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Quasiparticle Band Gaps of Graphene and Graphone on Hexagonal Boron Nitride Substrate NEERAV KHARCHE, SAROJ NAYAK, Computational Center for Nanotechnology Innovations, Department of Physics, Rensselaer Polytechnic Institute — Graphene holds great promise for post-silicon electronics; however, it faces two main challenges: opening up a band gap and finding a suitable substrate material. Graphene on hexagonal boron nitride (hBN) substrate provides a potential system to overcome these challenges. While theoretical studies suggested a possibility of a finite band gap of graphene on hBN, recent experimental studies find no band gap. We have studied graphene-hBN system using the first-principles density functional method and the many-body perturbation theory within GW approximation [1]. A Bernal stacked graphene on hBN has a band gap on the order of 0.1 eV, which disappears when graphene is misaligned with respect to hBN. The latter is the likely scenario in realistic devices. In contrast, if graphene supported on hBN is hydrogenated, the resulting system (graphone) exhibits band gaps larger than 2.5 eV. The graphone band gap is due to chemical functionalization and is robust in the presence of misalignment, however, it reduces by about 1 eV due to the polarization effects at the graphone/hBN interface.

[1] N. Kharche and S. K. Nayak, *Nano Lett.*, DOI: 10.1021/nl202725w, (2011).

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