage for the Au/GdI_2/Au junction in FM and AFM states with and without SOC. The values in brackets are the results without SOC. ↑ and ↓ represent the spin-up and spin-down channels, respectively.

Magnetic state	Conductance (Siemens)	TMR
FM	1.64×10^{-9} (1.73×10^{-9}) ↑; 5.71×10^{-12} (6.74×10^{-12}) ↓	570% (641%)
AFM	2.21×10^{-10} (2.20×10^{-10}) ↑; 2.20×10^{-11} (1.49×10^{-11}) ↓	

3. Project DOS of the Au/GdI_2/Au junction with AFM state

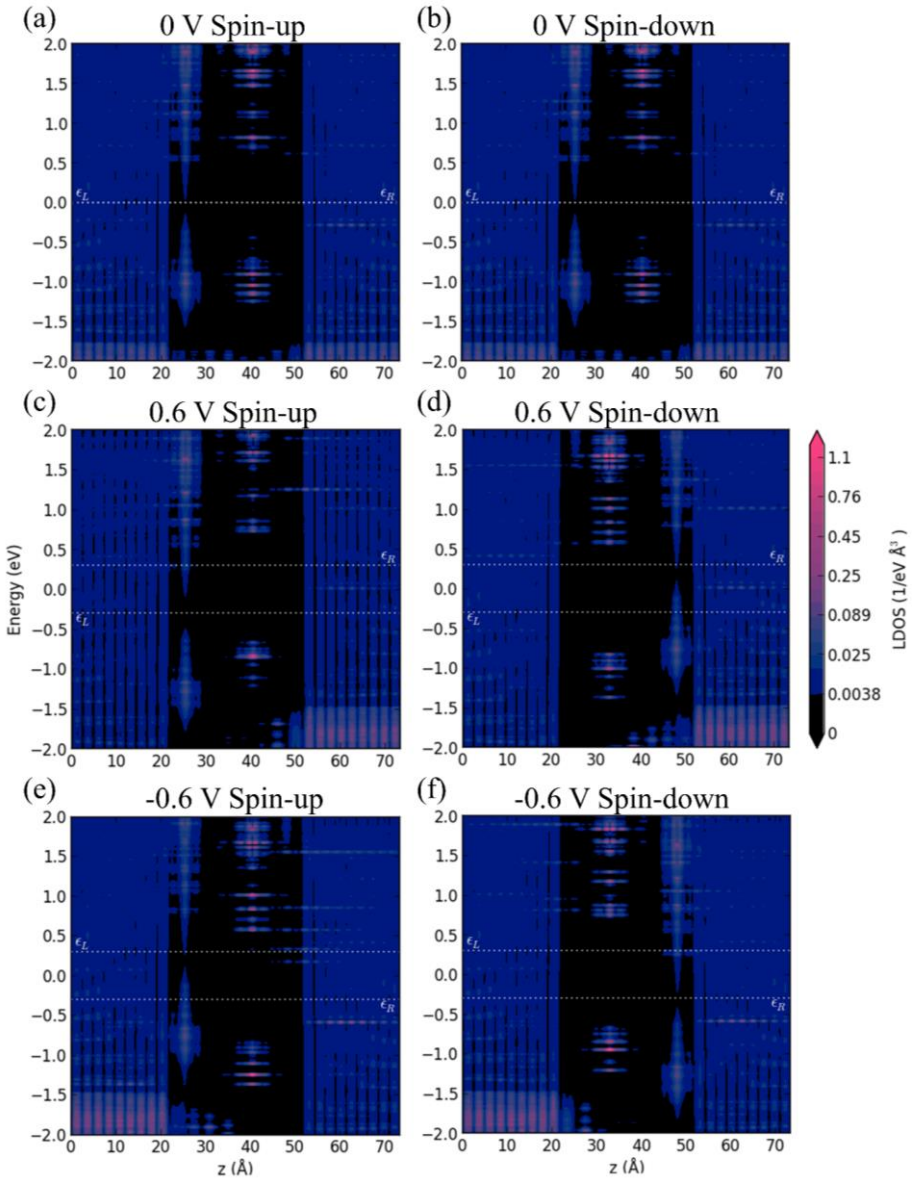

Fig. S5 The spin-dependent projected local density of states in the Au/GdI_2/Au junction with antiferromagnetic state at the bias voltages of zero, -0.6 and 0.6 V.