

## Half metallic g-C<sub>4</sub>N<sub>3</sub> on BN layer

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Half metallicity without any external factor in 2p materials may provide a new physics in spintronics. We have investigated structural, adsorptive, and magnetic properties of metal free graphitic carbon nitride (g-C<sub>4</sub>N<sub>3</sub>) layer on hexagonal BN layer (h-BN) using the van der Waals density functional theory. It is found that g-C<sub>4</sub>N<sub>3</sub> layer can be adsorbed on BN layer due to the change of lattice constant of the hybridized system. Interestingly, we have found that metal free half metallic behavior in g-C<sub>4</sub>N<sub>3</sub> can be preserved even on BN layer and the half metallicity originates mainly from the 2p<sub>xy</sub> planar orbitals of N atoms in g-C<sub>4</sub>N<sub>3</sub> layer. Characters of spin polarized planar orbitals suggest that our theoretical prediction can be verified using normal incidence of K-edge X-ray magnetic circular dichroism (XMCD) measurement.

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