

Hybrid Density Functional Study of 2D Graphene-Boron Nitride Nanostructures

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Graphene has attracted enormous research interest in the last few years because of its intriguing physics as well as application potential. Recent synthesis of 2D BNC nanostructures by doping graphene with a wide bandgap insulator boron nitride (BN) has unveiled new possibilities for this material [1]. BNC nanostructures are semiconductors and possess interesting properties that are distinct from the parent compounds. Reliable theoretical estimates can play a big role by predicting the feasibility and usefulness of still largely unexplored BNC nanostructures, and hence provide a route to engineer their electronic structures. We study electronic structures and magnetic properties of a variety of 2D BNC nanostructures using a hybrid exchange-correlation functional HSE (Heyd-Scuseria-Ernzerhof) in density functional theory (DFT). We show that their properties can be gradually tuned and are sensitive to composition and the type of configurations. In agreement with experimental observation, a strong tendency to phase-segregate exists for low concentration of BN in graphene.

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[1] L. Ci *et al.*, Nature Materials **9**, 430 (2010).