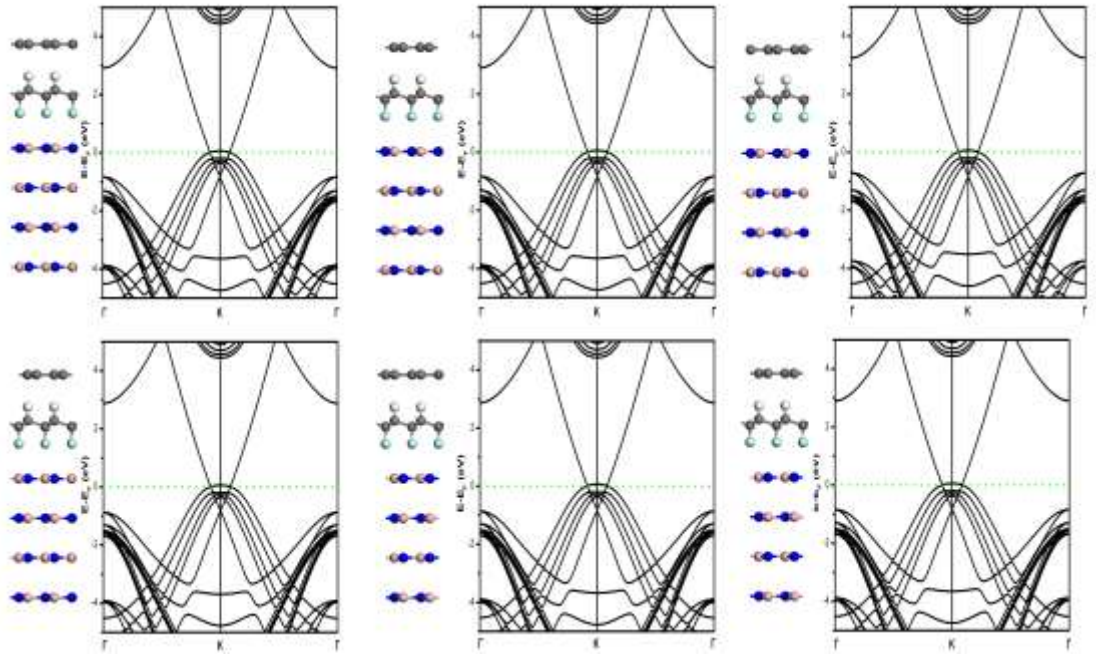
Electronic Supplementary Material (ESI) for RSC Advances

Utilisation of Janus Material for Controllable Formation of Graphene p-n Junctions and Superlattices

