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Yoshitaka Fujimoto

Tokyo Institute of Technology, Japan

Strain induced effects of hexagonal boron nitride atomic layers: a first-principles density-functional investigation

Since experimental realization of a graphene sheet, two-dimensional atomic-layer sheets have received much attention from the viewpoint of nanoscience and nanotechnology. Among them, hexagonal boron nitride (h-BN) atomic-layer sheets are also expected to be an important material since they possess several superior properties similar to a graphene. In the aspect of the electronic structures, both two materials exhibit considerably different features; graphene is a zero-gap material, whereas h-BN monolayer is a wide-gap material. One of the effective ways to tune electronic properties of nanomaterials is to apply strains to them. For example, the band gaps and the impurity states of h-BN monolayers are tunable by applying strains. In this talk, I will report strain effects on the stabilities and the electronic properties of h-BN atomic layers using first-principles density-functional calculations. I demonstrate the possible methods to tune the band gaps and the ionization energies of the impurity induced states in h-BN atomic layers. We also discuss the relationship among applied strains, band gaps and the impurity-related states of h-BN atomistic layers.

Biography

Yoshitaka Fujimoto received his PhD degree in Engineering from Osaka University, Japan. After receiving his PhD, he worked at the University of Tokyo and the University of Tsukuba. He joined Department of Physics, Tokyo Institute of Technology as an Assistant Professor. He has published more than 50 technical papers in peer-reviewed journals, reviews, book, book chapters, etc., and has served as referee of many international journals, organizations and committees in conferences.

fujimoto@stat.phys.titech.ac.jp

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