

## **Scientific report on STM – Laura Ciammaruchi**

During my STM at Pisa CNR – NANO, I shared with Dr. Lucia Sorba's group some experimental results already obtained at ICFO - regarding an innovative technique for achieving graphene hydrogenation - and based on those we designed targeted computational models aiming at reproducing the experimental findings, as well as at paving new ideas for improving them.

In brief, after discussion of the approach followed in order to get the experimental data, we created several models simulating various random configurations of functional groups attached to the graphene material, also considering different percentages in the distributions of functional groups decorating it. Additionally, we considered different levels of distortions with respect to a flat graphene cell, and we also created differently charged models in order to account for the various experimental setups adopted. Therefore, we considered strain, functional groups topology and charge as our three model variables.

The simulations provided by LS's group resulted especially useful in order to interpret certain experimental data as well as to point at additional tests to be performed, once I am back at ICFO.

During my stay at CNR – NANO, my partners and I also started the writing of the draft, that we will need to finalize when the last run of simulation will be completed.