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Electronic and magnetic properties of 2D BCN nanostructures[1]

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Recent developments of two-dimensional (2D) nanomaterials hold great promises for future electronics, optics and spintronics. Since the isolation and electronic characterization of graphene, other layered 2D crystals also have been synthesized. In particular, carbon can be combined with its neighboring atoms in the periodic table, boron and nitrogen as hexagonal BN (h-BN), to obtain hybrid BCN configurations. These BCN 2D nanostructures show a rich variety of physical properties, distinct from parent materials. Their electronic properties can in principle be tuned by varying the concentration of each of the three elements. We study electronic structures of a variety of 2D BCN nanostructures using hybrid functional HSE in density functional theory (DFT). We show that their electronic properties can be gradually tuned by composition and the atomic configuration of three elements. We demonstrate that the substitution-induced impurity states, associated with carbon atoms, and their interactions dictate the electronic structure and properties of C-doped h-BN. Stacking of localized impurity states in small C clusters embedded in h-BN forms a set of discrete energy levels in the wide gap of h-BN, leading to electronic structures of quantum dots made of carbon nano-domains for applications in optics and opto-electronics. We also show that half-metallic electron transport can be achieved by low concentration substitutional doping of only one sublattice of graphene by nitrogen or boron atoms. The delocalized spin-densities induced by the unpaired electrons at substitutional sites permeate only through the sublattice where the nitrogen (boron) atoms belong. For interacting nitrogen (boron) atoms located along the "zigzag" direction and in the same sublattice the ferro-magnetic spin-ordering is energetically favored, and substitution-induced impurity states selectively disturb the spin-polarized π-orbital of that same sublattice.

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