Graphane on SiO_2, transport in FHI-aims

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Hydrogenation of graphene on the α-quartz (0001) SiO_2 substrate is studied, considering different surface terminations in order to take into account the amorphic nature of the substrate. Our *ab initio* calculations show that the formation of graphane by hydrogen adsorption on graphene is energetically favored on hydroxyl- and oxygen-terminated surfaces, whereas silicon termination and reconstruction of the oxygen termination hinder adsorption. Our results indicate that in order to hydrogenate graphene on SiO_2 , it is benecial to oxygenize the surface and saturate it with hydrogen.

Using the lowest energy geometries of hydrogenated graphene on the α-quartz (0001) SiO_2 substrate, we form zigzag graphene nanoribbons by selectively removing hydrogens from the epitaxial graphane layer. In these ribbons the spin degeneracy of the free-standing antiferromagnetic zigzag ribbons is broken, and band gaps of different magnitude emerge for the opposite spin channels. This degeneracy breaking is due to a charge imbalance in the substrate below the ribbon, introduced through the asymmetric alignment of the substrate atoms with respect to the edges of the graphene ribbon.

Finally a small introduction to the Landauer-Büttiker transport calculations with FHI-aims is given.

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