Abstract Submitted
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Hybrid density functional study of 2D graphene-boron nitride (BCN) nanostructures[1] AMITA WADEHRA, HYOUNGKI PARK, JOHN W. WILKINS, The Ohio State University, ANTONIO H. CASTRO NETO, Graphene Research Centre, National University of Singapore and Boston University — Graphene has attracted enormous research interest in the last few years because of its intriguing physics as well as application potential. Recent synthesis of BCN nanostructures by doping graphene with a wide bandgap insulator boron nitride (BN) has unveiled new possibilities for this material [1]. BCN nanostructures are semiconductors and possess interesting properties that are distinct from the parent compounds. Reliable theoretical estimates can predict the feasibility and usefulness of still largely unexplored BCN nanostructures, and provide a route to engineer their properties. We study electronic structures of a variety of 2D BCN nanostructures using hybrid functional HSE 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. We also investigate magnetic properties of graphene containing substitutional nitrogen atoms, and their suitability for magnetic devices.

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

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