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Doping, strain engineering, and interlayer interaction in bilayer hexagonal boron nitride sheets[1] SUSUMU SAITO, YOSHITAKA FUJIMOTO, Tokyo Inst of Tech - Tokyo — We study electronic properties of bilayer hexagonal boron nitride (h-BN) sheets with different stacking sequences in the framework of the density-functional theory. The bulk h-BN material usually takes the so-called AA (or AA') stacking, corresponding to the "non-polar" bilayer h-BN sheet. On the other hand, the rhombohedral BN takes the ABC stacking, and the corresponding bilayer sheet has "upper" and "lower" layers which are not equivalent with each other. Interestingly, the energetics of stacking sequences for bilayer h-BN sheets is found to be different from that for bulk h-BN materials. We report that strain engineering for bilayer h-BN sheets can possess much wider possibilities than that for monolayer h-BN due to the modification of the interlayer interaction. We also study the substitutional C doping into bilayer h-BN sheets, and report the energetics and the strain effect for these C-doped sheets. Finally we discuss the similarities and differences between bilayer h-BN sheets and double-wall h-BN nanotubes.

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