Graphene on Pt step edges

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Understanding the coupling of graphene with its local environment is critical to integrate it in tomorrow's electronic devices. Previous studies have shown that highly perfect sheets of graphene can be obtained by epitaxial growth on metal surfaces, and for some transition elements, like Cu or Pt, the interaction is very weak and many characteristic properties of graphene are preserved [1,2]. In this work, we show the structure of graphene grown on Pt close to the steps where the flakes start to nucleate. To this end, we combine scanning tunneling microscopy (STM) experiments with density functional theory calculations (DFT) and non-equilibrium Green's functions (NEGF) methods to model the electronic transport.

RT-STM experiments on Pt have succeeded in mapping the structure of a graphene flake on a Pt steps edge showing atomic resolution not only on both the graphene and the metal but also on the boundary (see figure). By combining them with our ab initio simulations [3], we have been able to understand the competition between the interaction of graphene with the step and with the Pt surface that controls the structure and chirality of the flake edge and the observed Moiré structures. We have determined both the atomic and electronic structures of graphene zigzag edges on Pt steps. We observe that the stress induced by the boundary is relaxed straining the Pt atoms bonded to the carbons which are only slightly distorted from its graphene ideal positions (see figure). The electronic structure shows a localized state on the graphene edge that expands into the flake few unit cells and only in one of the sublattices. No signs of local magnetic moments were found.

References

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[2] P. Sutter et al, Phys. Rev. B, 80 (2009) 245411.

[3] M.M. Ugeda et al, Phys. Rev. Lett., 107 (2011) 116803.

Figures

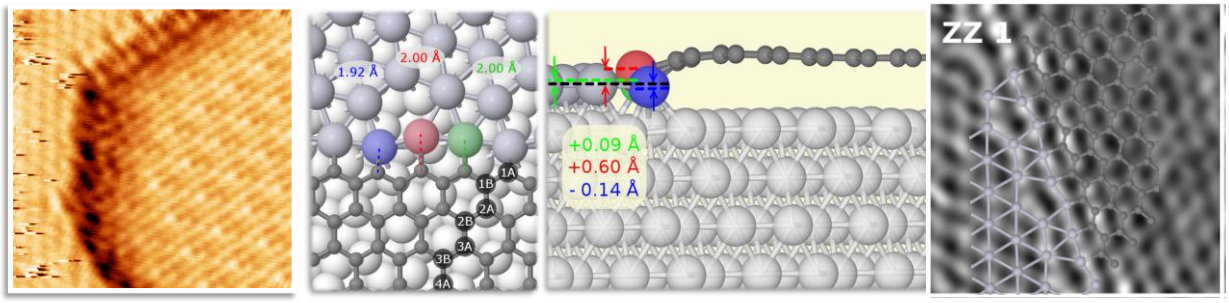

Figure 1: (Left panel) Experimental RT-STM image of a graphene flake on a Pt(111) step edge. (Central panel) Atomic structure of graphene zigzag edge on a Pt step calculated by a DFT method based on a plane wave basis set description (VASP). (Right panel) STM image with atomic resolution on the metal, the graphene and the boundary compared with the atomic structure calculated with DFT.