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Supporting Information

Tunable Schottky and Ohmic contacts in Ti_2NF_2/α-Te van der Waals heterostructure

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Table S1. The lattice constants, interlayer distances and binding energies of all stacking configurations, respectively.

Stacking configurations	T	V	H
Lattice constants (Å)	a=b=12.16	a=b=12.18	a=b=12.18
Interlayer distances (Å)	3.26	3.20	3.18
Binding energies (eV)	-1.19	-1.55	-1.56

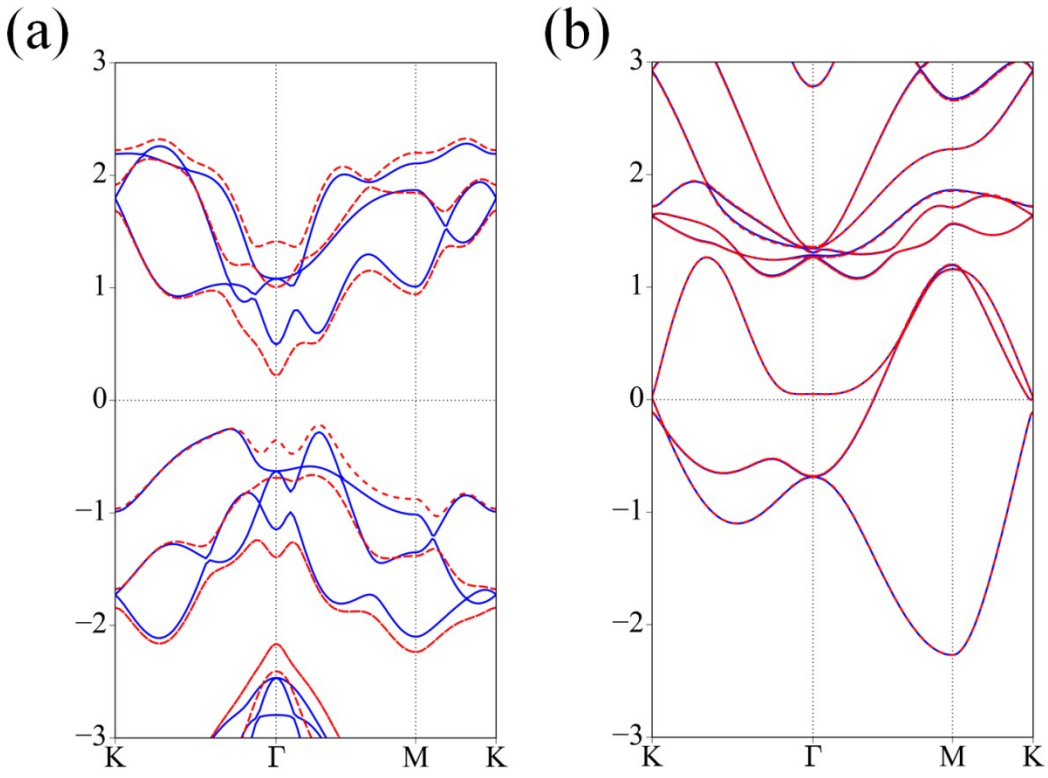

Figure S1. Band structures of (a) α-Te and (b) Ti_2NF_2 with (red, dashed line) and without (blue, solid line) inclusion of SOC.

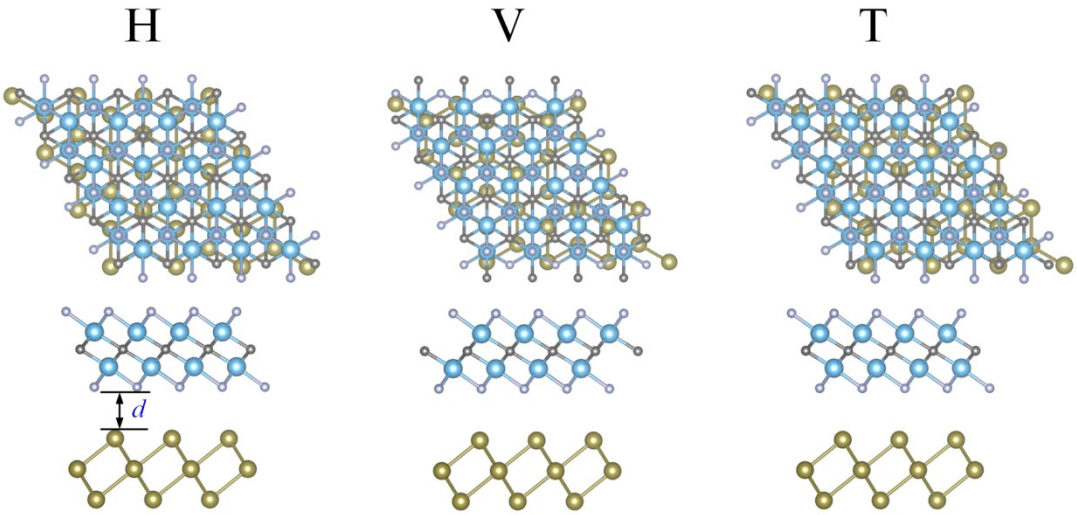

Figure S2. Top and side views of the optimized structures of the T, V, and H configurations for the Ti_2NF_2/α-Te vdW heterostructure.

