Substrate induced defects in graphene as opportunities for advanced applications

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All graphene amazing properties – large charge carriers mobility, extreme robustness combined with flexibility, broad band transmittance, huge surface to mass ratio, lubricity – rely on its being a perfect 2D crystal with the specific honeycomb symmetry[1]. However this status brings also some drawbacks [2]: its null density of states at the Fermi level limits its conducting properties; it is weakly interacting, which limits its potentialities as medium for gas storage. In addition, storage applications require building 3D media. On the other hand, perfect graphene is an ideal abstraction rather than a reality: epitaxially grown macroscopic 2D crystals display electronic doping, corrugations or localized defects [3], while using graphene flakes as precursors one can obtain nano-porous scaffolds with extremely complex and little ordered structure[4].

In this talk, it will be shown that the deviations from perfection of graphene are in fact opportunities to for specific applications. First, SiC supported epitaxial graphene will be examined. Density Functional Theory calculations show that the multi-stable corrugation of epitaxial monolayer graphene[5] and the steady-state rippling of its buffer carbon layer [6] could be exploited for chemical functionalization. Conversely, the quasi free-standing monolayer graphene obtained by H intercalation has with localized electronic states, with potential applications in optoelectronics[7,8].

Disordered graphene is more difficult to model. An algorithm to generate realistic models of graphene based scaffolds with given density, porosity and accessible surface is first illustrated and validated[9]. Adsorption of gases and electrolytes within these structures is subsequently simulated by means of Force Field based classical molecular dynamics, and its applications to hydrogen storage or for electrodes of batteries or supercapacitors is subsequently discussed.

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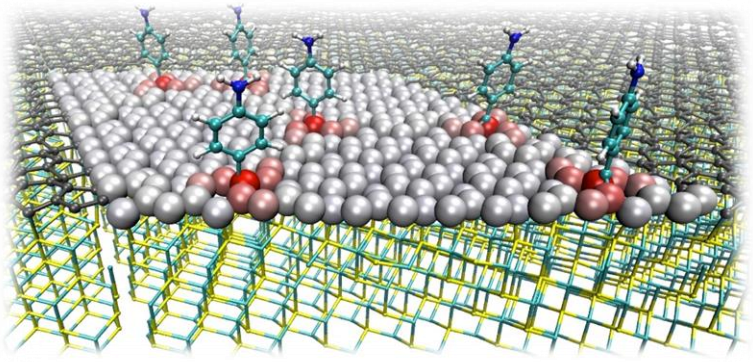

Tipo presentazione: orale

Area progettuale di riferimento:

SURFACES AND INTERFACES: NANOFABRICATION, IMAGING, AND SPECTROSCOPY

and

NANOSCALE THEORY, MODELLING AND COMPUTATION