Doping effect in graphene deposited on metals - scanning tunneling spectroscopy and density functional theory studies

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It is obvious that graphene electronics devices require metallic contacts. However, metal/graphene interaction is still not fully understood and demands experimental and theoretical studies. Particularly, it has been proved theoretically using density functional theory (DFT) and van der Waals density functional (vdW-DF) calculations that the unique conical dispersion relation around K/K' points in graphene is preserved on (111) surfaces of Al, Cu, Ag, Pt, and Au. However, this is accompanied with the change of position of the Dirac point (E_D) relative to the Fermi level (E_F) due to the presence of substrate (doping effect).

We describe influence of different substrates on graphene physical properties and focus on understanding of the metal-graphene contacts. Particularly, we will show detailed scanning tunneling microscopy/spectroscopy (STM/STS) and Raman spectroscopy (RS) studies of graphene interactions with Au(111) and Cu(111) substrates [1-3]. The obtained experimental results will be discussed in the frame of density functional theory (DFT) calculations. The representative results obtained for graphene/gold system are presented in Fig.1.

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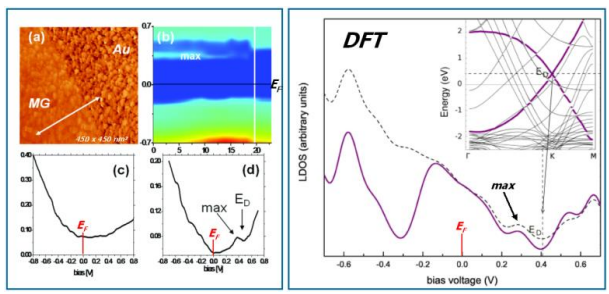

Fig.1. (a) 450 x 450-nm STM topography showing the details of graphene and Au borderline. (b) LDOS(*E*, line) map recorded on graphene/Au interface along arrow shown in panel (a). (d) The example of the LDOS profile recorded on Au region. (d) The example of the LDOS profile recorded on the graphene/Au region. Right panel shows DFT calculation of LDOS function using DFT method.

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