# COMPUTER DESIGN OF VACANCIES IN GRAPHENES

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In the present time carbon graphenes attract interest in the same degree, that nanotubes and fullerenes both from the applied and from fundamental points of views.

Influence of vacancies defects on electronic and phonon properties of graphenes is studied with models based on an elementary cell of 180 carbon atoms and 1, 2, 3, 6 and 24 vacancies. Ordered, with the single defects for a unit cell, and non-ordered, with the randomly located vacancies are calculated from the first principles and by the method of molecular dynamics [1].

Randomly oriented vacancies at low concentrations (from 1 to 6 for a unit cell) result in creation of characteristic defects of $V_1(5\text{-}9)$, as shown in Fig.1,a and at concentrations starting from 24 for a unit cell result in to the amorphisation of graphene with the different types of defects, as shown in Fig.1,b.

The electronic and phonon densities of the states are analysed. Switching of electronic conductivity from metallic to semiconducting is observed at an increasing of defect numbers from one and three vacancies to the large numbers of defects, as shown in Fig.2 and vacancies clusters. Characteristic phonon modes in an area ~19 and ~48 TGz is found in all these cases for future experimental determinations.

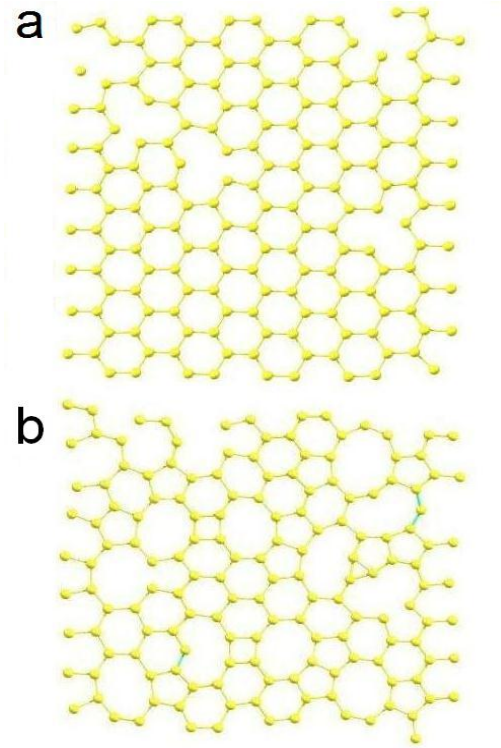


Fig.1 Optimized structures of graphenes with 6 (a) and 24 (b) non-ordered vacancies for a unit cell

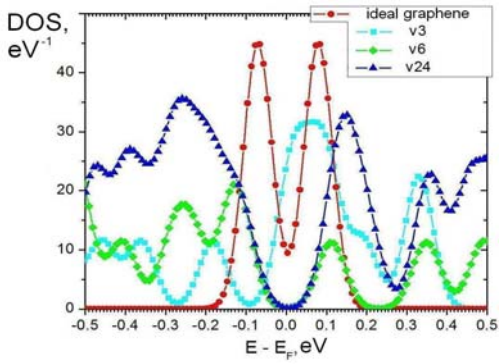


Fig.2 Densities of the electronic states of ideal graphene and graphenes with randomly oriented vacancies (from 3 to 24) for a unit cell

1. A.V. Pokropivny, Y. Ni, Y. Chalopin, Y.M. Solonin, S.Volz. Tailoring properties of graphene with vacancies. Phys. Stat. Sol. B (2014)