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Defect-mediated coupling between graphene monolayer and hexagonal boron nitride sheet SOHEE PARK, Department of Materials Science and Engineering, Seoul National University, GUNN KIM, Department of Physics, Graphene Research Institute and Institute of Fundamental Physics, Sejong University — Hexagonal boron nitride (hBN) offers an ideal substrate for graphene-based devices and promises to deliver higher device performances. A monolayer of graphene will be weakly coupled to a hBN substrate, but defects between the layers or within the hBN substrate are likely to enhance this coupling. We thus employed first-principles calculations to determine what effect such defects would have on the structural and electronic properties of graphene. We show in our paper that a boron (nitrogen) monovacancy in the hBN layer gives rise to p-doped (n-doped) graphene and that metal atom impurities may increase the energy of the Fermi level of graphene. We also demonstrate that the presence of monovacancies and some impurity atoms could induce residual scattering. However, we found that small triangular defect in hBN are unlikely to result in significant changes in the electronic transport of graphene.

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