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

*Tuesday, 10 July 2012 11:00 (20 minutes)*

### Abstract content <br> &nbsp; (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.

### Apply to be<br> consider for a student <br> &nbsp; award (Yes / No)?

Yes

### Level for award<br>&nbsp;(Hons, MSc, <br> &nbsp; PhD)?

PhD

### Main supervisor (name and email)<br>and his / her institution

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### Would you like to <br> submit a short paper <br> for the Conference <br> Proceedings (Yes / No)?

no

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