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Intrinsic Electron-Hole Puddles in Graphene on Hexagonal Boron-Nitride MENNO BOKDAM, TAHER AMLAKI, GEERT BROCKS, PAUL J. KELLY, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — When graphene is placed on top of hexagonal boron nitride (h-BN), the 1.7% lattice mismatch between the honeycomb lattices of graphene and h-BN leads to the formation of superstructures that are observed as moiré patterns in scanning tunneling microscopy images [1,2]. Using first-principles calculations and ignoring the incommensurability, we observed the formation of a dipole layer at the graphene|h-BN interface [3]. The strength and direction of this dipole layer depends sensitively on the local bonding of the carbon atoms to the substrate i.e. on the details of how the graphene layer is positioned on top of h-BN. The dipole layer is accompanied by a step in the electrostatic potential, which ranges from +120 to -30 meV depending on the configuration. Because the lattice mismatch is so small, the local bonding configuration varies slowly in a graphene|h-BN superstructure. We predict that the Dirac cone will follow the slowly varying potential created by the interface dipole layer even when screening effects are included. This then leads to the formation of regions of electron- and hole-doped graphene: intrinsic electron-hole puddles that will limit the mobility in this system. We make a comparison with graphene on molybdenum disulphide (MoS_2) where a dipole layer is also formed but where we do not expect intrinsic electron-hole puddles to be formed. [1] R. Decker et al., Nano Lett. 11, 2291-2295 (2011) [2] J.M. Xue et al., Nature Mat. 10, 282-285 (2011) [3] M. Bokdam et al., Nano Lett. 11, 4631-4635 (2011)

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