Supporting Information

Significantly Enhanced Magnetoresistance in Monolayer WTe_2 via Heterojunction Engineering: A First-principles Study

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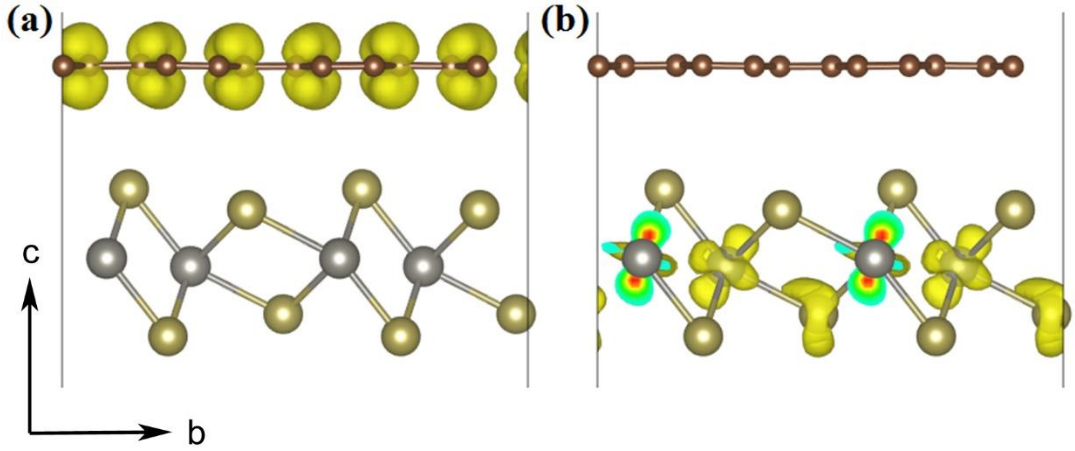

Figure S1. Charge density distributions of VBM (a) and CBM (b) of the graphene/WTe_2 heterojunction. For the charge density distribution iso-surface plot, the iso-value is 25 e/$Bohr^3$. The yellow and gray balls represent Te and W atoms, respectively.

Table S1: Effective mass m^* (m_0 is the mass of an electron), elastic modulus C (eV/Å^2) and deformation potential constant E_1 (eV), and room temperature carrier mobility μ ($\times 10^3$ cm^{2}V^{-1}s^{-1}) of the isolated WTe_2 monolayer and the WTe_2/graphene heterojunction.

	Direction	Carrier type	m^*	C	E_1	μ
WTe_2 monolayer	a-axis	hole	0.88	7.70	-10.35	0.03
		electron	0.31	7.70	-4.23	1.07
	b-axis	hole	0.54	9.15	0.55	20.50
		electron	0.25	9.15	-1.40	13.00
WTe_2/graphene heterostructure	a-axis	hole	-	57.46	-3.66	112.29
		electron	0.35	57.46	-6.78	2.31
	b-axis	hole	-	58.31	-3.50	126.67
		electron	0.30	58.31	-3.15	14.82

For the weak case, we should consider a parallel equivalent circuits of resistors made of graphene and WTe_2 to obtain the total MR resistance.Then, the total resistance (R_t) is related to that of graphene (R_{gr}) and WTe_2 (R_{wt}) as follows: $1/R_t = 1/R_{gr} + 1/R_{wt}$. And, the $MR = \frac{R(H)-R(0)}{R(0)}$, R(0) is the resistance when the external magnetic field equal to 0. We use the MR of WTe_2 (***B***^{2} for parabolic dispersion) and graphene (***B*** for a linear dispersion) and obtain:

$$MR_{wt} = \frac{R_{wt}(H) - R_{wt}(0)}{R_{wt}(0)} = \mu_e^2 B^2, (S1)$$

$$MR_{gr} = \frac{R_{gr}(H) - R_{gr}(0)}{R_{gr}(0)} = \mu_h B, (S2)$$

$$MR_t = \frac{R_t(H) - R_t(0)}{R_t(0)}, (S3)$$

And,

$$\frac{1}{R_t(0)} = \frac{1}{R_{wt}(0)} + \frac{1}{R_{gr}(0)}, (S4)$$

$$\frac{1}{R_t(H)} = \frac{1}{R_{wt}(H)} + \frac{1}{R_{gr}(H)}, (S5)$$

Here we make an approximation that when there is no external magnetic field, $R_{wt}(0) \approx R_{gr}(0) = R$. Because both graphene and WTe_2 are semimetals, when there is no external magnetic field, their resistances are very small. From (S4), we can obtain $R_t(0) = R/2$. Then, we can rewrite (S1-3) as:

