Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic properties and interface contact of graphene/$CrSiTe_3$ van der Waals heterostructures

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Table S1(a) Magnetic moment of atoms in the of graphene/$CrSiTe_3$ at d=3.19 Å

direction	Cr	Si	Te
In plane	3.38 μ_B	0.010μ_B	0.102μ_B
Z direction	0.02 μ_B	0.001μ_B	-0.010μ_B

Table S1(b) Magnetic moment of atoms in the of graphene/$CrSiTe_3$ at d=2.75 Å

direction	Cr	Si	Te
In plane	2.82 μ_B	0.001μ_B	0.062μ_B
Z direction	-0.68 μ_B	-0.004μ_B	-0.028 μ_B

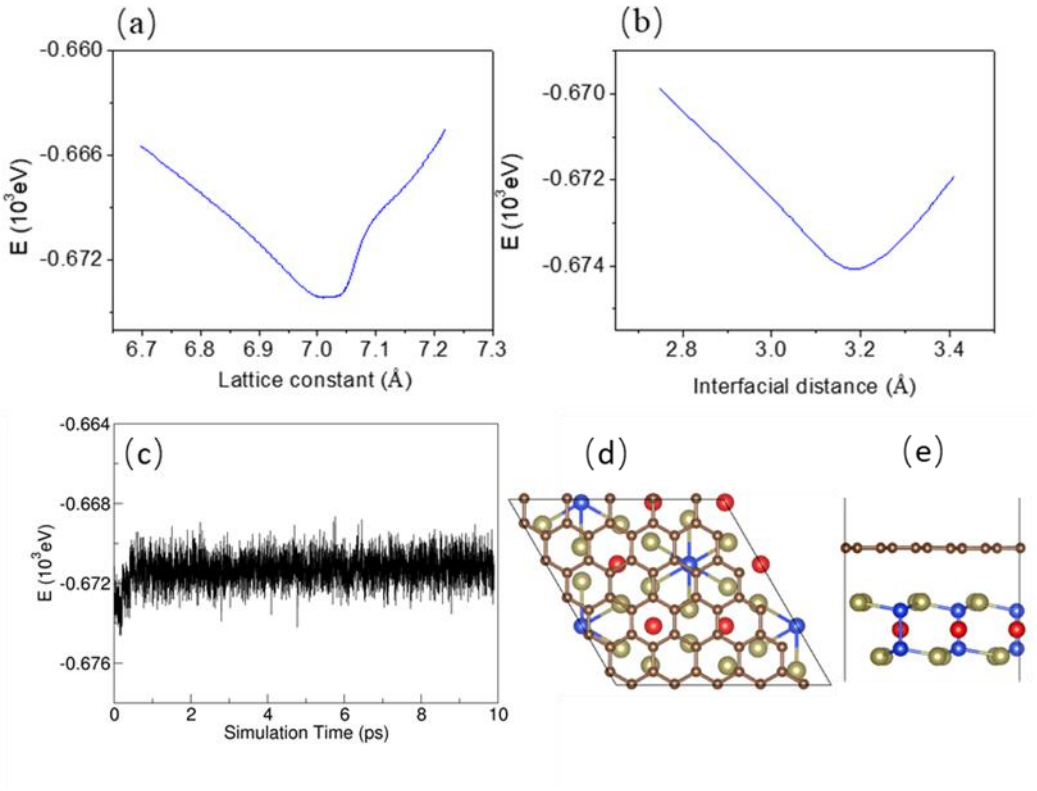

Fig. S1 (a) The calculated total energy of the Gr/$CrSiTe_3$ heterostructure as a function of the lattice constant of $CrSiTe_3$; (b) The calculated total energy of the Gr/$CrSiTe_3$ heterostructure as a function of the interfacial distance; (c) Ab initio molecular dynamics simulations of Gr/$CrSiTe_3$ at 300 K; (d) and (e) the final structure after 10 ps, showing that the Graphene/$CrSiTe_3$ heterostructure remains stable.

