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Accurate computational studies of carbon doped two-dimensional boron-nitride[1] HYOUNGKI PARK, AMITA WADEHRA, JOHN W. WILKINS, Department of Physics, The Ohio State University, ANTONIO H. CASTRO NETO, Graphene Research Centre, National University of Singapore, Singapore and Department of Physics, Boston University — Advances in development of atomic-layer crystals with a plethora of new materials are greatly extending the range of possible applications of these two-dimensional (2D) materials. One of these materials is the hexagonal structure of boron nitride (h-BN). Hexagonal BN has a wide band gap and a lattice constant similar to that of graphene. We show that even small quantities of C atoms can offer new functionalities and transform h-BN to be an amazing playground for 2D physics. Large-scale accurate density-functional-theory calculations with the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional reveal the electronic and the magnetic properties of h-BN with substitutionally embedded carbon atoms. Results of local magnetic moments induced by substitution and their interactions are presented for low C concentrations. We also show the electronic structures of quantum dots made of carbon nano-domains for applications in optics and opto-electronics.

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