Induced magnetic states upon electron-hole injection at B and N sites of hexagonal Boron Nitride bilayer: A DFT study

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Abstract

We have reported the electronic, magnetic, and optical properties of the top layer carbon-doped hexagonal Boron Nitride(h-BN) bilayer at B/N-sites using the density functional theory implemented in Quantumwise VNL-ATK package. The calculated structural and electronic properties of the h-BN bilayer are in agreement with the previously reported results. A single carbon doping on B and N sites modifies the large band gap semiconducting behaviour of h-BN bilayer similar to dilute magnetic semi-conducting material with a net magnetic moment of 1.001 μ B and 0.998 μ B , respectively. For double doping at B/N sites net magnetic moment increases to 1.998 μ B and 1.824 μ B , respectively. Whereas for triply carbon doped bilayer system at B/N sites, the system changes to metallic behaviour. Upon carbon doping at N-site, we obtained transition from Non-Magnetic semiconductor(Pristine) - Magnetic semiconductor(1C) - Half-Metal ferromagnetic(2C) - Metal(3C). Whereas, in case of doping at the B-site, we observed transition from Non-Magnetic Semiconductor(Pristine) - Magnetic Semiconductor(1C) - Metal (2C, 3C). Analysis from the PDOS plot of the car- bon doped systems reveals that the net magnetic moments are contributed by the 2p orbitals of carbon and partial contribution from the neighboring nitrogen and boron atoms, respectively. As 1,2C doping at the B-site reduces the energy band gap to 0.81-1.8 eV which falls in the visible spectrum and thus such system further opens up an opportunity to be utilised as a photocatalys material. Our carbon doped systems show a magnetic semiconducting behavior with a nite magnetic moment which is one of the criteria for a spintronic material. So, our system looks promising in this regard. Also, Carbon doping can be considered as a simple approach to tune the band gap of the Boron Nitride bilayer system.

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