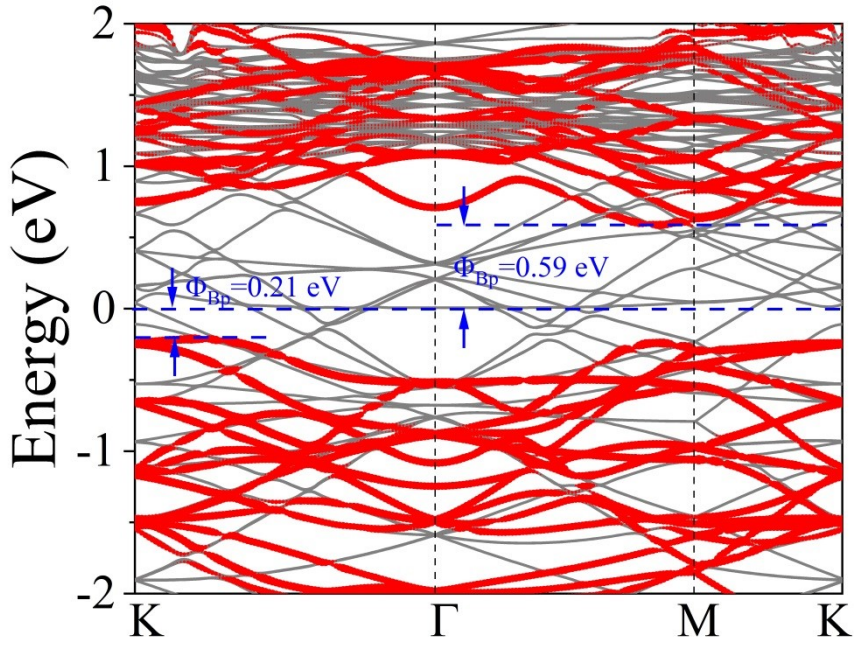

Figure S3. The band structure of V-type Ti_2NF_2/α-Te.

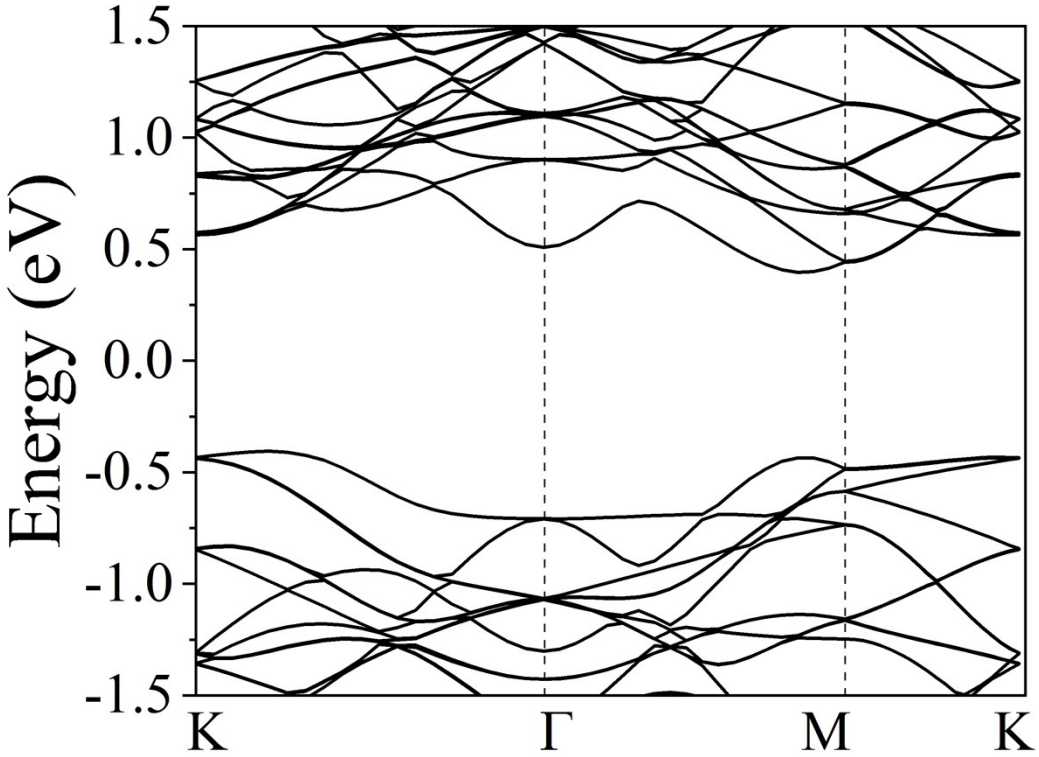

Figure S4. Band structure of standing alone α-Te with the strained lattice constants in the heterostructure.

