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Density Functional Theory Calculation of Hydrogenated Graphene

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Density functional theory (DFT) calculation was carried out to investigate the magnetic properties of hydrogenated graphene. Density of states, band structure, and spin density of hydrogenated graphene were calculated by using a pwscf DFT package. Spin-restricted calculation on the hydrogenated graphene gave a flat band near the Fermi level with a high density of states. Spin-unrestricted calculation gave a spin-splitting of flat band on the Fermi level, which corresponds to the magnetic moment in the hydrogenated graphene.