Decoupling graphene from a substrate

G. Profeta[1]

1 Department of Physical and Chemical Sciences and CNR-SPIN, University of L'Aquila (ITALY)

The intercalation of metals, semiconductors, oxygen and hydrogen under epitaxial graphene is an active topic in current graphene research due to the strong influence of the substrate on the electronic properties of graphene. The intercalant often forms a chemical bond with the substrate modifying the electronic properties of the 2D material on top. For example, H intercalation under graphene on SiC causes the formation of a SiH-graphene interface resulting in an unperturbed band structure; the intercalation of oxygen under graphene grown on Ni3Al alloy causes selective oxidation of Al atoms and formation of Al2O3--graphene interface.

For graphene on Ir(111), the oxygen intercalation results in a p-doping of graphene, intercalation of Si under graphene on Ni, Co and Fe results in the formation of corresponding silicides.

These promising results naturally point towards the question how the interface and the electronic structure for graphene and related 2D materials are affected by the type of intercalant.

In this work we studied, by means of experimental and theoretical approach, two specific interfaces involving different intercalants and substrates, namely: Germanium intercalation in graphene grown on Ni(111) substrate and Lithium intercalation in between the carbon buffer layer and the silicon-terminated face of silicon carbide.

Although the general aspects of the intercalation represent a fundamental aspect of the research in graphene technology, these two systems have interesting and peculiar physical motivations.

The Ge is promising due to its higher charge carrier mobilities when compared to Si while it is also compatible with CMOS technology. It has been shown that graphene can be grown on Ge by MBE and that graphene on H-terminated Ge and on Ge oxide surface have superb electronic properties that can even exceed the mobilities of free-standing graphene membranes.

Although, the electronic properties of such devices are strongly influenced by the interface structure, to date nothing is known about the interface structure between graphene and Ge.

Previous works on Ge intercalation were done for graphene on SiC for which the intercalated Ge is amorphous and no precise interface structures was reported.

On the other hand, lithium interaction with graphene attracts special attention for fundamental and technological reasons, related to the fabrication of Li-based batteries, possible piezoelectric effects, and a predicted superconducting phase.

In the present talk we present a complete structural and electronic characterization of these systems by means of density functional theory. A careful comparison with experimental results allows understanding the microscopic mechanism of the intercalation, the precise atomic configuration of the interfaces and the origin of the measured electronic properties.