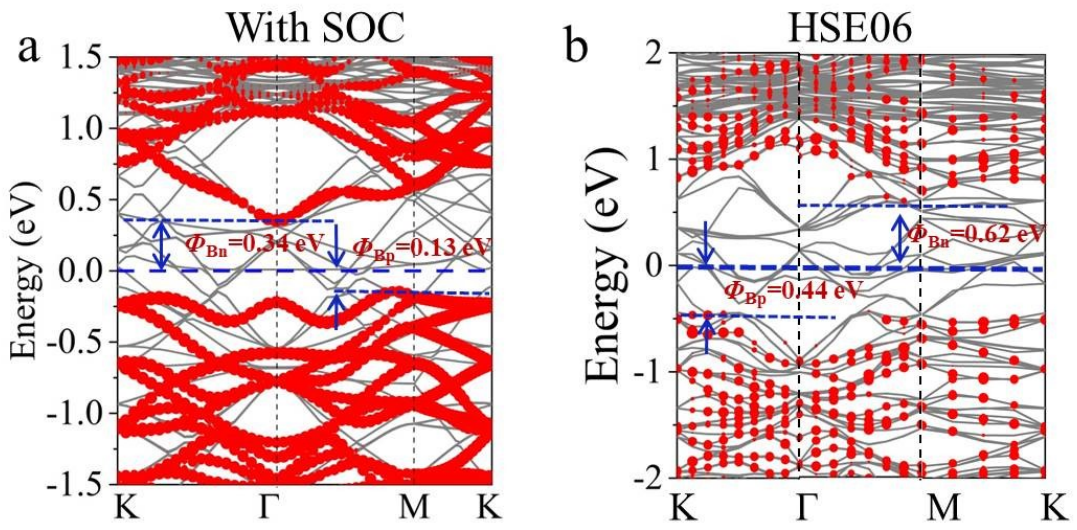

Figure S5. The projected band structures of Ti_2NF_2/α-Te heterostructure for (a) SOC and (b) HSE06 calculations, respectively.

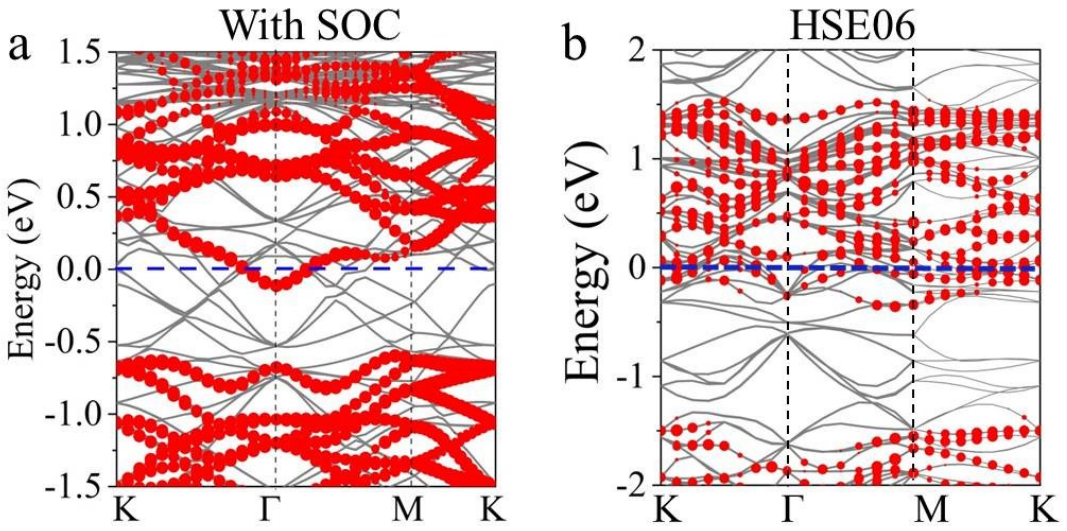

Figure S6. The projected band structures of Ti_2NF_2/α-Te heterostructure under -0.6 eV/Å for (a) SOC and (b) HSE06 calculations, respectively.

