

Point defects on graphene on metals

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Understanding the coupling of graphene with its local environment is absolutely critical to be able 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 Ir or Pt, the interaction is so weak that many characteristic properties of graphene, such as the Dirac cones, are preserved [1,2]. In this work, we show how the presence of a metallic substrate of this kind affects the properties of an atomically tailored graphene layer. After growing a pristine monolayer on a Pt(111) surface, we have deliberately created single carbon vacancies on the graphene sheet, and studied its impact in the electronic, structural and magnetic properties. To this end, we combine low temperature scanning tunneling microscopy (LT-STM) experiments [3] with density functional theory calculations (DFT) and non-equilibrium Green's functions (NEGF) methods to model the electronic transport [4]. The DFT calculations have been performed using the PBE functional empirically corrected to take into account dispersion interactions [5]. Some of our results are displayed in Figure 1. For the non-defective graphene adsorbed on Pt(111), our calculations show that the periodic modulations typically observed by STM on the Moiré patterns can be explained as a purely electronic effect, because the simulated image is anticorrelated with the topmost regions of the corrugated sheet. For the vacancies on graphene/Pt(111), the calculations help us to associate the STM images observed with the positions of the atoms. Our experiments reveal a broad electronic resonance which is shifted above the Fermi energy, and resembles that previously observed near the Fermi level on graphite [6]. Vacancy sites become reactive, leading to an increase of the coupling between the graphene layer and the metal substrate at these points. This gives rise to a rapid decay of the localized state and the quenching of the magnetic moment associated with carbon vacancies in free-standing graphene layers.

References

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Figures

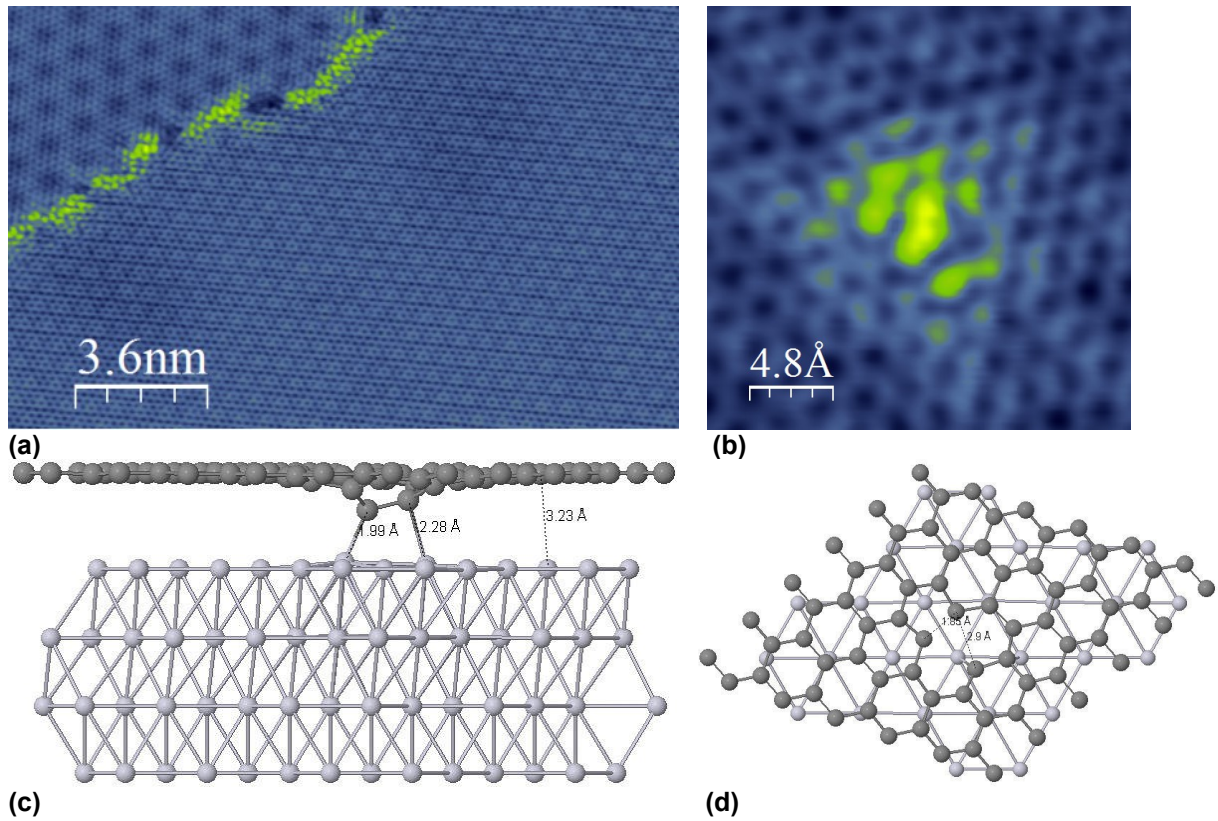


Figure 1. (a) $14 \times 20 \text{ nm}^2$ STM image of the pristine graphene/Pt(111) surface showing two different Moiré structures: an $R19 \times R19$ on the upper left side and a 3×3 in the rest of the image. Sample bias: 50 mV, tunneling current: 1.0 nA. (b) STM image of a single vacancy on graphene/Pt(111). Sample bias: -30 mV, tunneling current: 0.8 nA. (c) and (d) One of the possible adsorption sites for a single vacancy in graphene on Pt(111). The supercell used is fully displayed in (c). In (d) we show only the topmost Pt layer for clarity.