

Boron and nitrogen doping of graphene from first principles

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Similarly to the case of doping in the silicon industry, the addition of foreign atoms in sp^2 carbon nanostructures modifies its electronic properties [1,2]. However, in contrast with standard semiconductors, the position and configuration of the foreign atoms plays a significant role in nanostructures due to quantum confinement of the electrons [2], and indeed, many geometries have recently been identified in scanning tunneling microscopy (STM) images [3,4]. Our conventional interpretation of doping would suggest that nitrogen atoms, by having one more electron than carbon, induce an n-type doping to carbon-based nanostructures [5,6]. Similarly, boron atoms which lack one electron with respect to carbon would p-dope the material [2].

This work compares different configurations for nitrogen and boron atoms incorporated into graphene. Their properties are investigated using first principles calculations. Their total and local density of states reveal specific signatures of the defect, which could be correlated with experimental scanning tunneling spectroscopy (STS) measurements. STM images are presented in order to aid the identification of these defects.

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

In summary, we present a comprehensive study of different kinds of boron and nitrogen defects in graphene. We show that the configuration of the incorporated atoms defines the electronic properties of the resulting doped material. In addition we show that specific and accurate STM and STS analyses can be obtained from first principles calculations.

References

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Figures

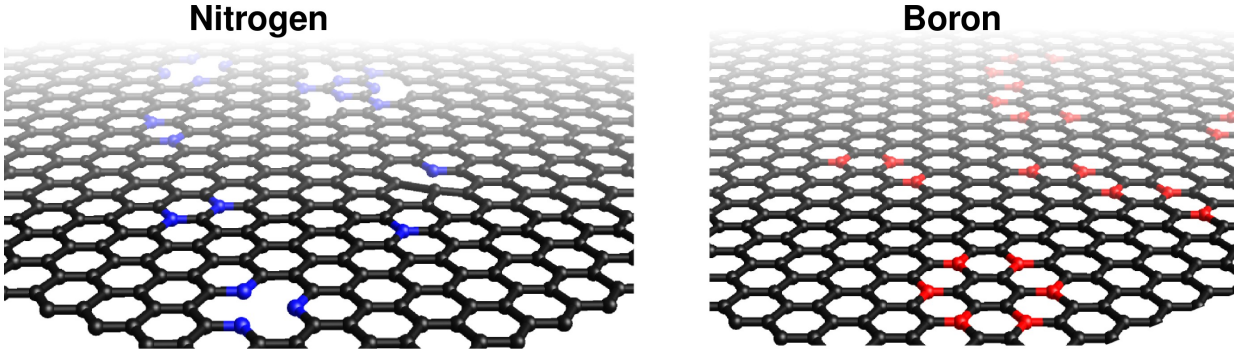


Figure1. Schematic image showing the different kinds of doping structures for both nitrogen and boron in graphene.