**Nitrogen-doped graphene : a theoretical point of view**

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The introduction of local defects such as vacancies or doping impurities is a well-documented way to tune the electronic properties of graphene. In such a context, nitrogen is a natural substitute for carbon in the honeycomb structure due to both its ability to form $sp^2$ bonds and its pentavalent character. However, a clear correlation between the atomic configuration of the chemically modified graphene and the electronic properties remains a challenging task.

Scanning tunneling microscopy and spectroscopy (STM/ STS) are unique tools to measure local electronic properties of graphene and correlate them with their atomic structure [1]. The present work, based on both ab initio DFT, semi-empirical tight-binding (TB) electronic structure calculations and analytical calculations (Green function formalism [2]) aims at looking for interference effects generated by different types of defects. As a first step, the case of simple substitution of nitrogen, where long-range Coulomb effects are expected, will be presented. The Coulomb impurity screening problem in graphene which has been the subject of some debates is discussed [3] and elucidated within a local TB formalism based on the recursion method. This approach is extended to other defects such as vacancy, simple- and double-substitution of nitrogen or pyridine configurations. All the results presented here are discussed in the light of recent experimental STM data [5,6].

## References

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## Figures

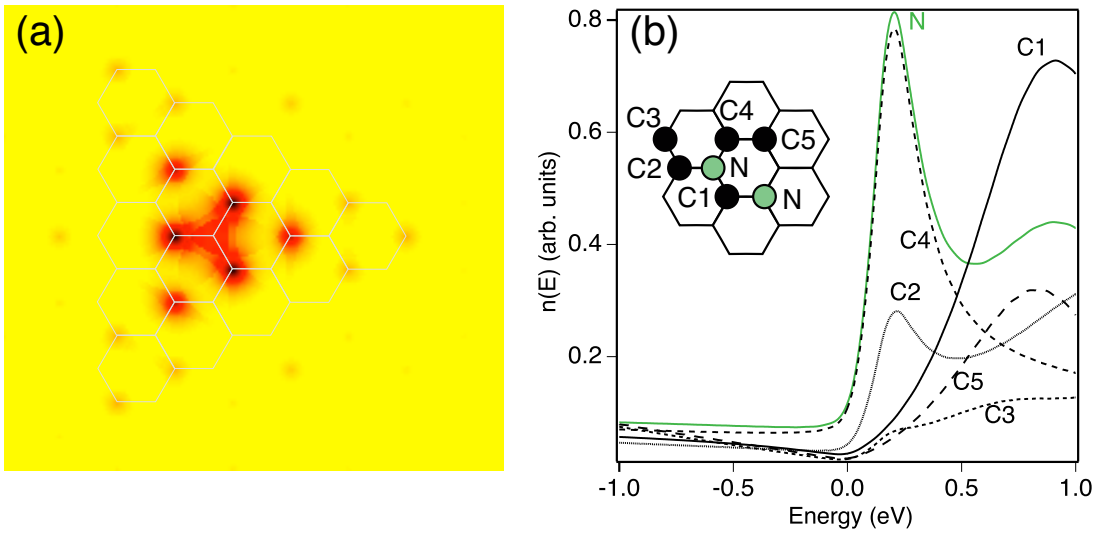


Fig. (a). Map of the local density of states at zero energy in the presence of a vacancy. (b) Local density of states on the nitrogen atom and carbon atoms around a second neighbour nitrogen pair.