

# Nanostructured graphene catalyzes the reaction between two organic molecules

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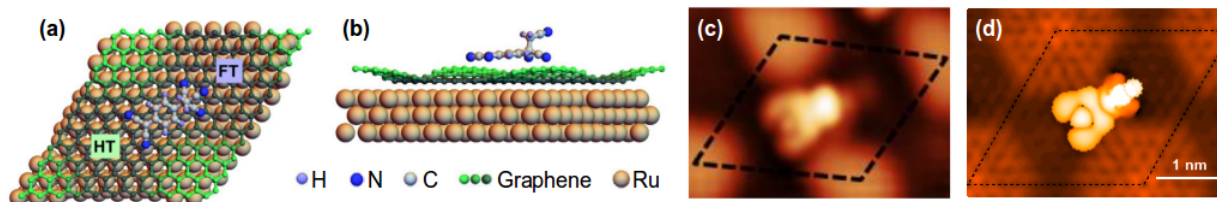
The graphene-substrate interaction can be a powerful tool to tune the electronic properties of graphene [1]. A paradigmatic example is the graphene/Ru(0001) interface. The lattice mismatch between the two systems gives rise to a strong corrugation in graphene, dramatic variations of the graphene-metal interaction, and a strong modulation of the electronic properties at the nanometer scale [2]. Furthermore the graphene/Ru(0001) interface can be used as an adsorption template for organic molecules, like TCNQ [3], due to the low reactivity of graphene. On the other hand, organic radicals (CH<sub>2</sub>-CN·) have also been employed to covalently pattern the graphene/Ru(0001) surface with high spatial selectivity [4].

In view of these results, a natural development is determining the role of supported graphene as a catalytic agent, studying the chemical reaction that may take place when multiple molecular species are adsorbed on the graphene/Ru(0001) surface. In this talk I will present our recent results on this topic [5], analyzing the adsorption of a TCNQ molecule on a graphene/Ru(0001) surface, previously functionalized with CH<sub>2</sub>-CN· radicals. By means of Density Functional Theory (DFT) calculations we determined that the graphene/Ru(0001) surface promotes the formation of TCNQ-CH<sub>2</sub>CN, in which the two molecules are bonded by means of a C-C covalent bond, a reaction that would hardly take place under non catalyzed conditions. The new TCNQ-CH<sub>2</sub>CN molecule has no magnetic moment, due to charge transfer from the surface. More interestingly, the reaction can be fully reversed by injecting electrons in the LUMO of the molecule by the STM tip. The TCNQ-CH<sub>2</sub>CN/TCNQ duo can hence be used as a reversible magnetic switch, controlled by a chemical reaction. On the other hand, our study shows that the TCNQ molecule can be used as a chemical “mop”, with which strongly bound addends can be removed from the graphene surface.

## References

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## Figures



**Figure 1.** (a-b) Top view and side view of the unit cell including the ruthenium substrate, the corrugated graphene and the TCNQ-CH<sub>2</sub>CN molecule as obtained in the DFT calculations. (c-d) STM images of the TCNQ-CH<sub>2</sub>CN on the surface, as obtained in the STM measurements (c) and in the DFT calculations (d).