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Electronic Structure of Boron-doped Graphene Nanoribbons on Metallic Substrates: Ab Initio Studies and Scanning Probe Measurements[1] FANGZHOU ZHAO, TING CAO, ZAHRA PEDRAMRAZI, CHEN CHEN, GIANG NGUYEN, ARASH OMRANI, HSIN-ZON TSAI, DANIEL RIZZO, TRINITY JOSHI, CHRISTOPHER BRONNER, WON-WOO CHOI, RYAN CLOKE, TOMAS MARANGONI, FELIX FISCHER, MICHAEL CROMMIE, STEVEN LOUIE, Univ of California - Berkeley — Graphene nanoribbons (GNRs) have been a very promising candidate for nanoelectronic devices because of their tunable electronic structure with varying width and edge termination. Introducing boron dopants in the backbone of the GNRs further creates new dopant states in the band gap of pristine GNR. In this work, we used density functional theory calculations to investigate the electronic structure of freestanding boron doped GNRs as well as that of GNRs on gold substrate. We find that the boron dopant states change dramatically with doping concentration and interaction with the substrate. The boron atoms bind strongly to the gold substrate, resulting in new features in the GNR's electronic structure. Our calculated results are in good agreement with experimental measurements by scanning tunneling microscopy and spectroscopy.

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