Electronic Supplementary Information for

Tunable valley polarization and high Curie temperature in two-dimensional GdF$_2$/WSe$_2$ van der Waals heterojunction

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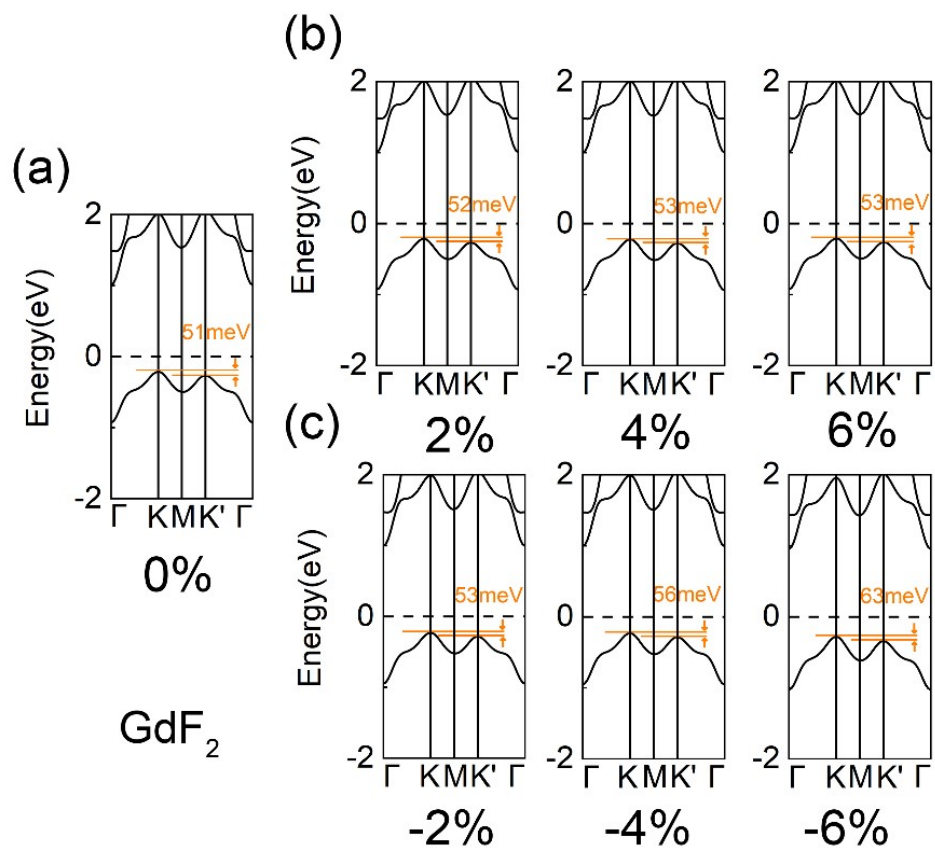wangxc@email.tjut.edu.cn (Xiaocha Wang)

