Graphene-Graphane ribbons on substrate

Ari Harju[1], Mari Ijäs[1], Paula Havu[1], Pirjo Pasanen[2]

[1]Aalto University School of Science, Espoo, Finland
[2]Nokia Research Center, Helsinki, Finland
ari.harju@aalto.fi

Ever since the first experimental discovery of graphene and its extraordinary electronic properties [1], the search for practical applications for this new material has been intense. As the lack of a band gap is a hindrance for applications, various methods have been suggested to induce a gap, among them cutting the material into thin stripes, graphene nanoribbons (GNRs). Confinement induces a width- and edge- dependent gap [2], but manufacturing these experimentally with atomic precision is challenging. An interesting possibility to generate graphene nanoribbons is by selective dehydrogenation of graphane [3], the fully hydrogenated graphene.

We have theoretically studied the stability of the one-side hydrogenated graphene on the oxygen-terminated silicon dioxide surface. Scanning and relaxing around 500 initial configurations, we have found the two most stable graphane configurations shown in Fig. 1. Both configurations are insulators but their band gaps differ considerably. The quarter-hydrogenated configuration has only a small band gap of 0.46 eV, and for the half-hydrogenated graphene the magnitude is 3.7 eV. Whereas our simulations show that graphene binds to the silicon dioxide via the van der Waals forces, graphane binds to the surface covalently.

We have formed graphene ribbons on graphane by removing hydrogens from the half-hydrogenated configuration, see Fig. 2. In experiments, this can be done using STM tip [4]. For the electronic structure of the resulting ribbons, both antiferromagnetic and ferromagnetic spin order were found, the antiferromagnetic ones being lower in energy. In addition, the coupling of the graphene to the substrate leads to an interesting electronic structure: As the substrate is not symmetric on the two edges, see Fig. 2, and because the edge atoms in the ground state have opposite spins, the spin symmetry of the ribbons is broken by the substrate and the two spin channels turn out to have gaps of different magnitude. As a result, the system shows a half-semiconducting band structure. The gaps in ribbons typically get smaller as the ribbons get wider, and in this case the electronic structure might change to half-metallicity.

References

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Figures

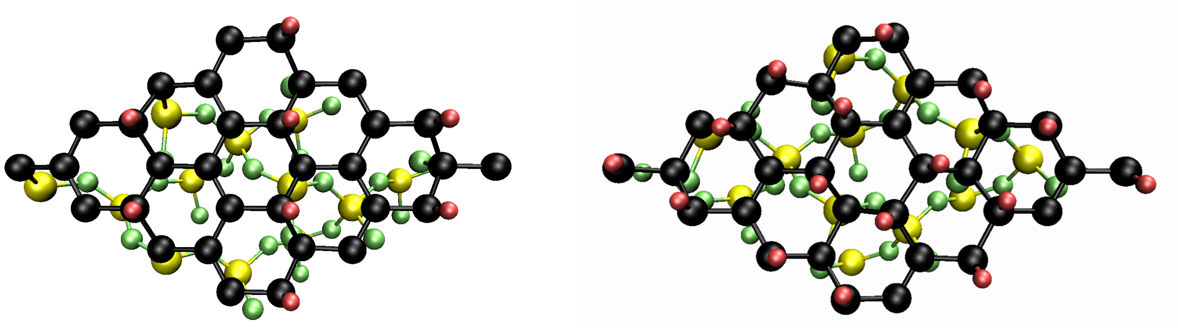

Figure 1: *Quarter- (left) and half-hydrogenated (right) graphanes on substrate.*

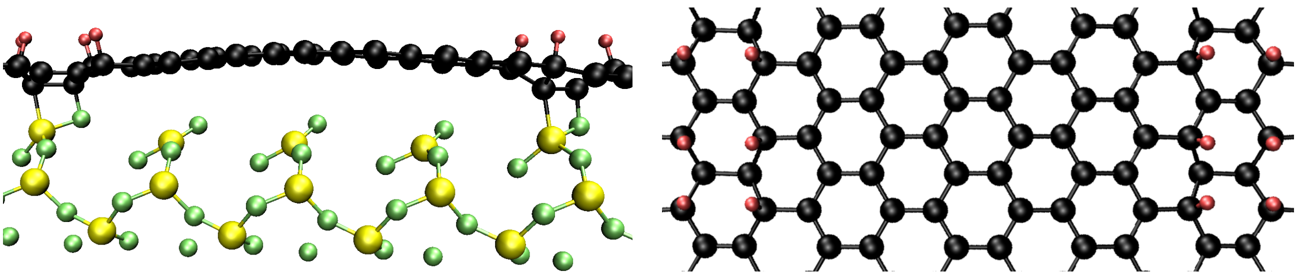

Figure 2: *Graphene ribbon created by removing rows of hydrogen.*