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Metal free half metallic graphitic carbon nitride on BN layer JISANG HONG, ARQUM HASHMI, Department of Physics, Pukyong National University — We have investigated structural, adsorptive, and magnetic properties of metal free graphitic carbon nitride (g-C_4N_3) layer on hexagonal BN layer (h-BN) using the optB88-vdW van der Waals density functional theory. The free standing g-C_4N_3 layer is known to have (2×2) surface reconstructed structure with 0.3 $\mathring{A}$ buckling feature. However, the surface reconstruction disappears on BN layer and the g-C_4N_3 layer becomes flat. Interestingly, the g-C_4N_3/BN hybridized system has a new lattice constant which differs from that of either BN or g-C_4N_3 and this lattice change is responsible for adsorption of g-C_4N_3 on BN layer. More surprisingly, we have observed half metallic behavior in g-C_4N_3 even on BN layer. We propose that our theoretical prediction can be verified using normal incidence of K-edge X-ray magnetic circular dichroism (XMCD) measurement and also our finding indicates that the g-C_4N_3/BN system can be utilized for novel metal free spintronics material.

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