

Electronic structure of stripped graphene nanoribbons delimited by sp³ defect lines:
A density functional theory study

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Abstract

Graphene has been touted as the miracle material because of both its exceptional mechanical and electronic properties. However, owing to its semimetallic properties (absence of a band gap) its applications in electronic remain limited. Graphene nanoribbons (GNRs) appears as a particularly interesting alternative. Indeed, the electronic structure of GNRs can be tuned from a metallic to a semiconductor behavior through a tailored quantum confinement and edge effects.¹⁻⁴ To provide semiconducting properties to graphene with sufficiently large gaps, sub-5nm GNRs are required in order to reach graphene-based FETs with proper on/off ratio at room temperature.¹⁻³

The formation of covalent bonds transforms the sp² carbons of graphene to sp³, opening a band gap and generating semiconducting regions.⁵ This approach has been successfully applied for other carbon nanostructures such as fullerenes and carbon nanotubes.^{6,7}

In this work, we perform Density Functional Theory (DFT) calculations of the geometric and electronic structures of stripped graphene delineated by chemical defects. We show that the bonding of hydrogen atoms on specific carbon atoms along the armchair direction effectively breaks the π -delocalization and opens a band gap. The density and the positions of such defects at the surface of graphene have been varied while simultaneously probing the influence on the electronic structure of the resulting periodical disruption in π -conjugation.

References

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