Fig. S1 The band structure of GdF_2 when (a) no strain is applied, (b) tensile strain and (c) compressive strain are applied.
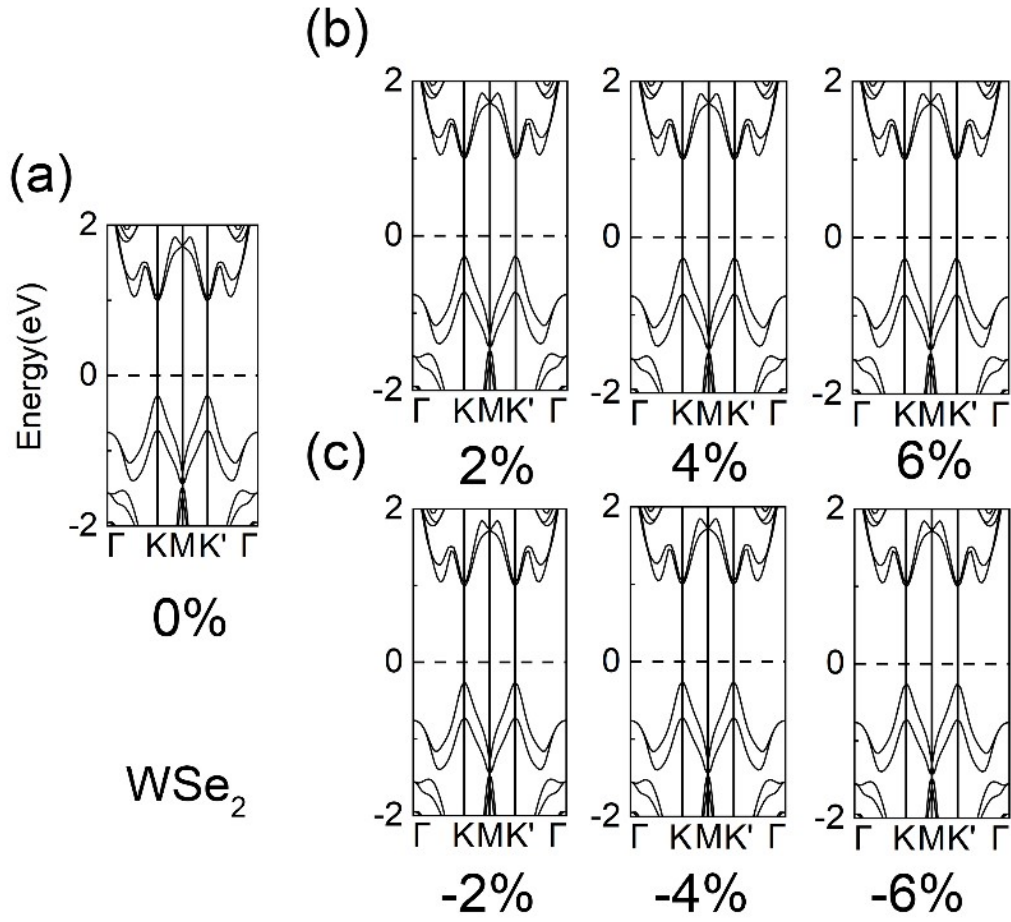
Fig. S2 The band structure of WSe_2 when (a) no strain is applied, (b) tensile strain and (c) compressive strain are applied.
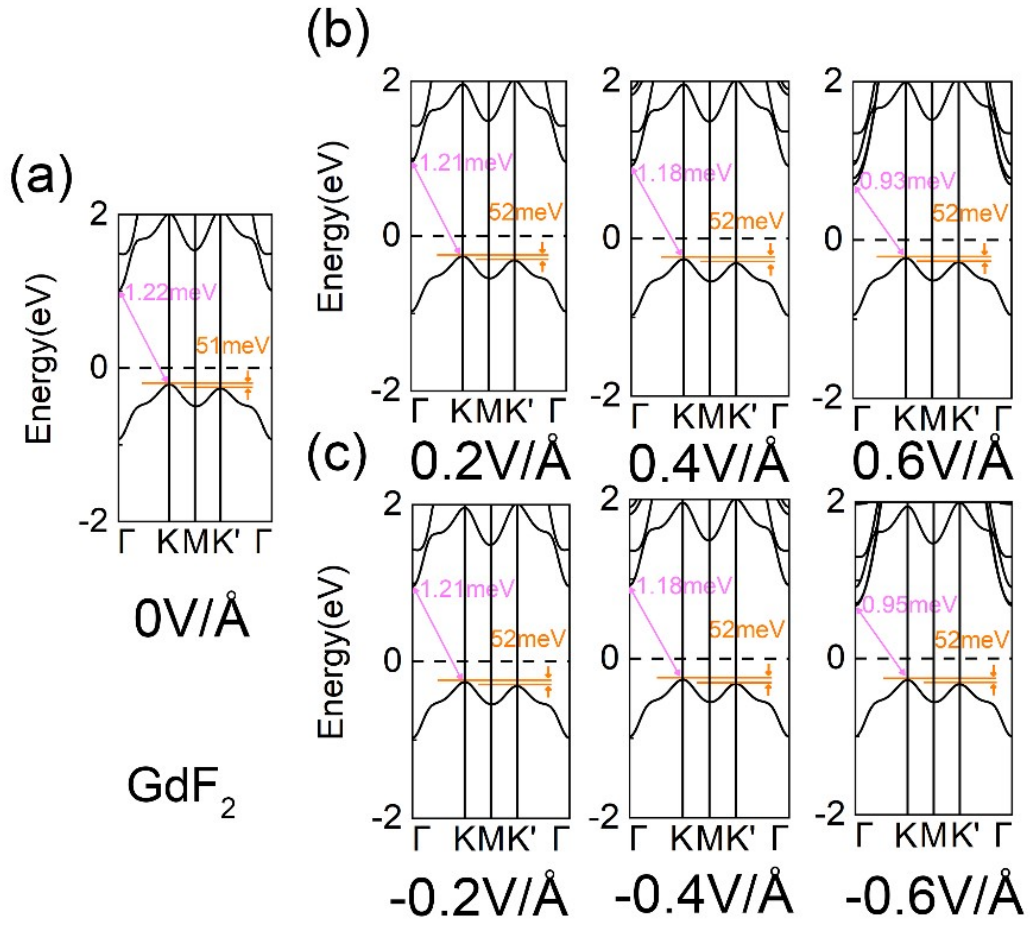
Fig. S3 The band structure of GdF$_2$ (a) without external electric field, (b) with

