Structural, Electronic, and Magnetic Properties of the Two-Dimensional Graphene-BN System Studied by First-Principles Simulations

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The single-atom sheet of a hybrid system of graphene and boron nitride (monolayer thick sheets of hexagonal BN) has been recently explored experimentally having several applications in mind [1]. This 2D atomic layer that goes beyond graphene may be produced with a variety of compositions and therefore may exhibit a wide range of structural and electronic properties. This gives an opportunity of band-gap engineering to span the entire range of materials from metals to insulators. A BN/graphene interface with atomically sharp boundary has been also recently synthetized extending even more the applicability of those hybrid materials [2]. In order to get more insight about the properties of these new systems, we performed extensive first-principles calculations based on density functional theory to determine their structural, electronic, and magnetic properties. Several aspects for those systems were considered with an emphasis on: the mechanical properties of graphene with BN domains of different shapes and sizes, the details of the bonding and dipole formation at the BN/graphene interface, and the presence of magnetic properties involving local magnetic moments at the BN/graphene interface and in defects in the graphitic network.