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Supporting Information

Electrostatic gating-driven transition from Schottky contact to *p-n* junction in moiré patterned Ars/Gra heterostructure

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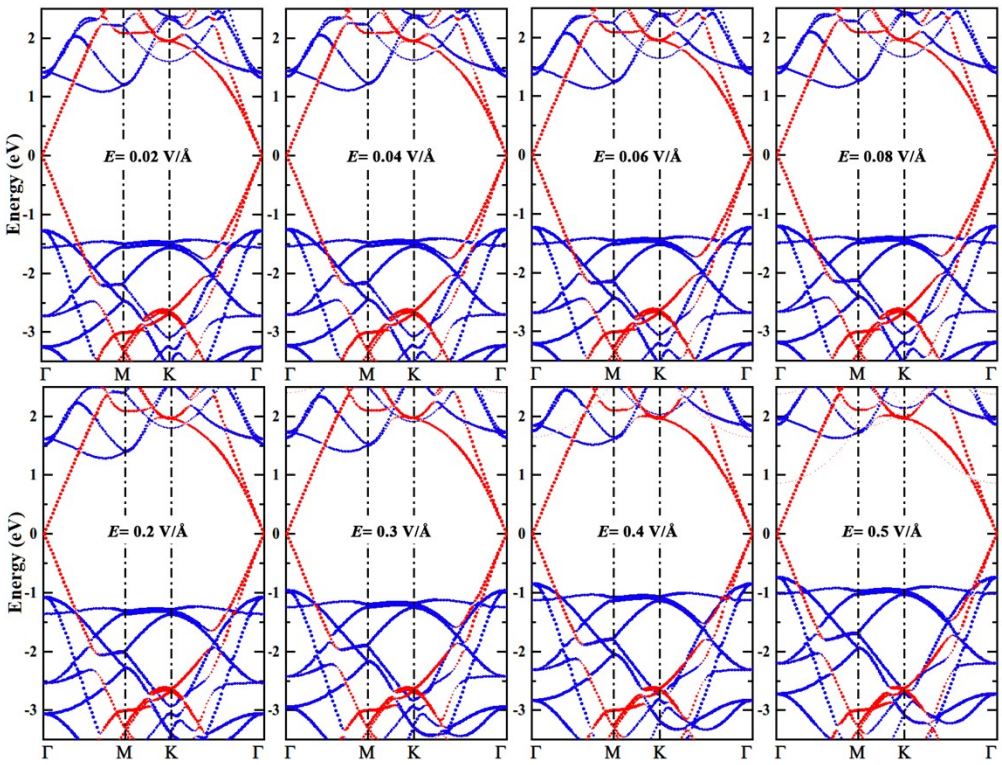

Fig. S1. The influence of electronic on projected bands of ordered stacking (3×3)-(2×2) Ars/Gra heterostructure. As the electric field increases gradually from 0.2 to 0.50 V/Å, the corresponding shift of the Dirac point refereed as Fermi level can be clearly identified. The Fermi level is set to zero.

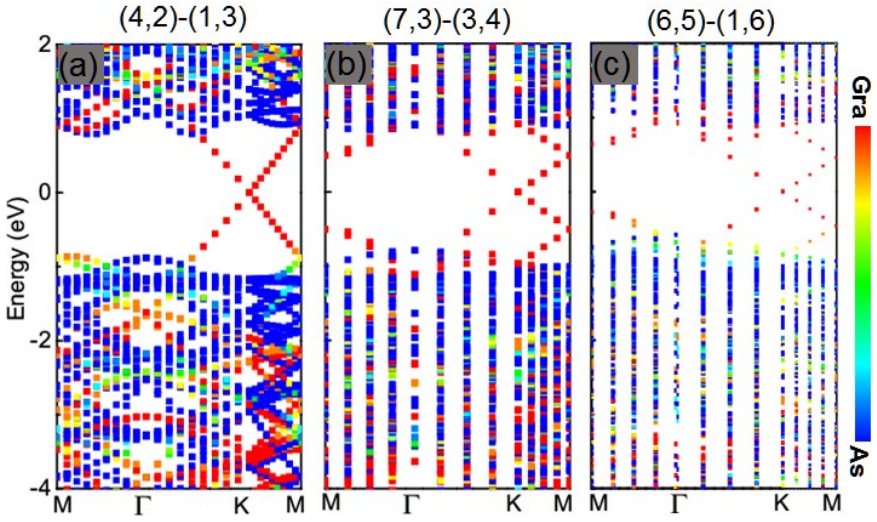

Fig. S2. Calculated the projected bands of three different Moiré structures using PBE functional.

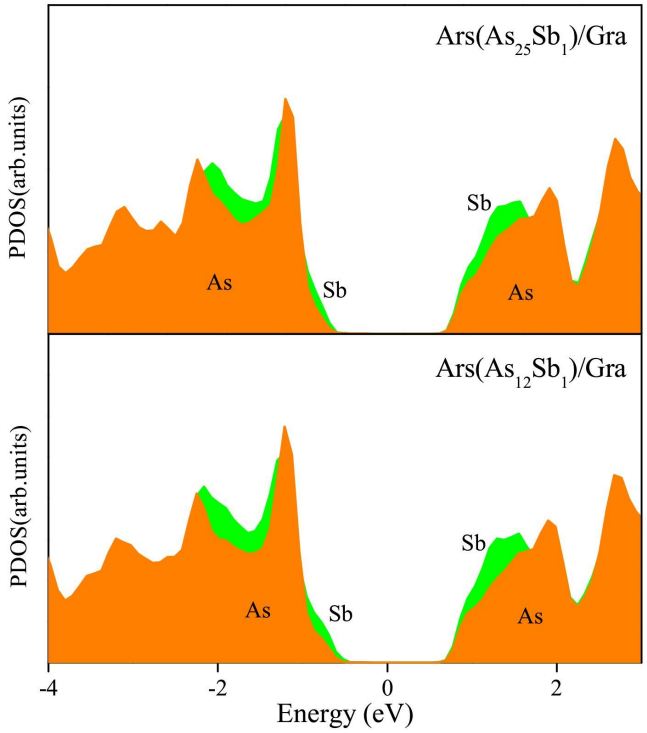

Fig. S3. The influence of doping concentration of Sb atom on the PDOS of moiré patterned Ars/Gra heterostructure, upper low concentration and lower high concentration. We clearly see that the impurity bands becomes more abundant and shift higher above the VBM. The Fermi level is set to zero.

Table SI. listed the binding energy E_b (mev/Å^2), lattice constants a (Å), number of atoms (n), twisted angles θ (°) and lattice mismatch LM (%) of ordered stacking and different Moiré patterned Ars/Gra van de Waals heterostructures.

	Ordered stacking	Moiré patterns		
	(3×3)-(2×2)	M(4,2)-(1,3)	M(7,3)-(3,4)	M(6,5)-(1,6)
E_b	-17.3	-12.8	-15.8	-12.7
a	7.404	13.059	21.936	23.646
n	26	82	232	268
θ	0.00°	32.53°	8.59°	23.68°
LM	2.59%	0.44%	0.007%	0.43%

Table II. Calculated the formation energy (E_f) of different impurity and defects. The host *M*(4,2)-(1,3) Moiré patterned heterostructure is selected.

	As-T	As-H	Gra	inter	Sub-1	Sub-2
structure						
Ef (eV)	-0.86	-0.82	-0.21	-0.34	0.40	0.35