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Van der Waals density functional studies of hydrogen adatoms on bilayer graphene

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Abstract content
   (Max 300 words)

We present a comparative density functional study of the adsorption of hydrogen atoms on bilayer graphene. Two different exchange-correlation functionals are employed to explore the possible configurations of hydrogen adsorption at 50% coverage. Using the non-local van der Waals density functional, we identify three distinct competing configurations that retain the coupled bilayer structure at 0 K. One of the configurations undergoes a spontaneous transformation from hexagonal to tetrahedral structure, under hydrogenation, with the energy of formation of -0.06 eV (GGA) and -0.37 eV (vdW-DFC09x).This configuration has a finite band gap of around 3 eV, whereas all other competing configurations are semi-metallic.

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Main supervisor (name and email)
and his / her institution

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