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Computer simulation of STM images of vertical heterostructures of graphene/hexagonal boron nitride with intercalated atoms[1] GUNN KIM, JUNSU LEE, Sejong Univ — Using density functional theory, we did computational simulations of scanning tunneling microscopy of vertical graphene/hexagonal boron nitride heterostructures with an intercalated atom (Li, K, Cr, Mn, Co or Cu). A plane-wave basis set was employed with a kinetic energy of 400 eV. The form of the Perdew-Burke-Ernzerhof type was utilized for the exchange-correlation energy functional. To obtain the more accurate result, the van der Waals interaction was also considered. In the computer-simulated scanning tunneling microscopy (STM) images in the Tersoff-Hamann scheme, we demonstrated that the single impurity atom between Gr and hBN sheets is detectable. We observed three different STM patterns on the graphene side. These can be classified by group 1 (Li, Co, and Cu), group 2 (Cr and Mn), and group 3 (K), which have hexagonal, circular, and wide bright spot patterns around the impurity atom, respectively. Although Co and Cu are both in group 1, the Co atom shows stronger d orbital character than the Cu atom. Interestingly, in the case of the Co atom, the simulated STM images are quite different at bias voltages of -0.1 V and +0.1 V. While C p_z-Co d_{yz} hybridization occurs at the bias voltage of -0.1 V, C p_z-Co d_{xz} hybridization occurs at the bias voltage of +0.1 V.

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