$$R_{wt}(H) = (\mu_e^2 B^2 + 1)R, (S6)$$

$$R_{gr}(H) = (\mu_h B + 1)R, (S7)$$

$$R_t(H) = \frac{(MR_t + 1)R}{2}, (S8)$$

Combine equations of (S5-8), we obtain the total MR as:

$$\mathrm{MR}_t = \frac{2\mu_h \mu_e^2 B^3 + \mu_e^2 B^2 + \mu_h B}{\mu_e^2 B^2 + \mu_h B + 2}, (S9)$$

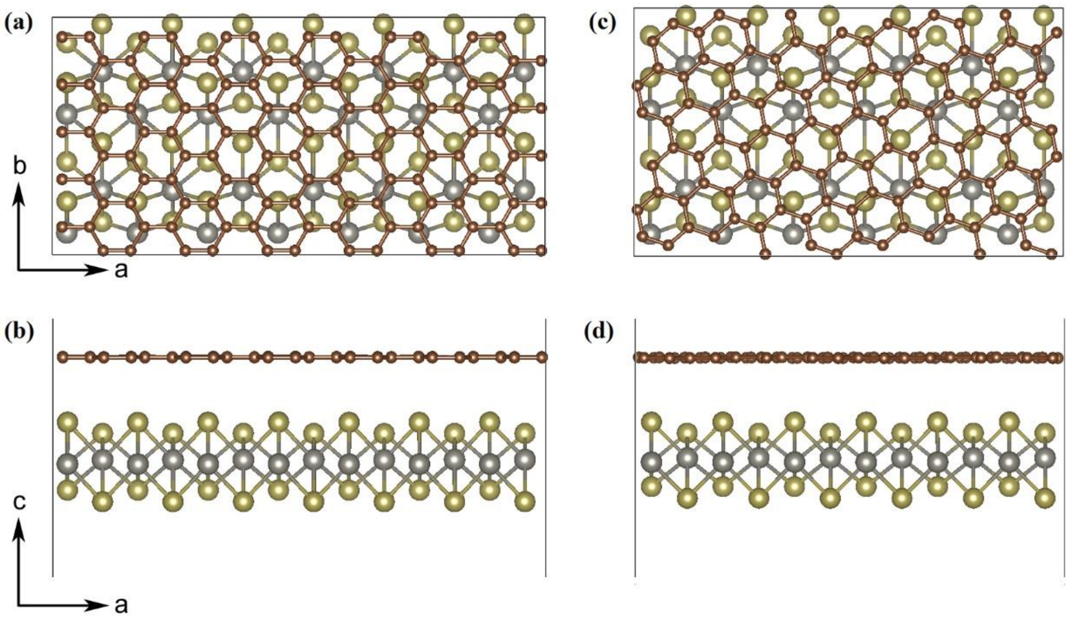

Figure S2. Top and side views of the geometric structure of the WTe_2/graphene heterojunction with different angle, θ. (a)(b) and (c)(d) show the $\theta = 30°$ (a 2×7 supercell of WTe_2 is used to match a $5\times 6\sqrt{3}$ supercell of graphene) and $\theta = 10.8°$ (a 2×6 supercell of WTe_2 is used to match a $2\sqrt{21}\times 2\sqrt{7}$ supercell of graphene) heterojunction for top and side view, respectively; ***a*** , ***b*** and ***c*** represent the lattice vectors. Brown, yellowish and gray balls represent C, Te and W atoms, respectively.

Table S2: Effective mass m^* (m_0 is the mass of an electron), elastic modulus C (eV/Å^2) and deformation potential constant E_1 (eV), room temperature carrier mobility μ (×10^3 cm^{2}V^{-1}s^{-1}) and MR when the external magnetic field B=14.7T of the WTe_2/graphene heterostructure with different angle θ.

θ	Carrier type	m*	C	E_1	μ	μ_e*μ_h	MR
0°	hole	-	58.31	-3.50	126.67	1877.25	4056.54
	electron	0.30	58.31	-3.15	14.82		
10.8°	hole	-	62.07	-3.79	115.60	1406.85	3040.06
	electron	0.33	62.07	-3.26	12.17		
30°	hole	-	57.36	-3.65	115.18	299.46	647.12
	electron	0.33	57.36	-6.77	2.6		