

Accurate Computational Studies of Carbon Doped Two-Dimensional Boron-Nitride

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The great success of graphene has vastly extended the range of possible applications of an atomic-layer two-dimensional (2D) crystals with a plethora of new materials. One of these materials is the 2D hexagonal structure of boron nitride (h-BN). h-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 study 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 will be presented for low C concentrations. We will also show the electronic structures of quantum dots made of carbon nano-domains for applications in optics and opto-electronics.

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