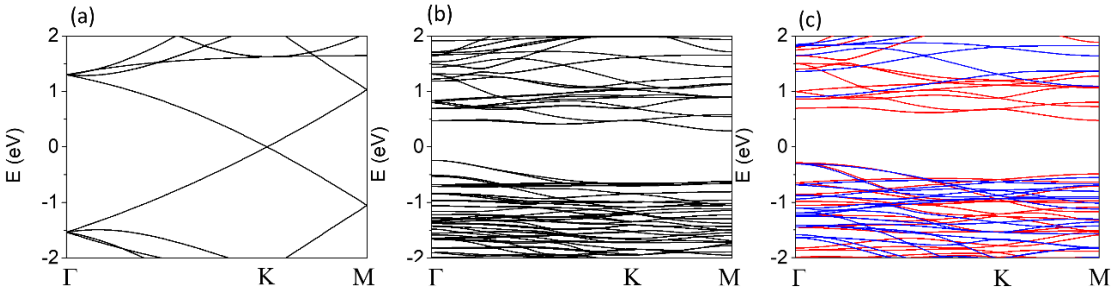

Fig. S2 (a) Band structures of graphene; (b) Band structures of $CrSiTe_3$ ML with SOC interaction and (c) The spin-polarized band structure of the $CrSiTe_3$ ML, red for spin-up and blue for spin-down.

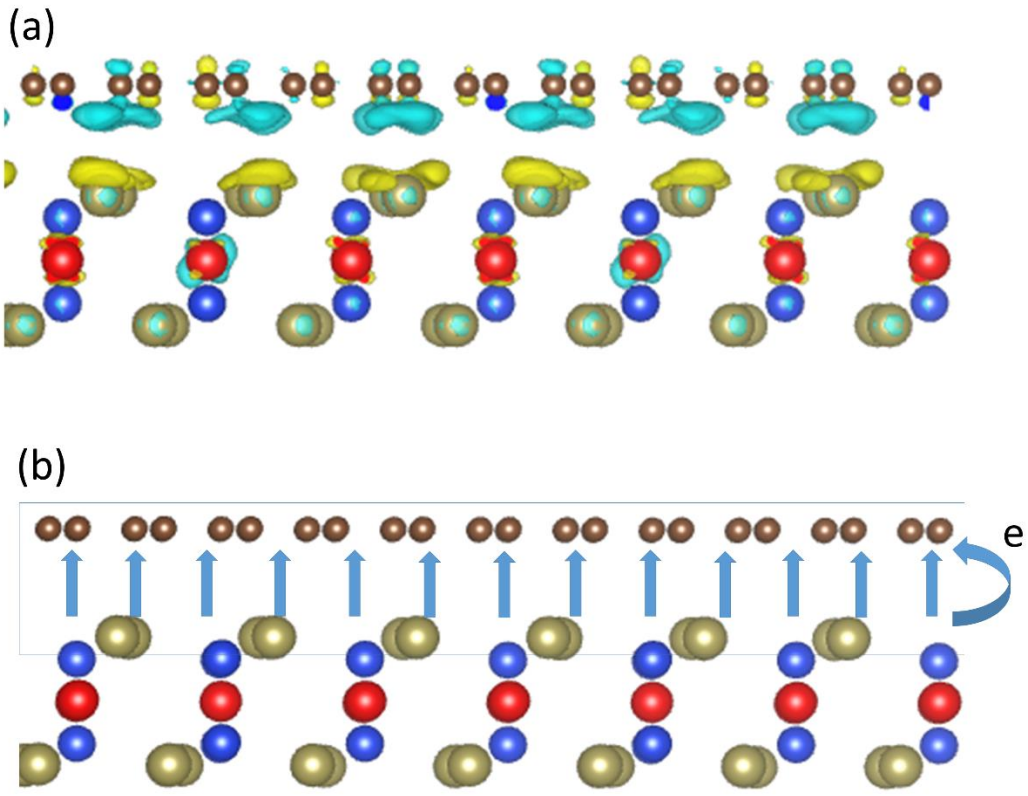

Fig. S3 (a) Charge density difference of the graphene/$CrSiTe_3$ at the interfacial distance d=2.75 Å. The isosurface refers to isovalues of 0.001 e $Å^{-3}$. (b) Schematic diagram of the built-in electric field at the graphene/$CrSiTe_3$ interface.

