

**The strong influence of configurations of graphane islands to electronic properties of
graphene/graphane mixing structure**

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Graphene is one of the most interesting materials synthesized in the last years which two-dimensional nature along with the fascinating electronic properties attracts the great attention from the scientific community. Graphene has unique electronic properties such as the linear dispersion law leading to zero effective mass for electrons and holes. It already applied as solar cell [1], liquid crystal device [2], molecular sensor [3] and nano-sized transistor prototype [4].

Moreover, electronic properties of graphene can be drastically changes by only partial hydrogenation. It was predicted that adsorption of only one hydrogen atom onto graphene area at $\sim 2 \text{ nm}^2$ can open the small band gap of 0.45 eV [5]. Furthermore, adsorption of hydrogen in the periodically arranged lines changes the properties of graphene similarly to graphene ribbons [6]: graphene confined by hydrogen lines displays band gap depended upon the distance between lines and their orientation.

We considered the various concentration of the adsorbed hydrogen atoms from 2% to 56.3%. Note that the hydrogen content is not an absolute parameter that determines the electronic properties of the structures, due to the fact that the electronic structure of the superlattices also depends on the particular location of adsorbed atoms. In the Fig. 1 the atomic geometry and electronic structure of graphene with different content of adsorbed hydrogen is shown.

We begin our study from considering of the structures with far-arranged ($\sim 2 \text{ nm}$) pairs of adsorbed hydrogen atoms (begin of nucleation process, see Fig. 1). Even at such low hydrogen concentration we observed the opening of the band gap.

The electronic structure of the partially hydrogenated graphene is sensitive to particular arrangement of adsorbed hydrogen atoms.

We studied this effect in more details by considering graphene with concentration of adsorbed hydrogen 56.25% with various distribution of adsorbed hydrogen atoms on the surface.

We investigated two different configurations of graphane islands ($\begin{array}{cc} A & A \\ A & A \end{array}$ or $\begin{array}{cc} A & B \\ B & A \end{array}$) and didn't find significant difference between their electronic structure.

References

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Figures

Fig. 1 The evolution of the electronic properties of graphene superlattice. Atomic geometry (in the left), band structure (in the center) and density of states (in the right) of graphene superlattice with concentration of hydrogen a) 6.25% ($E_{gap} = 0.07$ eV) and b) 6.25%, ($E_{gap} = 0.43$ eV). DOS of superlattice and graphene are marked by solid and dotted lines, respectively. The Fermi energy is marked by horizontal (in the case of band structure) and vertical (in the case of density of states) line

