Spatially resolved electronic characterization of hydrogenated graphene by scanning tunneling spectroscopy

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Abstract
Graphene has attracted great research interest in the past years due to its extraordinary mechanical [1] and electronic [2] properties. Graphene has a very high electrical conductivity due to extremely high carrier mobility governed by ballistic carrier transport, i.e. transport without scattering over macroscopic distances. The linear band dispersion of graphene close to the Dirac points results in electrons behaving as massless Dirac fermions [2].

Due to the aforementioned properties, graphene is a promising candidate for fabrication of ultrafast transistors but since graphene is a semimetal, the on/off ratio of current switching is inefficient. Therefore many different mechanisms have been proposed on how to modify graphene into semiconductor by opening a bandgap at Dirac point. One possible route to achieve this is by hydrogenation of graphene. We have successfully demonstrated, that a bandgap of at least 450 meV [3] is induced in graphene on Ir(111), which is sufficient for application in electronic devices.

The poster will present preliminary data of LDOS mapping of hydrogenated graphene on Ir(111). The hydrogenation of graphene has already been investigates extensively by our group. Graphene on Ir(111) possesses a superstructure (Moiré structure) due to lattice mismatch between the substrate and graphene. Hydrogen does not adsorb with same probability to all sites in the Moiré - it has been shown that at lower coverages hydrogen preferentially binds to the fcc and hcp parts of the moiré. In these regions the density functional theory (DFT) calculations show that the most stable structure is obtained when a C atom binds alternately to H and Ir. This result can also be understood from geometrical considerations since the optimal geometry for sp³ hybridization is tetrahedral with angles of 109.5° between each bond. Since the formation of a C-Ir bond stabilizes H adsorption, only regions where a C atom is directly above an Ir atom are hydrogenated, which explains why hydrogen is adsorbed in a periodic fashion until high coverage. When hydrogen is adsorbed to the surface a local graphene-like structure is created which, according to calculations is insulating [4]. Our hypothesis is that the periodic modulation with insulating regions leads to confinement of electrons and hence opens a bandgap [6]. This hypothesis has been challenged by other studies where a bandgap was observed by hydrogenation without periodic modulation [5]. We propose to investigate this experimentally by atomic resolution mapping of the LDOS using low temperature STS measurements which should shed light on this matter.

Future work includes LDOS mapping of hydrogenated graphene on several different substrates which do not show the periodic modulation, e.g. SiC(0001) and Pt(100). We have demonstrated that these substrates show different hydrogen adsorption scheme compared to Ir(111): At very low coverages, graphene on SiC is geometrically modulated due to interactions with the underlying buffer layer. It has been shown that hydrogen preferentially binds to convex areas at low coverage resulting in quasi periodic adsorption following the 6 x 6 SiC reconstruction as imaged in fig. 2a [6]. At higher coverage, disordered hydrogen clusters are observed, fig. 2b. Adsorption on Pt(100), on the other hand, shows no site preference and disordered hydrogen structures are observed, fig. 3 [7]. By investigating the electronic behaviour of these systems, we should be able to comment on whether the periodic arrangement plays an important role for the bandgap opening or not.

References

**Figures**

![Hydrogenated graphene on Ir(111)](image)

**Figure 1** Hydrogenated graphene on Ir(111) a) Clean graphene where the Moiré is easily observed, b) at low coverage H binds in dimers at fcc and hcp sites. When increasing the coverage c), ring shaped clusters are formed and finally at highest coverage d), e) these merge to form elongated H clusters. f) is fourier transform of e) shows that the Moiré periodicity is preserved.
Figure 2: STM images of hydrogenated graphene on SiC, a) at low coverage hydrogen binds as ortho or para dimers at sites following the $6 \times 6$ reconstruction of SiC, b) when the coverage is increased no site preference is observed. Hydrogen binds in larger disordered clusters.

Figure 3: STM images of hydrogenated graphene on Pt(100) both at low a) and high b) coverage no ordering of hydrogen adsorption is seen.