At the edges of graphene nanoribbons

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Graphene has many excellent and unique properties, and it has become very intensively studied a material. For some applications, such as electronic devices, a band gap is however required, whereas the pure graphene is a semi-metal. This can be achieved by restricting the spatial extent of the graphene sheet into one or zero dimensions.

We first determine, by means of density functional theory, the stability and the geometry of one-dimensional graphene nanoribbons (GNRs) edges in the environment composed of common gases such as hydrogen [1, 2], oxygen, water, ammonia and carbon dioxide [3]. From thermodynamical analysis we find that the most stable structures with either armchair or zigzag edge reconstruction are characterized by a non-metallic/non-magnetic nature, and are compatible with Clar’s sextet rules, well known in organic chemistry. These results are particularly relevant to both synthesis of GNRs where the most recent experimental routes are either via water- and/or ammonia-containing solutions, and preparation of nanoribbons by “opening” carbon nanotubes in atmosphere of gaseous oxygen. We further analyse the electronic structure by simulating the scanning tunnelling microscope images. They are found to faithfully reflect the expected electronic configuration.

We also study the confinement of the electrons of graphene in the vicinity of the Fermi energy by hybridising nanoribbons or zero-dimensional dots in a plane with an insulating material, hexagonal boron nitride. Such structures have recently been demonstrated in experiments [4, 5]. The electronic states appear as very similar to those in saturated GNRs.