Study of the substrate influence on the properties of physisorbed self-assembled molecular layers: Azabenzene 1,3,5-Triazine on graphite and graphene on metals

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Abstract

The properties of molecular overlayers on inorganic substrates depend on a delicate balance between intermolecular and overlayer-substrate interactions [1]. Here we present a combined experimental and theoretical study of azabenzene 1,3,5-Triazine layers grown on both graphite and graphene on Pt(111). VT-STM experiments (see fig. 1) show large overlayer islands with Moiré structures on both substrates [2]. While in both cases the last layer is graphene, the atomic arrangements, the measured molecule diffusion barriers and the growing properties are different [2]. This system is, therefore, a perfect model for the study of the properties of physisorbed self-assembled molecular layers [1]. We have carried out ab initio DFT calculations (using VASP) trying with all the functionals available (LDA, PBE and hybrids) and different approaches for the van der Waals interactions [3] to fully characterize the intermolecular (H bonds and vdW) and molecule-substrate (vdW attraction and Pauli repulsion) interactions (see fig. 2). We have found that the graphene layer, even for these physisorbed molecules, modifies the intermolecular interactions respect to an isolate layer but not significant differences are found between graphite and graphene on Pt substrates. This exhaustive characterization shows the theoretical limitations to describe these weakly interacting systems even with state-of-the-art approaches.

References

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[2] Martinez-Galera et al, JPhysChemC, **115**, 11089 (2011); JPhysChemC, **115**, 23036 (2011)
[3] S. Grimme et al, J Comp Chem, **27** (2006) 1787; Klimes et al, J Phys: Condens Matter, **22**, 022201 (2010)

Figures

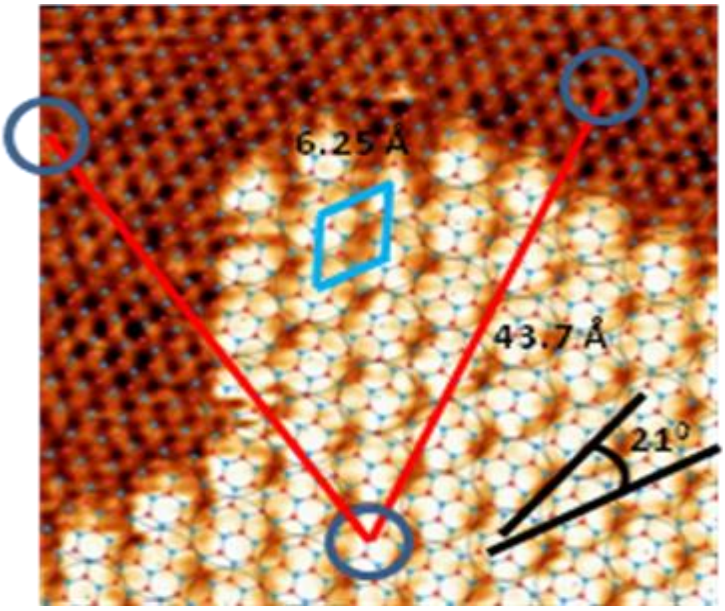

Figure 1. VT-STM experimental image of the graphene + Pt system

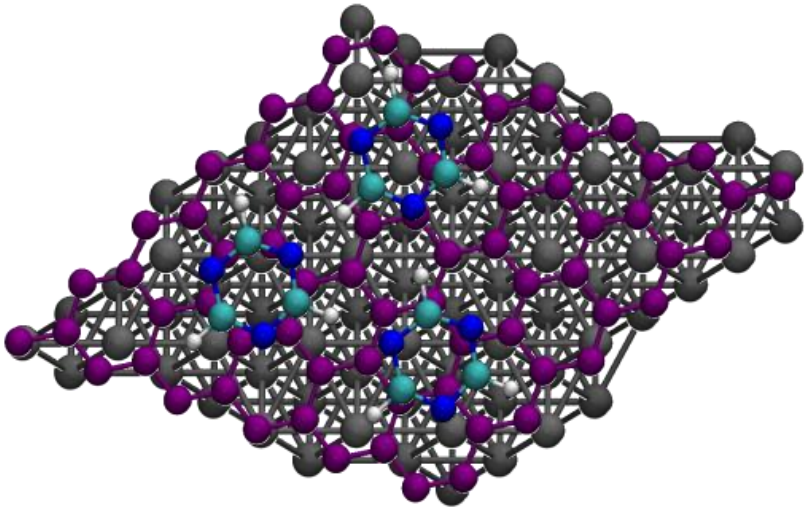

Figure 2. Ball-stick scheme of the theoretical simulation for the graphene + Pt system