

Boron and nitrogen doping of graphene from first principles

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The modification of the electronic properties of sp^2 carbon nanostructures by the controlled addition of foreign atoms into the carbon lattice has been widely proposed and investigated [1,2], in close analogy to the doping of silicon in the semiconductors industry. However, in contrast with conventional materials, the effect of foreign atoms in nanostructures is expected to depend significantly on the position and surrounding of each atom due to the quantum confinement of the electrons [2]. In principle, the fact that nitrogen atoms contain one additional electron than carbon, suggests that nitrogen doped carbon nanostructures will exhibit the characteristics of an n-type material [3,4]. Similarly, boron atoms which lack of one electron with respect to carbon atoms are good elements to achieve a p-doped material [2]. Furthermore, recent experiments on graphene reveal through scanning tunneling microscopy (STM) images, that B and N doping can occur in different kinds of geometries [5,6].

This work explores different configurations for nitrogen and boron atoms incorporated onto graphene, and investigates their effects and properties using ab-initio electronic structure calculations. The computed total and local density of states reveal specific signatures for each type of defect, which could be correlated with experimental scanning tunneling spectroscopy (STS) measurements. In addition, STM images are presented in order to aid the eventual large scale identification of these defects.

Our calculations, and recent experimental observations suggest that the classically assumed nitrogen incorporations into graphitic structures (i.e., single substitution and pyridinic), are not necessarily the most common. It is generally true, however, that substitution defects (single, double substitution) dopes graphene with electrons, and vacancy-nitrogen complexes (e.g. pyridinic, or single nitrogen + vacancy) add holes to the system. In contrast, boron atoms are usually found in substitution for carbon atoms in graphene. However, these are rarely observed isolated, but rather showing a tendency to form islands.

In summary, we present an extensive study of the properties of different kinds of boron and nitrogen doping in graphene. We show that the structural details of the incorporated atoms can be extremely important for the electronic properties of the resulting doped material. In addition we show that specific fingerprints in STM and STS analysis can be obtained accurately from ab-initio calculations.

References

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Figures

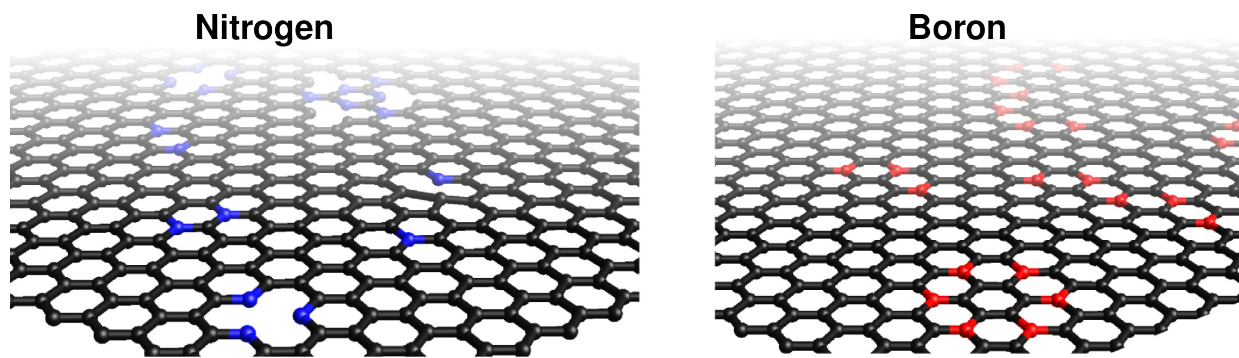


Figure1. Schematic image showing the different kinds of doping structures for both nitrogen and boron in graphene.