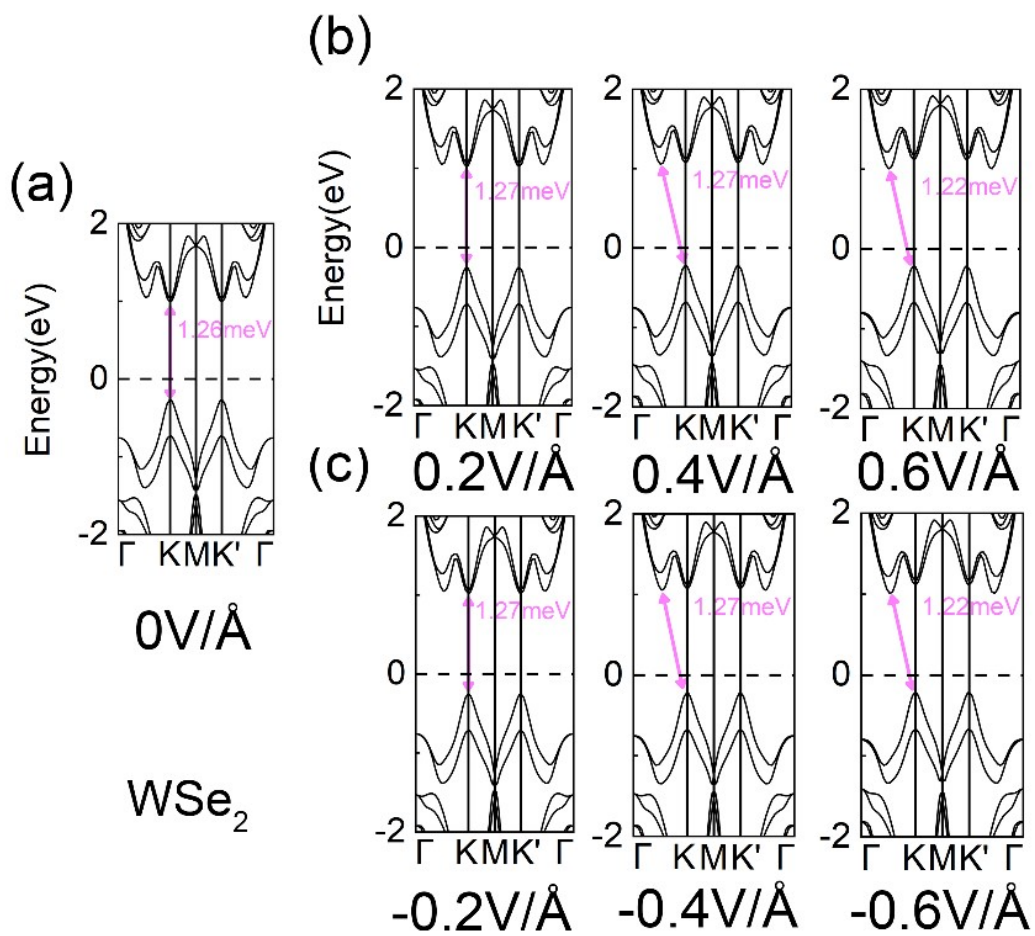positive electric field and (c) negative electric field.

