Ab Initio Calculations of Hydrogen Adsorption on Graphene

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Recent reports of large hydrogen adsorption on carbon nanotube materials have raised the question whether such materials could be used for hydrogen storage. The very favorable weight ratio, and the feature that the properties of carbon nanotube materials can be engineered to a remarkable degree through control of chirality, tube diameter and through doping among others, make carbon nanotubes a very promising hydrogen storage material.

To get a better insight into hydrogenation of carbon nanotubes, the most stable configurations of hydrogen on single graphitic sheets were examined. As hydrogen can attach both from above and from below a horizontally positioned graphitic sheet, the number of configurations of partially hydrogenated graphene is very large even for rather small periodic cells. Therefore an *ab initio* electronic structure method was combined with a cluster expansion to effectively sample the configuration space. For un-curved graphene one particular configuration was found to be much favored over all others. How the results for flat graphene carry over to the case of curved graphene will be discussed.