Supporting Information

Rectifying behavior in twisted bilayer black phosphorus nanojunction mediated through intrinsic anisotropy

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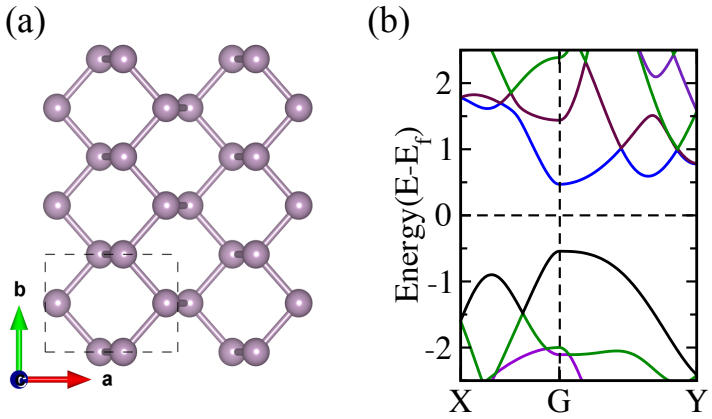

Fig. S1: Schematic picture for monolayer BP, dotted lines represent the unit cell (b) The band structure of the monolayer

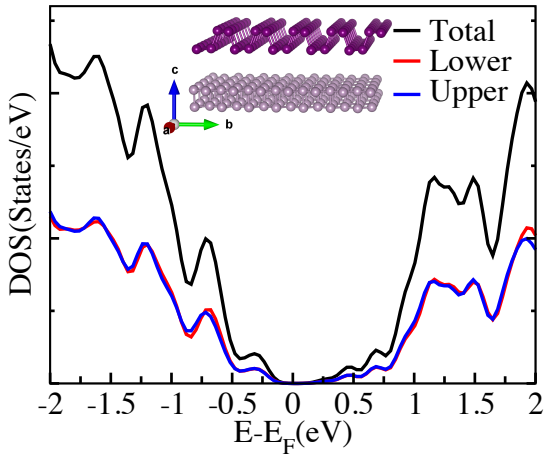

Fig. S2: Total and projected density of states of 90º twisted bilayer, blue and red curves show the density of states projected in lower and upper layers respectively