Fig. S4 The band structure of WSe$_2$ (a) without external electric field, (b) with positive electric field and (c) negative electric field.

Table S1. In Model1-6, the total energy (eV) of the GdF_2/WSe_2 heterojunction, and the

energies of the ML GdF_2 and WSe_2, respectively.

	E_{GdF_2/WSe_2}	E_{GdF_2}	E_{WSe_2}
Model-1	–50.093901	–27.652289	–21.641195
Model-2	–50.165071	/	/
Model-3	–50.157111	/	/
Model-4	–50.161071	/	/
Model-5	–50.1607	/	/
Model-6	–50.094409	/	/

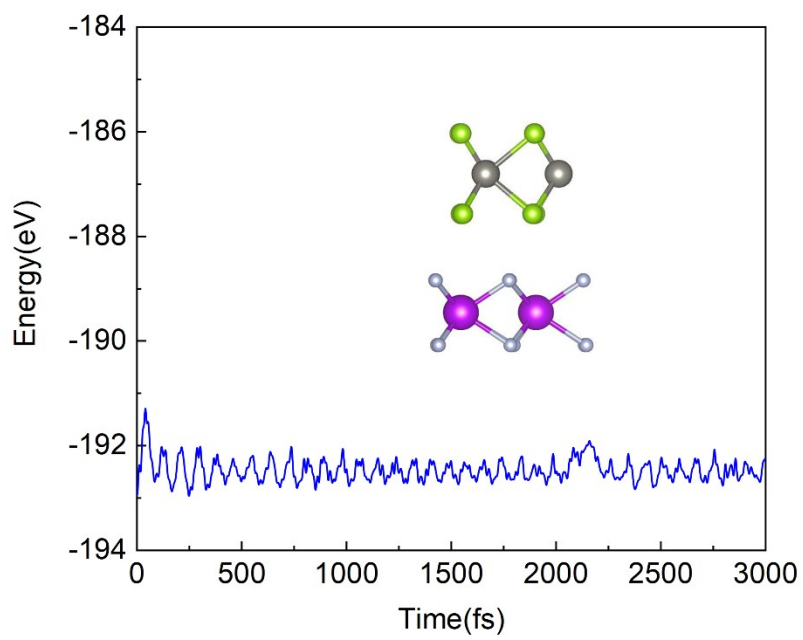**Fig. S5** Variation of the total free energy during the 3000 fs AIMD simulation of the GdF$_2$/WSe$_2$ supercell at 300K.

