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Impurity induced states in monolayer hexagonal BN[1] SUSUMU SAITO, YOSHITAKA FUJIMOTO, TAKASHI KORETSUNE, Department of Physics, Tokyo Insitute of Technology — Ever since the experimental production of graphene, it has attracted much attention as a future device material with monoatomic-layer thickness although the material has metallic electronic transport properties. In this respect, a monoatomic layer of hexagonal boron nitride (hBN) can be even more interesting device material to be used in the future since it possesses semiconducting electronic properties with the fundamental energy gap. We study the electronic properties of the hBN monolayer in the framework of the density-functional theory and the many-body theory with Hedin's GW approximation. Both donor and acceptor-type states induced by the substitutional C impurity atom at B and N sites respectively are studied in detail. In addition, we also study the impurity states induced by the substitution of the cluster of atoms in hBN by the graphene flake. These impurity states are found to be generally rather deep, and therefore we discuss the possible methods to change the ionization energies of these impurity-induced states [1].

[1] Y. Fujimoto, T. Koretsune, and S. Saito, to be published.

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Susumu Saito
Department of Physics, Tokyo Insitute of Technology

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