Ab Initio Calculations of Nitrogen Functionalization of Graphene

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Abstract

A new way of incorporating single nitrogen atoms in a graphene sheet, which involves a treatment in the late afterglow part of a plasma, has been developed by an experimental team[1,2]. It aims to maximize the substitutional, or graphitic, doping while minimizing the damage done to the graphene. With the software package ABINIT[3,4], we have carried out some first-principles calculations of different configurations of doping nitrogen atoms in a graphene sheet. We obtained the formation energies of the structures to study whether they are realistic configurations. We found that vacancies in the graphene sheet facilitate the incorporation of nitrogen atoms and, in particular, that the substitutional doping has the lowest formation energy. We also studied the energetic of nitrogen atoms adsorbed above the carbon plane because it plays a role in the process of functionalization. Using the Nudged Elastic Band method (NEB), we were able to calculate energy barriers for the diffusion and the in-plane absorption of these atoms.

References

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