One-dimensional extended lines of defects from di-vacancies in graphene

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Graphene is interesting both as an exceptional system for the study of new quantum phenomena, and as novel material for exciting applications. In particular, the outstanding electronic properties of graphene make it a promising material for the future of nanoelectronics. However, graphene cannot be integrated as a building block for pure carbon-based transistor devices due to the lack of a good I_{ON}/I_{OFF} ratio associated to the absence of a gap. Since the outstanding transport properties of graphene originate from its specific structure, modification at the atomic level of the graphene lattice is needed in order to impact its electronic properties. Thus, topological defects, defined as the introduction of non-hexagonal rings in the carbon lattice preserving the connectivity of the network, play a very important role on graphene and related nanostructures. Indeed, recent experimental observations show that arrays of topological defects exist at the boundary between two domains of graphene grown with different orientations [1]. Such arrays of defects have been studied and are found to have interesting electronic properties [2,3]. However, formation of such lines of defects is difficult to control because it depends on the kinetics at the growth of graphene.

In this work we explore various architectures of extended lines of defects that could arise from the reconstruction of di-vacancies in graphene (Fig.1). Different approaches have been successful for the controlled introduction of single vacancies in graphene under a transmission electron microscope or via scanning tunneling lithography. Furthermore, single vacancies are very mobile, and tend to form di-vacancies, which are more stable and tend to be reconstructed with topological defects. Using a first-principles approach, we study the electronic and quantum transport properties of extended lines of defects that could arise from the reconstruction of di-vacancies. In addition, we present simulated STM images in order to help the identification of these systems experimentally. In particular, we find that some of these systems exhibit conduction channels and localized states which could enhance the chemical reactivity of graphene [4]. Therefore, these extended lines of defects open the possibility of arranging molecules or atoms in a linear fashion, thus behaving as a 1D template.

References

[1] J. Lahiri, Y. Lin, P. Bozkurt, I. I. Oleynki, and M. Batzill. Nat. Nano, **5** (2010), 326.
[2] O. V. Yazyev and S. G. Louie, Nat. Mater., **9** (2010), 806.
[3] O. V. Yazyev and S. G. Louie, Phys. Rev. B, **81** (2010), 195420.
[4] A. R. Botello-Méndez, X. Declerck, M. Terrones, H. Terrones. Nanoscale *(in press)*

Figures

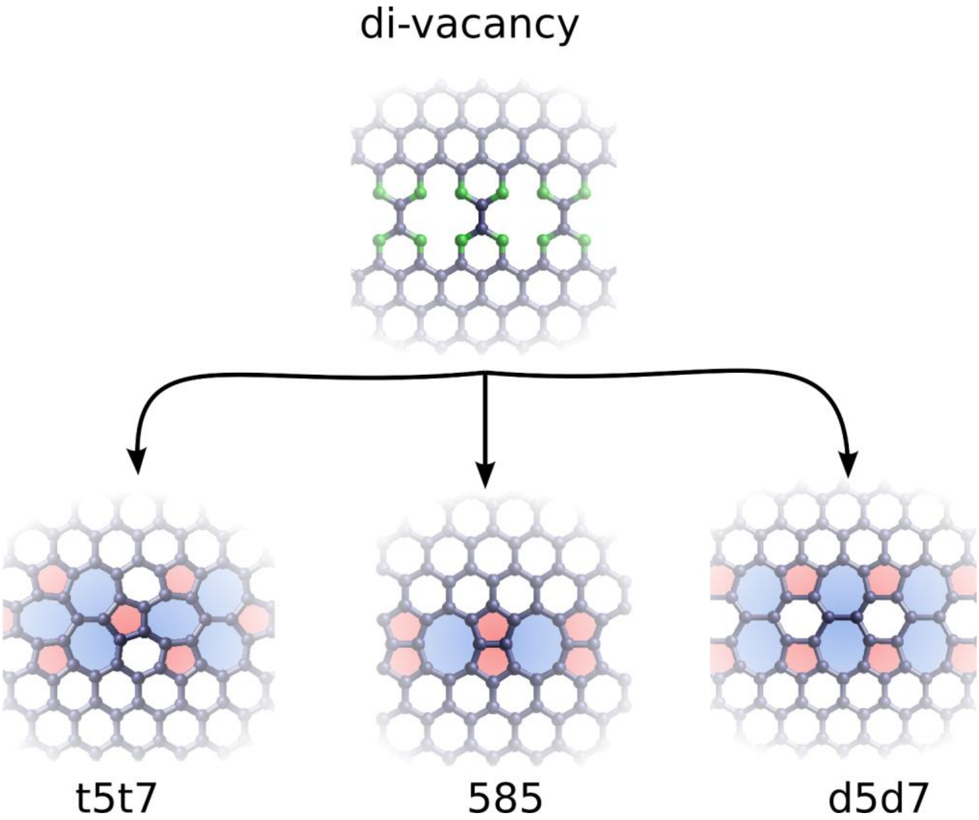

Figure 1. Molecular model of the formation of extended lines of defects in graphene from the reconstruction of divacancies