SW-P013

Ab Initio Investigations of Shapes of the h-BN Flakes on Copper Surface in Relation to h-BN Sheet Growth

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The hexagonal boron nitride (h-BN) sheet, a 2D material like graphene sheet, is comprised of boron and nitrogen atoms. Similar to graphene, h-BN sheet has attractive mechanical properties while it has a wide band gap unlike graphene. Recently, many experimental groups studied the growth of single BN layer by chemical vapor deposition (CVD) method on the copper substrate. To study the initial stage of h-BN growth on the copper surface, we have performed density functional theory calculations. We investigate several adsorption sites of a boron or nitride atom on the Cu surfaces. Then, by increasing the number of adsorbed B and N atoms, we study formation behaviors of the BN flakes on the surface. Several types of BN flakes atoms such as triangular, linear, and hexagonal shapes are considered on the copper surface. We find that the formation of the BN flake in triangular shape is most favorable on the surface. On the basis of the theoretical results, we discuss the growth mechanism of h-BN layer on the copper surfaces in terms of its shapes in the initial stage of growth.

Keywords: h-BN, growth mechanism, Cu surface, CVD

SW-P014

First-principles Study of MoS2 Nanostructures with Various Adsorbates

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Recently, molybdenum disulfide (MoS2) nanostructures have been investigated for applications of lithium-ion batteries, solar cell, and gas sensors. In this regard, we have studied atomic and electronic properties of MoS2 nanostructures with adsorbed atoms and molecules using density functional theory calculations. Our calculations reveal that the several atoms such as H, C, N, and F are chemically bound to several sites on the two-dimensional (2D) MoS2 surface. On the other hand, various contamination molecules such as CO, CO2, NO, NO2, and NH3 do not bind to the surface. Next, adsorption of various molecules on the one-dimensional (1D) armchair MoS2 nanoribbon is investigated. Contrary to the case of 2D MoS2 monolayer surface, some molecules (CO and NO) are bound well to the edge of the MoS2 nanoribbon. We find that the molecular states due to adsorption are located near the Fermi level, which makes the band gap narrower. Therefore, we suggest that monolayer MoS2 nanoribbons be used as the gas sensors or detectors.

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Keywords: MoS2, adsorbates, gas sensor