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Stabilities and electronic structures of B and N defects in bilayer graphene[1] YOSHITAKA FUJIMOTO, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology — Since its discovery, atomically thin monolayer of graphene has received a lot of attention. The few-layered sheets of graphene have also attracted great attention both scientifically and technologically since they exhibit different electronic structures from monolayer graphene. One of the effective ways to tune the electronic properties of carbon-based nanomaterials is to dope them with B and N atoms. Here, we study energetics and electronic properties of B and N defects in bilayer graphene, based on the first-principles density-functional theory. All kinds of dopant sites and stacking patterns (AA and AB) of bilayer sheets are studied and the site-dependent and independent behaviors of the dopants are found. We also report the electronic structures and study the STM images of doped bilayer graphene. While B-doped and N-doped defects show different STM images, the STM images are shown to be similar for AA and AB stacking patterns in both B- and N-doped defect cases.

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