# Behavior of different types of graphene nanoribbons with water molecules

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## Abstract

Graphene is the ideal candidate for the manufacture of next generation electronic devices because of its very high carrier mobility and quantum-hall effect. However, the absence of band-gap limits its usage for some purposes, like digital switching, where a high value of the on-off current ratio is an essential requirement. Fortunately, this limitation can be overcome by inducing quantum confinement and edge effects as in the case of narrow width graphene nanoribbons (GNRs) with controllable widths and smooth edges [1]. Therefore producing high quality GNRs at low cost on a large scale and in a reproducible manner is a very interesting target nowadays.

Moreover, another issue of concern is that the synthesis of graphene by conventional methods involves the use of toxic chemicals and these methods usually result in the generation of hazardous waste and poisonous gases [2]. Therefore, there is a need to develop green methods to produce graphene by following environmentally friendly approaches. One process that involves such a material as water can be a good candidate for this aim.

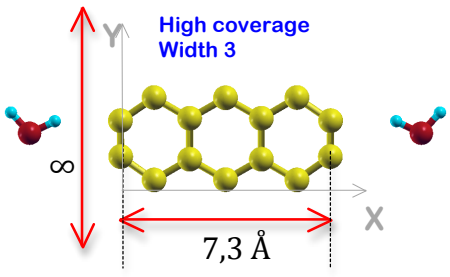
We have used a Tight-Binding code (DFTB+) to analyze the interaction of water molecules with the edges of bilayer graphene nanoribbons changing the water concentration and the molecules orientation, the nanoribbon width and the kind of edge, zig-zag or armchair. Besides, we have studied the difference between using pure carbon nanoribbons and nanoribbons with their dangling bonds passivated with hydrogen atoms.

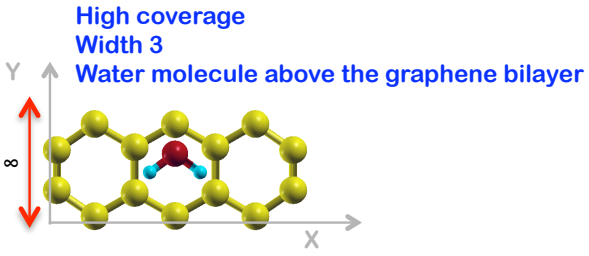
## References

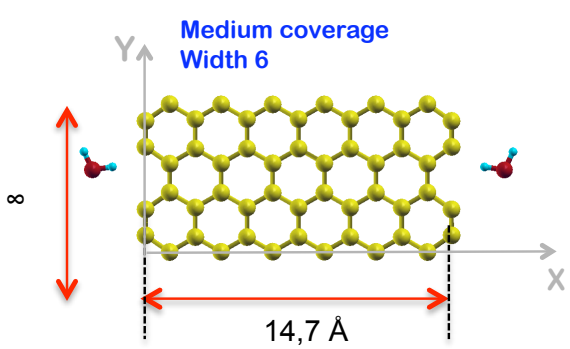
[1] T.S. Li, Y.C. Huang, M.F. Lin &S.C. Chang, Philosophical Magazine, **Conductance of bilayer grapheme nanoribbons with different widths** (2010) 3177.

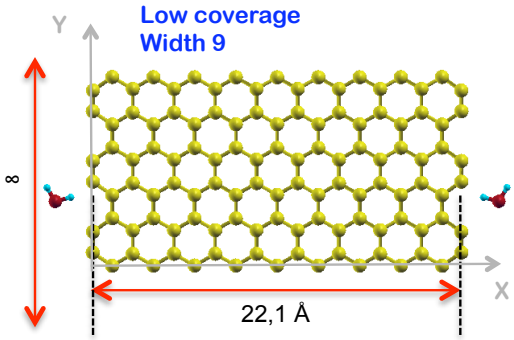
[2] K. Samba Sivudu and Yashwant Mahajan, Centre for Knowledge Management of Nanoscience and Technology (CKMNT), **Mass production of high quality graphene: An analysis of worldwide patents** (2012) http://www.nanowerk.com/

## Figures




Medium coverage
Width 6
Y
X
∞
14,7 Å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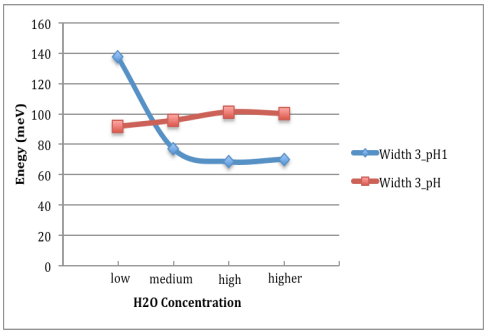
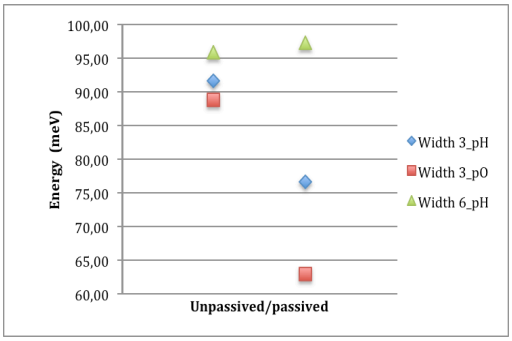
Width 9
Y
X
∞
22,1 Å


160
140
120
100
80
60
40
20
0
Enegy (meV)
low
medium
high
higher
H2O Concentration
Width 3_pH1
Width 3_pH


100,00
95,00
90,00
85,00
80,00
75,00
70,00
65,00
60,00
Energy (meV)
Unpassived/passived
Width 3_pH
Width 3_pO
Width 6_pH