

Supplementary Information

Controlling the bandgap in graphene/h-BN heterostructure to realize electron mobility for high performing FETs

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A1. Asymmetric Structure of graphene/h-BN

In order to maintain the stability, accuracy and efficiency, we use the $3 \times 3 \times 1$ supercell structure where one graphene sheet of $3 \times 3 \times 1$ dimension is set on $3 \times 3 \times 1$ h-BN, acting as the substrate with a vacuum gap of 9.8 \AA between the layers. The angle between the graphene sheet, i.e. the host sheet and the substrate, i.e. h-BN is kept at 14° to get stable configuration with 0.4 % lattice mismatch. 48 carbon (C) atoms are there in the graphene sheet and 56 atoms of boron (B) and nitrogen (N) are present in the h-BN sheet. As a sum of 104 atoms of C, B and N are considered for computation. This two layer system is considered as the asymmetric structure where the valley K and K' are folded onto the Γ point. For the case where these valley points act as the valley degree of freedom are kept under Brillouin zone folding. Due to variation in bandgap with the reference applied field, the system will give topological properties. The effect of spin-orbit coupling has also been studied in presence of electric field. The band structure for asymmetric system has been shown in Figure S1.

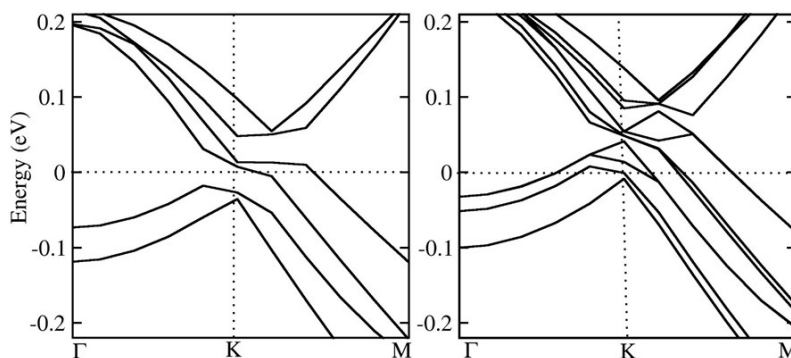


Figure S1: Band structure of asymmetric heterostructure with $3 \times 3 \times 1$ graphene sheet on h-BN without (a) and with (b) SoC.

A2. Symmetric Structure of graphene/h-BN

Accordingly, we use the $3 \times 3 \times 1$ supercell structure where one graphene sheet of $3 \times 3 \times 1$ dimension is set on $3 \times 3 \times 1$ h-BN, acting as the substrate in the layer structure. One graphene sheet is sandwiched between two sheets of h-BN with a gap of 19.6 Å. The angle between the graphene sheet, i.e. the host sheet and the substrate, i.e. h-BN is kept at 11° to get stable configuration with 0.28 % lattice mismatch. 48 carbon (C) atoms are there in the graphene sheet and 56 atoms of boron (B) and nitrogen (N) are present in the h-BN sheet. As a sum of 160 number of C, B and N atoms are considered for computation in the trilayer system. This three layer system is considered as the symmetric structure where the valley points K and K' has been folded onto the Γ point to calculate band structure. The effective electric field of h-BN opens a trivial gap without SoC. When the SoC has been taken into account, the symmetric heterostructure of graphene/h-BN is almost gapless (Fig. S2). From both DFT and TB parameters, it is noticed that the spin-orbit coupling strength is superior then the substrate field value, i.e. $t_{SO} > |U_{h-BN}|$, so the gap is falling under topological gap supporting both TB and DFT methods mentioned in the work.

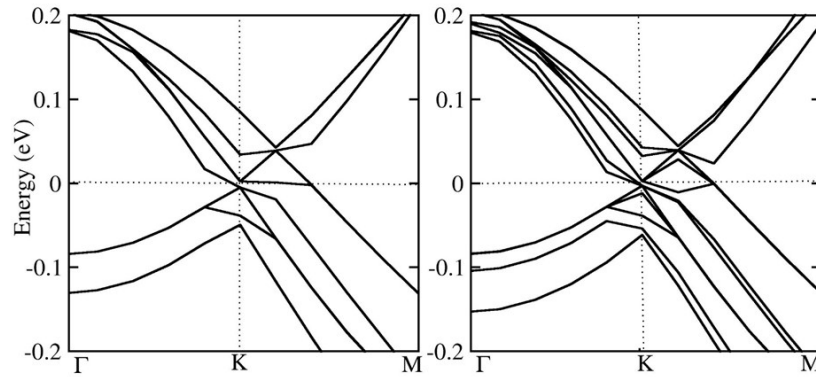


Figure S2: Band structure of Symmetric heterostructure with $3 \times 3 \times 1$ graphene sheet sandwiched between h-BN sheets without (a) and with (b) SoC.