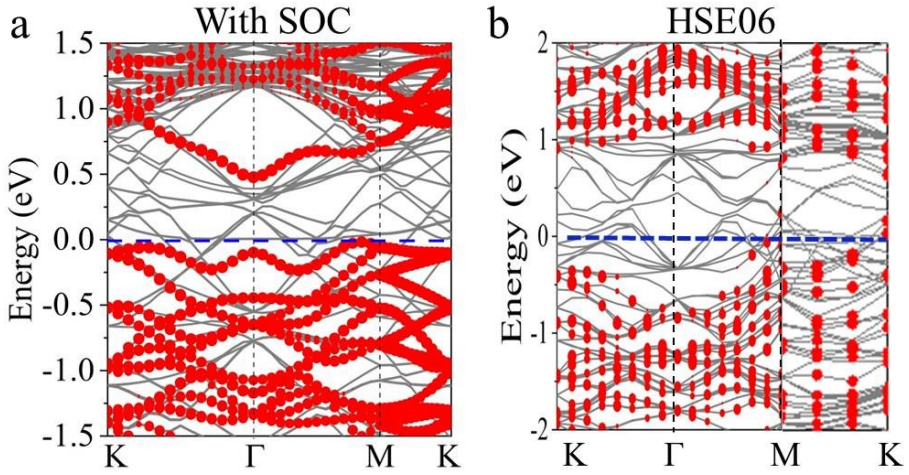

Figure S7. The projected band structures of Ti_2NF_2/α-Te heterostructure under 0.6 eV/Å for (a) SOC and (b) HSE06 calculations, respectively.

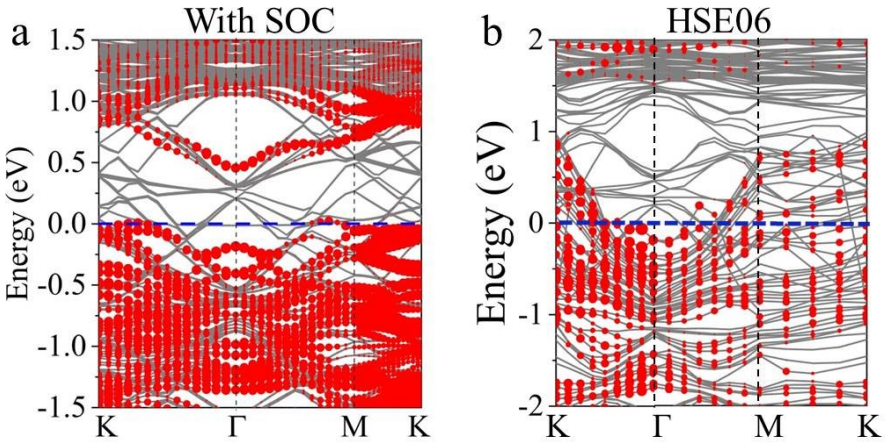

Figure S8. The projected band structures of Ti_2NF_2/α-Te heterostructure with interlayer distance 2.0 Å for (a) SOC and (b) HSE06 calculations, respectively.

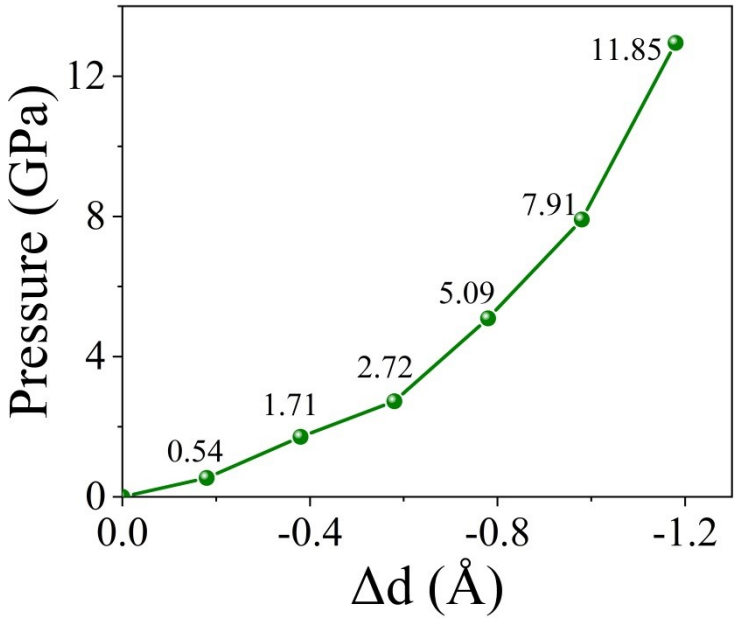

Figure S9. The calculated effective external vertical pressure as a function of the reduced interlayer distance Δ*d*.