Abstract Submitted
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Doping, adsorption, and polarity of atomic-layer materials: A predictive theory from systematic first-principles study[1] SUSUMU SAITO, YOSHITAKA FUJIMOTO, Department of Physics, Tokyo Institute of Technology, TAKASHI KORETSUNE, RIKEN Center for Emergent Matter Science — Based on the extensive first-principles electronic-structure study of various doped hexagonal boron-nitride (h-BN) atomic layers as well as that of various doped graphene and carbon nanotubes, we propose a simple but predictive theory of polarity in doped atomic-layer materials. We first report the electronic structure of the pristine h-BN, h-BN layers with B and B_3N vacancies which have been experimentally produced and observed frequently, and doped h-BN layers, and show that both p-type and n-type h-BN layers can be produced in a variety of ways. We next review the electronic structure of doped graphene and carbon nanotubes and the effect of the H adsorption which can even change the polarity of the system. Finally we propose a simple but predictive theory which is based on the number of valence electrons of each system, and can explain the polarities of all the h-BN, graphene, and nanotube-based systems studied so far.

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