Hydrogen interaction with statically and dynamically rippled graphene

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Hydrogen can be either physisorbed in graphene, interacting with carbon by Van der Waals, forces or chemisorbed by chemically bonding to it[1]. Physisorption is often considered as a mean for H storage, but the gravimetric density (GD, related to gas internal pressure) reaches reasonable values only at low temperatures[1,2]. H chemisorption allows modulating the electronic properties of graphene with possible applications in nano-electronics. In addition, it leads to acceptable GD and stable binding, but the loading and release kinetics are slow at room temperature, due to high chemi-de-sorption barriers[1,3].

We propose that rippling in graphene could be exploited to enhance its interaction with hydrogen[4]. By means of experimental measurements on naturally corrugated graphene grown on SiC[5] combined with multi-scale simulations[6,7] we show that hydrogen preferentially binds on convex areas and is unstable within concavities. We demonstrate by simulations that a curvature interchange mechanically induced by e.g. by coherent flexural phonons can be used to enhance the desorption kinetics and actively transport physisorbed molecular hydrogen eventually increasing the internal pressure of the gas[6]. We are currently evaluating the possibility of obtaining curvature control by mean of external electric fields, exploiting the flexoelectric properties of the pristine or N/B substituted graphene, or by mechanical pulling of graphene sheets on corrugated substrates. These results can be used to design devices for hydrogen storage and in advanced nano-electronics.

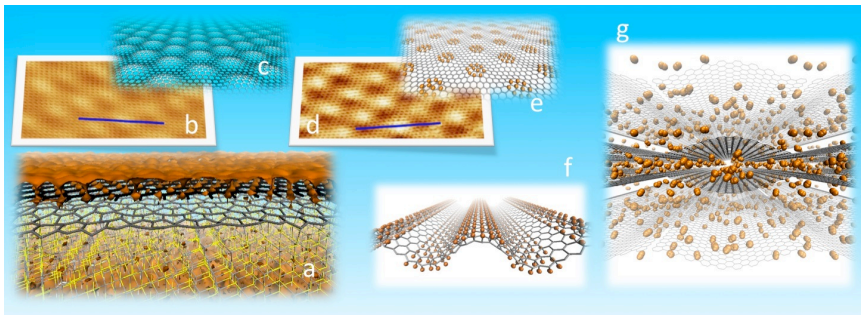

Fig. 1. a: Representation of buffer layer (grey) and first monolayer (black with electronic density in orange) of graphene on SiC (grey and yellow). b: STM image and c: ball&sticks representation of the rippled monolayer. d: STM image and e: ball&sticks representation of the rippled hydrogenated monolayer. f: hydrogenated wave-like ripples in a monolayer. e: physisorbed hydrogen in multilayers with ZA phonons.

References

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