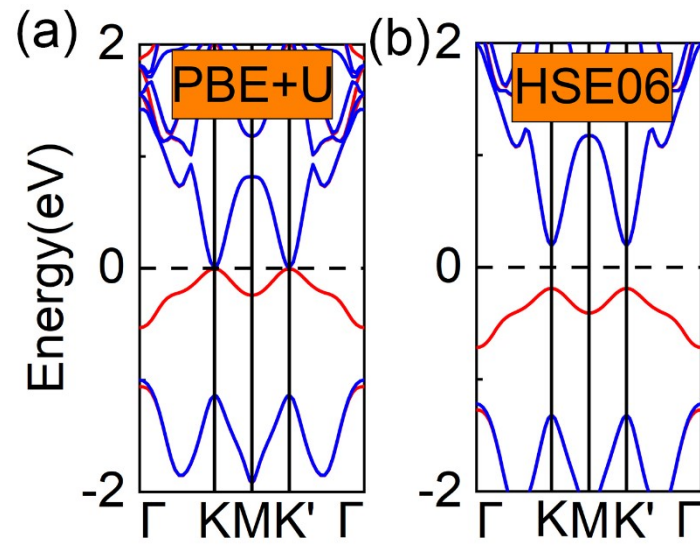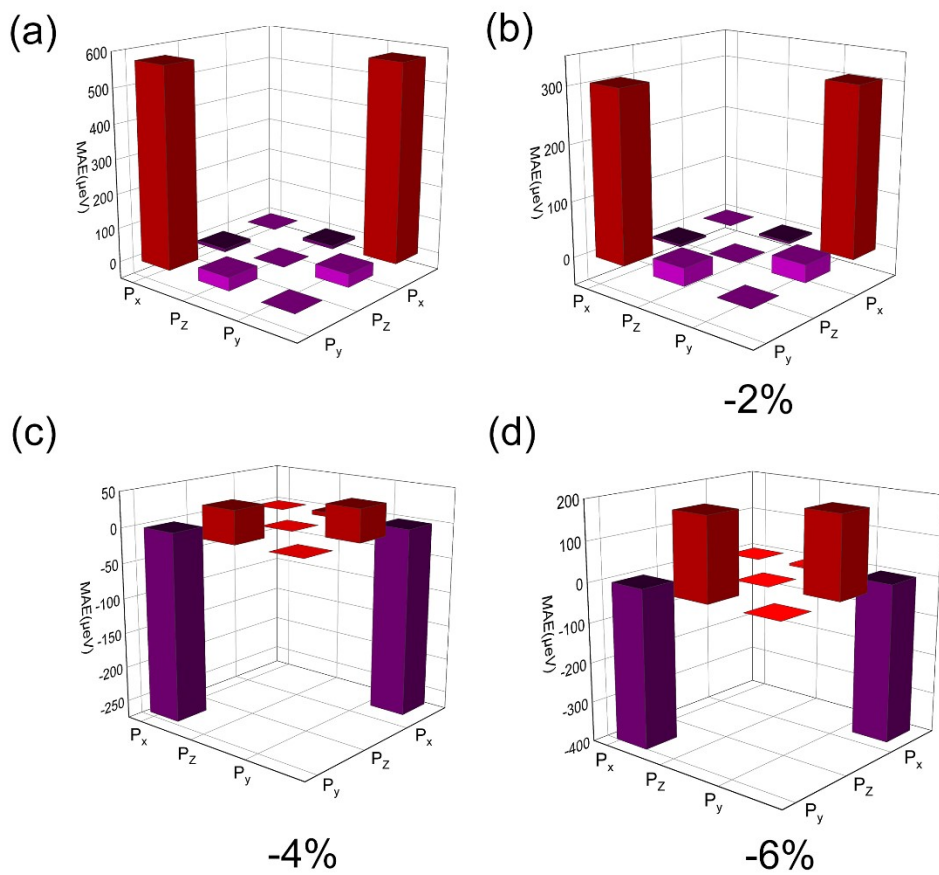**Fig. S6** The band structures of GdF_2/WSe_2 calculated by the (a) PBE+U and (b) HSE06.