Xian. Fei. Chen, Yong. Fu. Zhu,* Qing. Jiang*

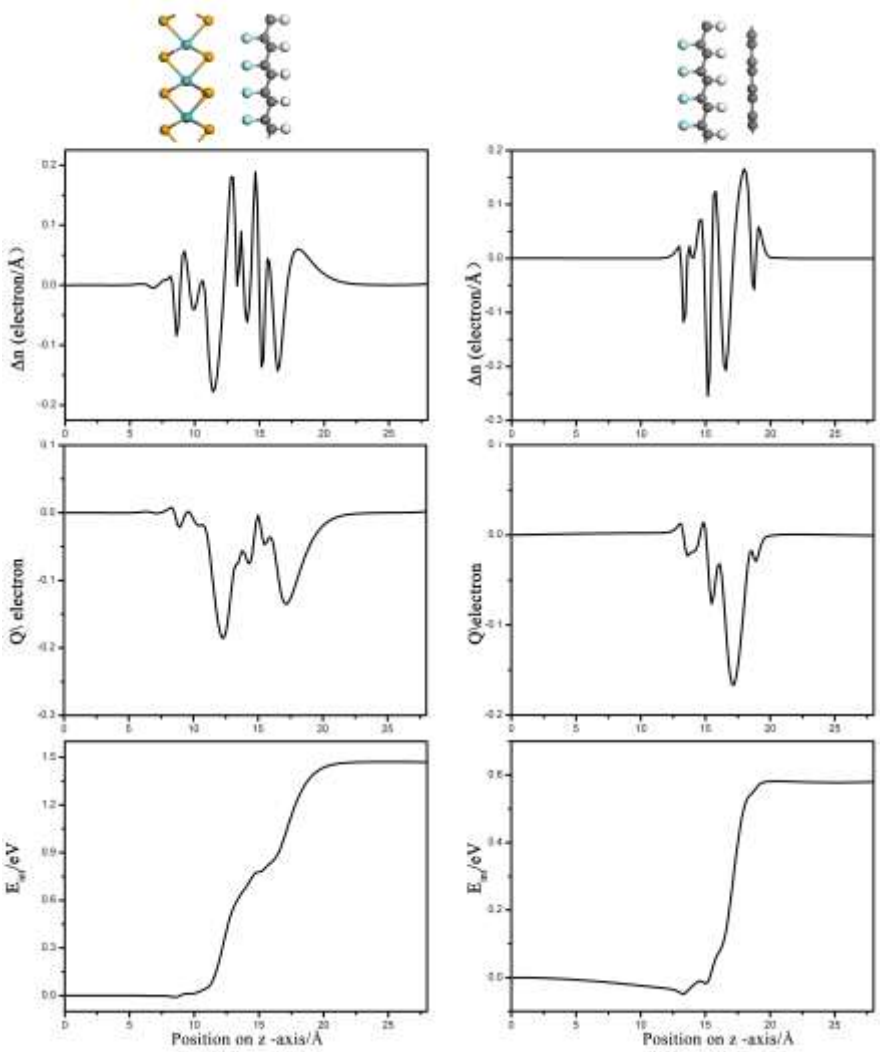
Figure S1 Atomic structures and calculated band structures of other configurations of BN/F-G-H/Graphene. The Fermi levels are set to zero as indicated by the green dot lines.

We can found that the Fermi levels shift upward, representing a p-type doping in graphene and closer examination demonstrates that the doping concentration in graphene shows little relationship with the relative disposition of graphene, buffer layer, and BN substrate.



* Corresponding author. Tel/Fax: 86–431–85095876. E–mail address: yfzhu@jlu.edu.cn, jiangq@jlu.edu.cn

Figure S2 Charge rearrangements upon inserting H-G-F, $\Delta\rho(z)$, net charge transfer, Q, as well as the resulting change in electrostatic energy, E_{int}, for $MoSe_2$/F-G-H, F-G-H/Graphene，BN/F-G-H and F-G-H/Graphene.



