

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Strain, stabilities and electronic properties of hexagonal BN bilayers¹ YOSHITAKA FUJIMOTO, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology — Hexagonal boron nitride (h-BN) atomic layers have been regarded as fascinating materials both scientifically and technologically due to the sizable band gap. This sizable band-gap nature of the h-BN atomic layers would provide not only new physical properties but also novel nano- and/or optoelectronics applications [1]. Here, we study the first-principles density-functional study that clarifies the biaxial strain effects on the energetics and the electronic properties of h-BN bilayers [2]. We show that the band gaps of the h-BN bilayers are tunable by applying strains. Furthermore, we show that the biaxial strains can produce a transition from indirect to direct band gaps of the h-BN bilayer. We also discuss that both AA and AB stacking patterns of h-BN bilayer become feasible structures because h-BN bilayers possess two different directions in the stacking patterns. [1] Y. Fujimoto and S. Saito, Phys. Rev. B 93 (2016) 045402. [2] Y. Fujimoto and S. Saito, submitted to Phys. Rev. B.

¹Supported by MEXT Elements Strategy Initiative to Form Core Research Center through Tokodai Institute for Element Strategy, JSPS KAKENHI Grant Numbers JP26390062 and JP25107005.

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Date submitted: 11 Nov 2016

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