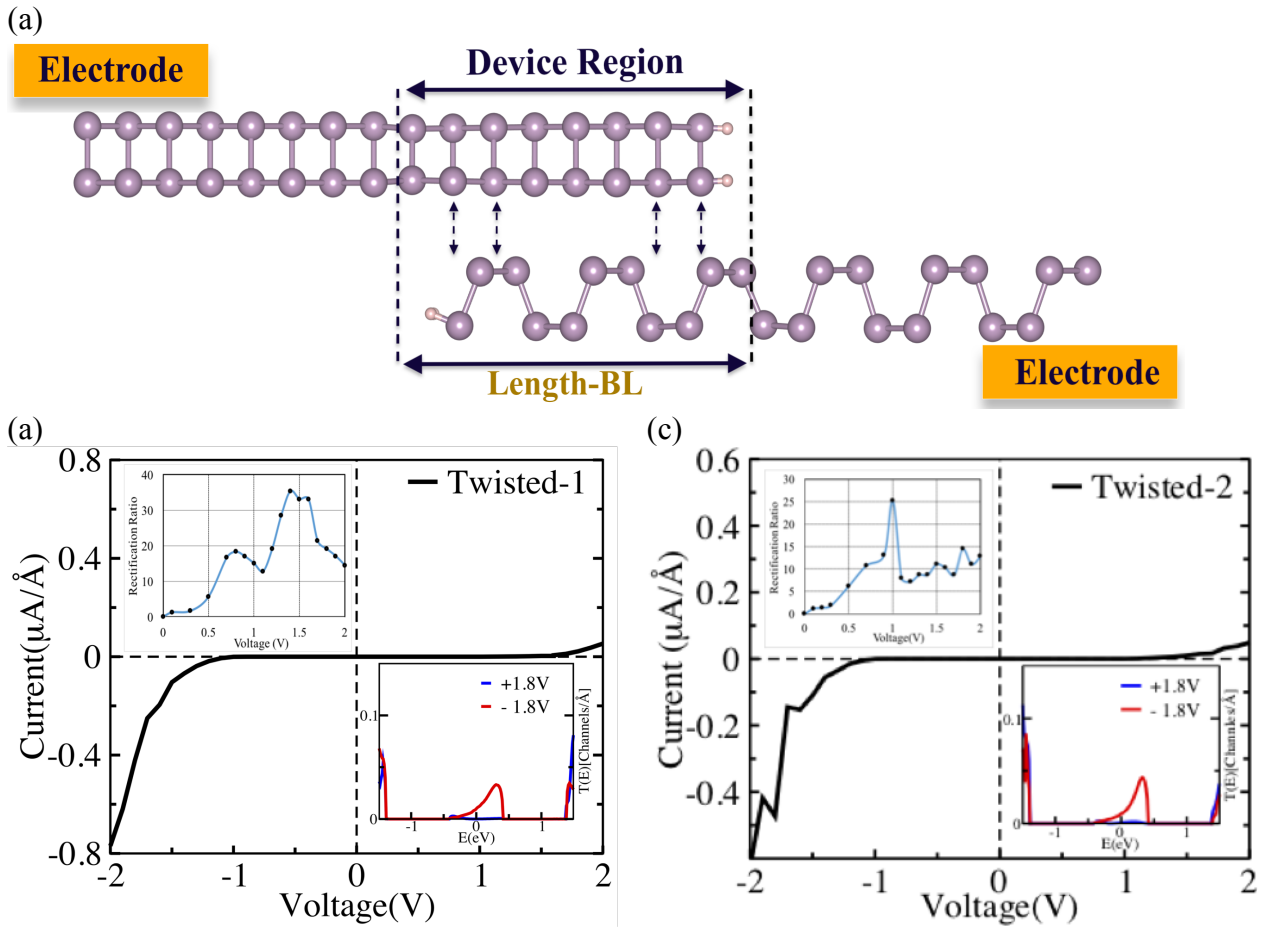

Fig. S3: (a) Schematic picture of twisted bilayer devices, Length-BL denotes the length of the bilayer region, (b) Current-Voltage Characteristics of small junction (length-BL= 10.33 Å), Upper inset shows the rectification ratio of the same devices and the lower insets show the transmission function at ±1.8V bias for both the devices (c) Current-Voltage Characteristics of big junction (length-BL= 16.22 Å), insets show rectification ratio and transmission function at ±1.8V

To understand the suitability of rectifying property of twisted bilayer nanojunction. We studied two more devices where we modulated the junction length of the twisted bilayer (Length-BL). The schematic picture is shown in Fig S3(a), where we defined the Length-BL region schematically. Further I-V characteristics show that both the devices are the potential rectifier. We see the higher current as 0.8 μA/Å at 2-volt bias in the device where the length of the bilayer is 10.33 Å, and the rectification ratio is 35 at 1.4 V bias. Whereas in the device having the junction length as 16.22 Å, shows the current as 0.65 μA/Å at 2 V bias. We also see the rectification ratio maximum at 1V bias is 25. Lower insets of the Fig. S3(b,c) show, the transmission functions at ±1.8V bias, where we can see that the negative bias has higher transmission than that of positive bias. Which is responsible for the rectifying properties of these devices. These transmission functions are relative as our primary device which has been adequately discussed in the main text.

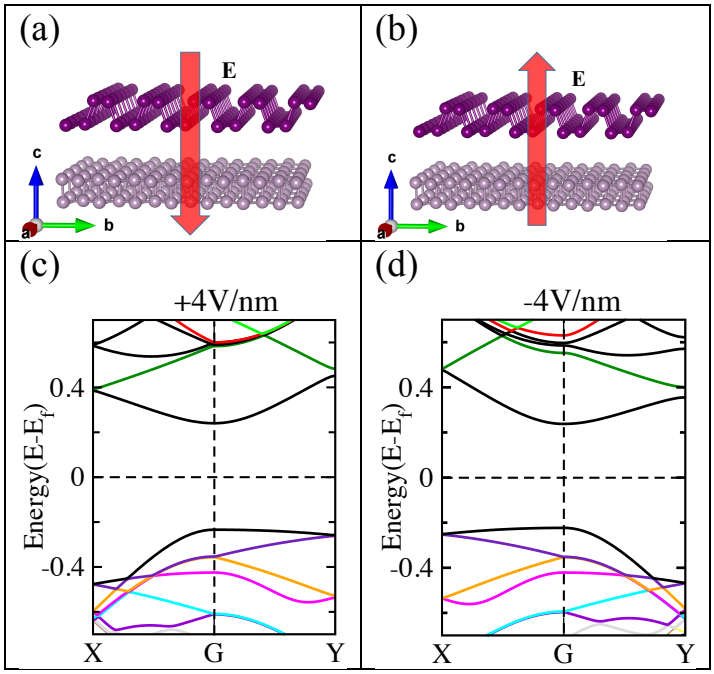

Figure S4: Electronic structure of 90º twisted bilayer BP under the vertical electric field (a,b) show the schematic picture for structure and applied electric field, (c,d) stand for band structure under the out of plane electric field 4V/nm and -4V/nm respectively