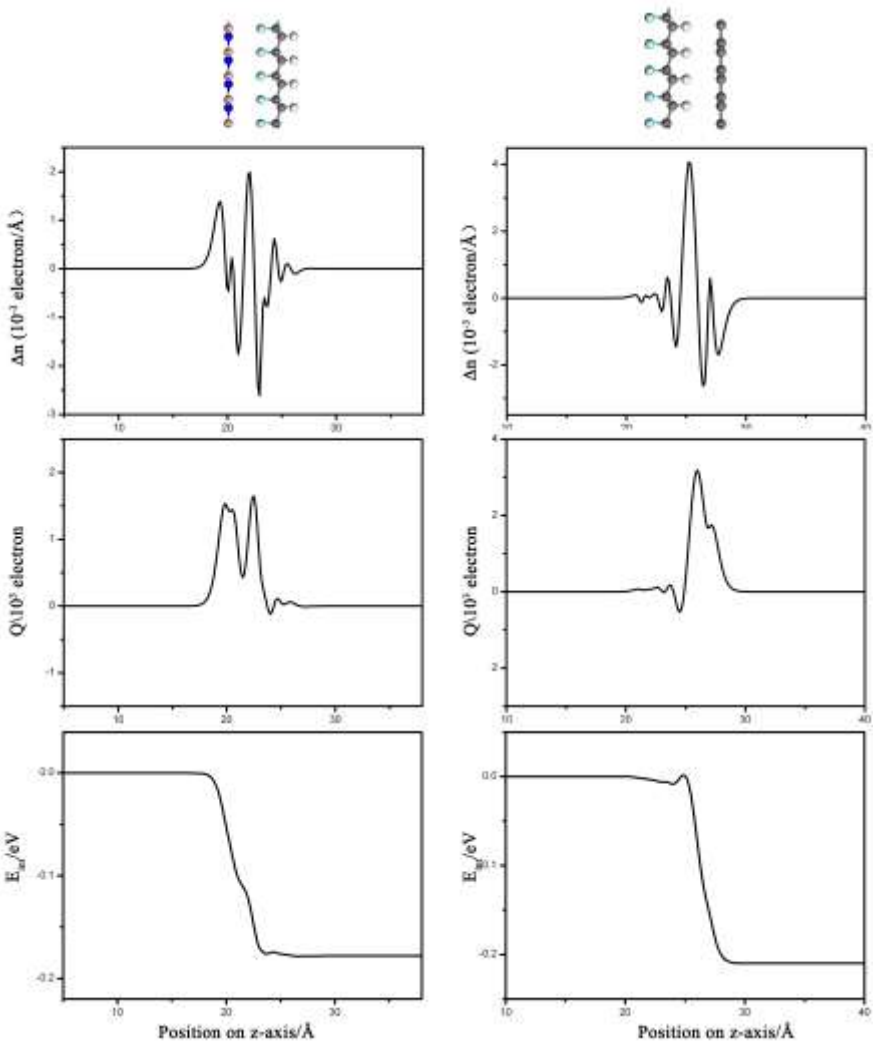


Figure S3 (a) Work function, W_{BN}, of the 4-ML BN and that for graphene W_G (e). Interface dipole layer induced potential energy steps between BN and F-G-F denoted as $\Delta E_{BN/F\text{-}G\text{-}H}$ (b) and that between F-G-H and graphene layer denoted as $\Delta E_{F\text{-}G\text{-}H/graphene}$ (d). (c) Potential energy step, ΔE_{vac}, across the F-G-H layer. (f) The plane-averaged electron potential energy of the combined system.

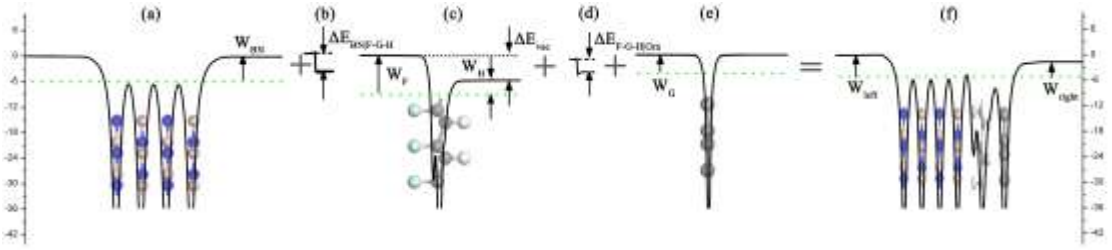


Figure S4 Optimized atomic structures and corresponding band structure of BN|H-G-F|Graphene. The bands derived from graphene and H-G-F layers are highlighted via pink and green curves, respectively.

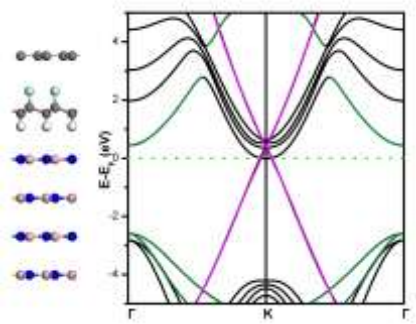


Figure S5 Dependence of the graphene Dirac point relative to the system Fermi level plotted as a function of an external field for both BN/F-G-H/Graphene and BN/H-G-F/Graphene. The Fermi level is set to zero in all plots.