A novel synthesis route with large-scale sublattice asymmetry in boron doped graphene on Ni(111)

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One of the most promising ways to functionalize graphene, among the multiple developed approaches, is incorporation of heteroatom in the carbon sp2 lattice, as it is proven to be an efficient and versatile method for controllably tuning the chemistry of graphene. [1,2] Here, we present a unique, contamination free and versatile method of creating boron reservoir in the bulk of Ni(111) single crystal, which allows the preferential sublattice incorporation of boron atoms in the graphene network during the standard chemical vapor deposition growth process. We combine experimental (LEED, STM, XPS,) and theoretical (DFT, simulated STM) studies to understand the structural and chemical properties of the substitutional boron dopants in these highly reproducible flat layers of doped graphene. Along with previously observed B fcc defect [3], we have observed for the first time, two defects namely, B top and B Oct site in the subsurface. Extensive high resolution STM investigations confirm the presence of low as well as high concentration regions of boron doping in graphene grown on Ni(111) single crystal, suggesting non uniform boron incorporation. The low concentration boron doped regions do not show a specific choice of sublattice for incorporation, whereas in the high boron concentration regions, one of the sublattice is preferred for the incorporation. This generates an asymmetric sublattice doping for as grown boron doped graphene layer. This asymmetric doping has been theoretically predicted to possess the notable band gap [4,5] This novel route of boron incorporation in graphene network can therefor result as a suitable candidate for electronic applications.

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