Sublattice localized electronic states in atomically resolved graphene-Pt(111) edge-boundaries

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Understanding the connection of graphene with metal surfaces is a necessary step for developing atomically-precise graphene-based technology. 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 [3], 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 at (STM) experiments with density functional theory calculations (DFT) and non-equilibrium Green's functions (NEGF) methods to unveil the atomic structure of a border-like edge between a Pt(111) step and a graphene zigzag edge. RT-STM experiments have succeeded in mapping the structure of a graphene flake on a Pt step edge showing atomic resolution not only on both the graphene and the metal but also on the boundary (see Fig. 1).

By combining the experiments with our ab initio simulations, 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 can conclude then that the tendency to form passivated zigzag graphene terminations plays a relevant role in the formation and orientation of the stable Moiré patterns. The unsaturated C atoms strongly interact with the Pt step, preserving a zigzag structure quite close to the ideal configuration. However, on the other side, Pt edge atoms experience a 3-fold reconstruction that stabilizes the structure. Our combined approach also reveals the interesting electronic properties of this nanoscopic system including, as stated by the simulations, the preservation of the G-edge state shifted to energies at about +0.8 eV above Fermi level, highly localized in one of the graphene sublattices and confined to the G-Pt interface. This state spreads out inside the first Pt row resulting in a high quality G-metal electric contact that could be relevant for designing future atomically precise graphene metal leads [4]. No signs of local magnetic moments were found.

References

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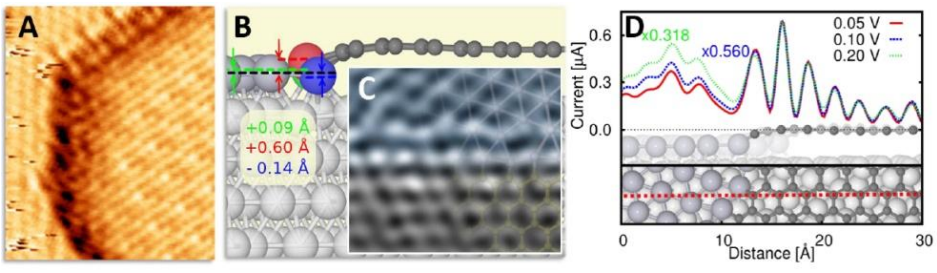

Figure 1. A) Experimental RT-STM image of a graphene flake on a Pt(111) step edge. B) Atomic structure of graphene zigzag edge on a Pt step calculated by a DFT method based on VASP. C) STM image with atomic resolution on the metal, the graphene and the boundary compared with the atomic structure calculated with DFT. D) Simulated STM profiles at constant height (2.75 Å) for different bias voltages.