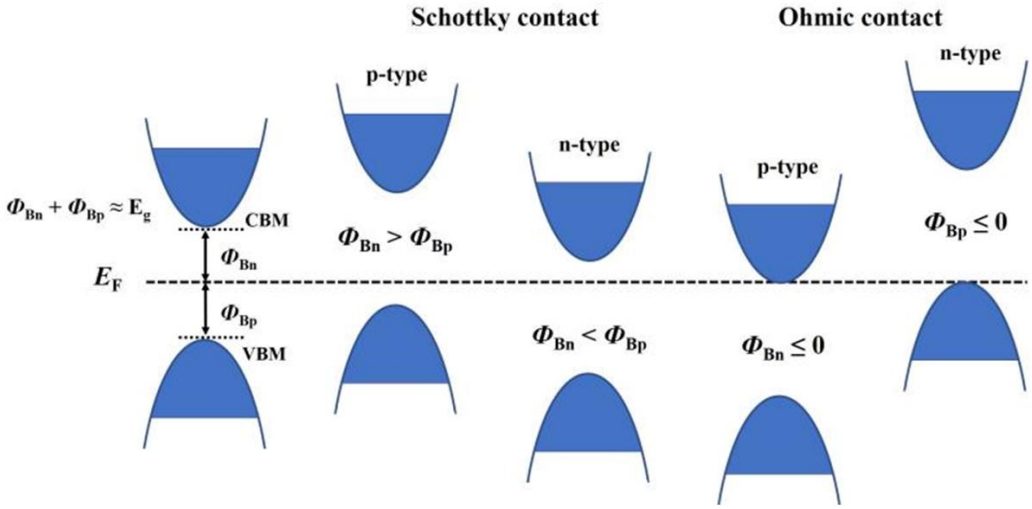

Fig. S4 Diagrammatic illustration of the p-type and n-type Schottky and Ohmic contact at the interface region.

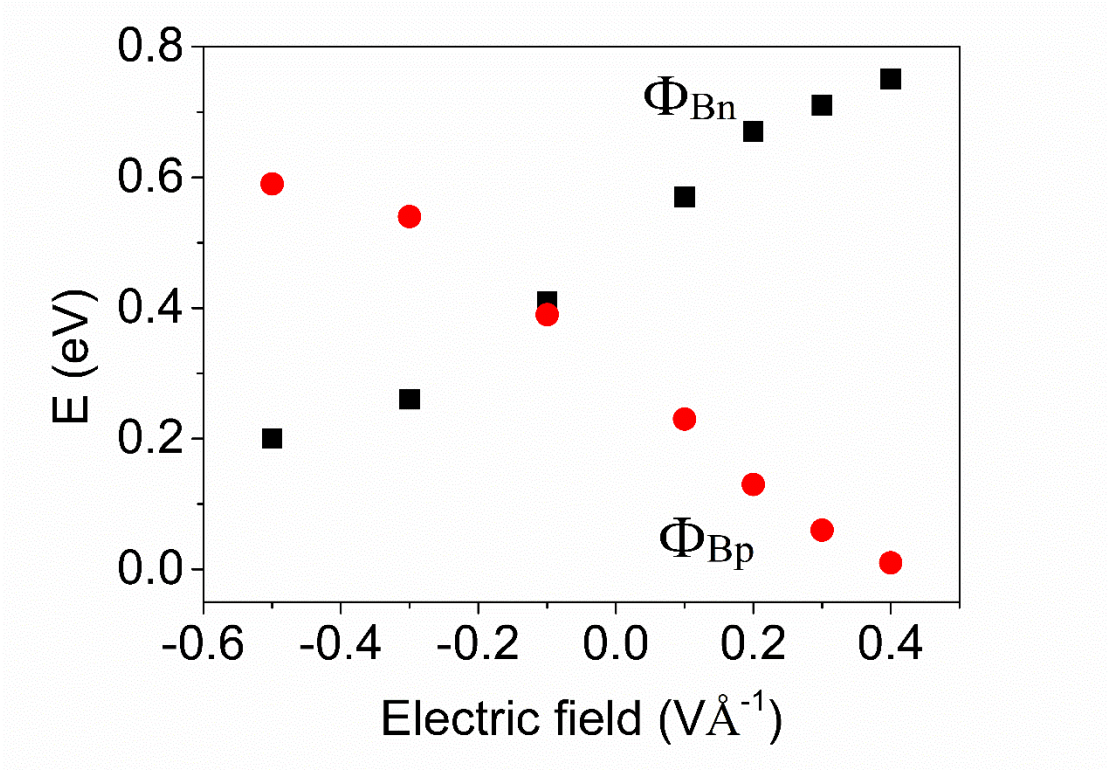

Fig. S5 The SBH of the graphene/$CrSiTe_3$ as a function of the external electric field. The n-type Schottky barrier (Φ_{Bn}) noted in black color is the energy difference between the E_{CBM} and the E_F, while the p-type Schottky barrier (Φ_{Bp}) noted in red color is the energy difference between the E_F and the E_{VBM}.