Fig. S7 Oribital resolved MAE of Gd-p in the GdF$_2$/WSe$_2$ heterojunction at (a) no strain, (b) –2% stain, (c) –4% strain and (d) –6% strain.
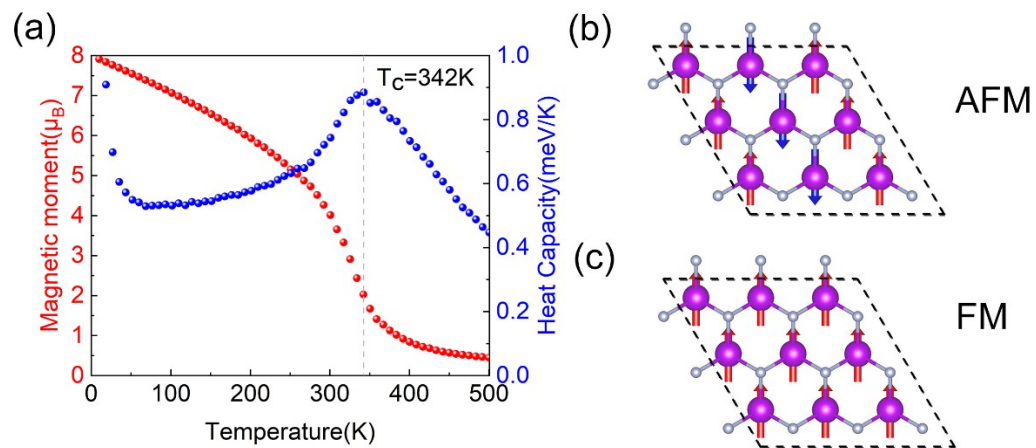
Fig. S8 Curie temperature of the monolayer (a) GdF_2. The (b) AFM and (c) FM states of the GdF_2: red arrow shows the direction of spin-up and the blue arrow shows the direction of spin-down.
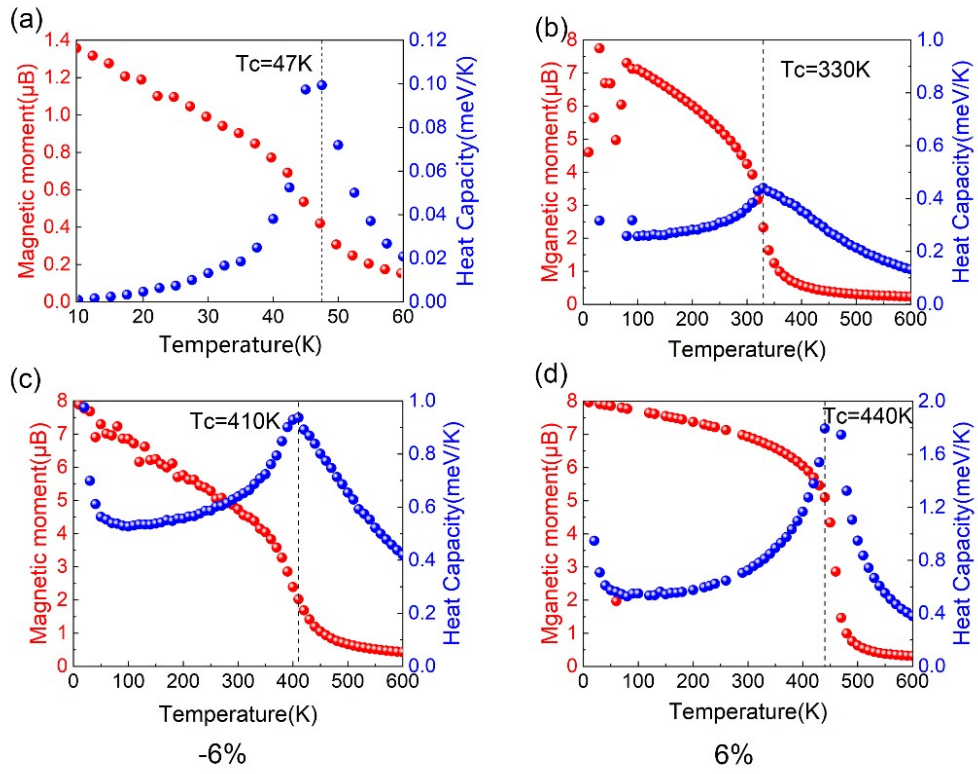
Fig. S9 (a) The Tc of CrI$_3$. The Tc of GdF$_2$/WSe$_2$ when (b) no strain is applied, (c) −6%

strain and (d) 6% strain are applied.