Electronic Supplementary Information (ESI)

Graphene/Janus B$_2$P$_6$ heterostructure with controllable Schottky barrier via interlayer distance and electric field

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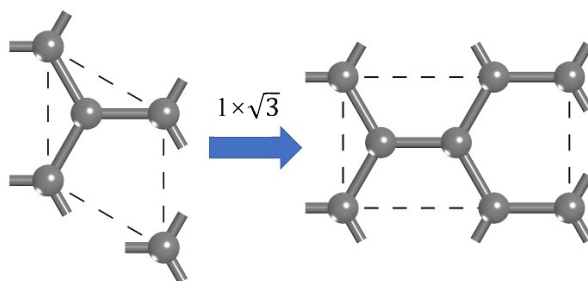
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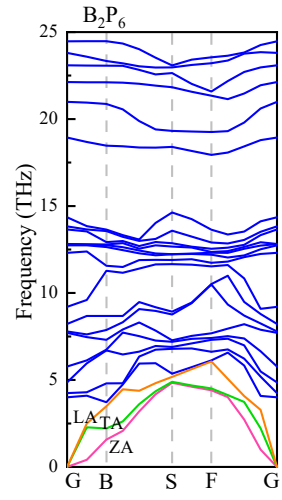[c] 111 Research Center, Hubei University of Technology, Wuhan 430068, China

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Table S1. The fractional coordinates parameters of monolayer B$_2$P$_6$ using GGA-PBE.
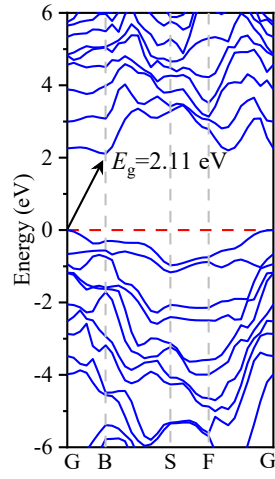
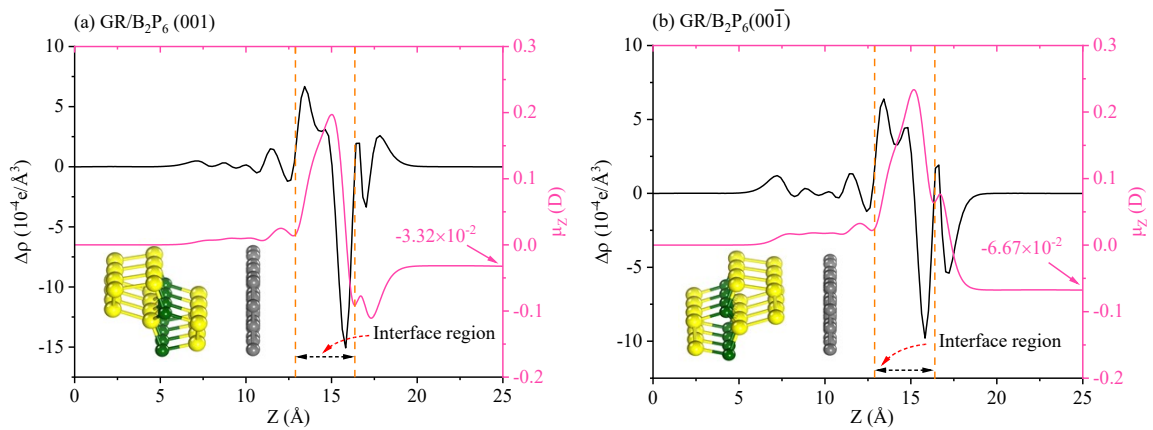| fractional coordinates	atom							
	B$_1$	B$_2$	P$_1$	P$_2$	P$_3$	P$_4$	P$_5$	P$_6$
x	0.495	0.973	0.502	0.226	0.156	0.634	0.613	0.892
y	0.262	0.762	0.763	0.263	0.262	0.762	0.263	0.763
z	0.117	0.111	0.000	0.005	0.093	0.085	0.193	0.189

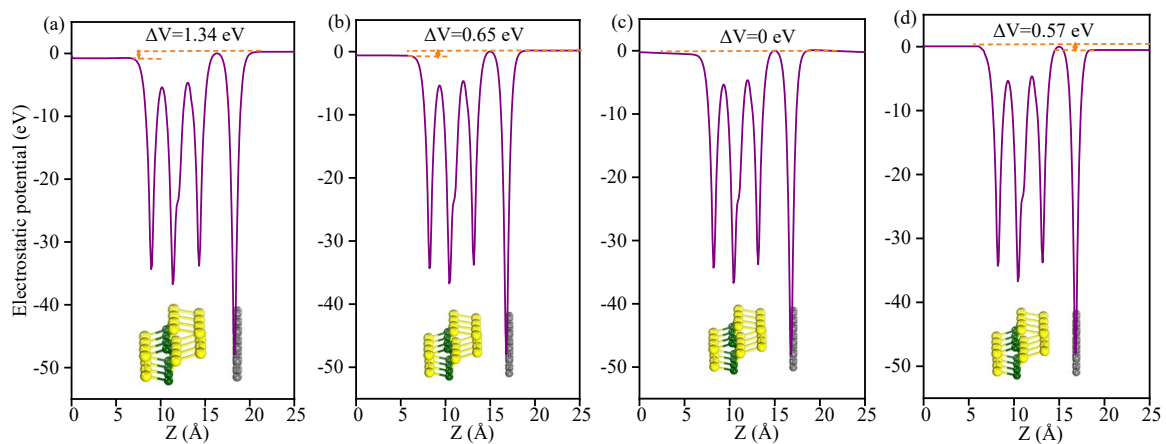**Fig. S1.** The redefined monolayer GR.

Fig. S2. Phonon dispersion curves of Janus B_2P_6 monolayer.

Fig. S3. Energy band structure of monolayer Janus B_2P_6 using hybrid functional HSE06.

Fig. S4. Planar-averaged charge density differences (black line) and dipole moments (pink line) of (a) GR/B$_2$P$_6$(001) and (b) GR/B$_2$P$_6$(00$\bar{1}$) heterostructures.

Fig. S5. The electrostatic potential for GR/B_2P_6(00**Error!**) heterostructure with various external electric field. (a)−(d) represent the external electric field 0, -0.025, -0.050 and -0.075 V·Å^{-1}.