Hydrogen Storage in Graphene

S. Heun

NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, 56127 Pisa, Italy

The realization of innovative hydrogen storage materials has worldwide strategic importance. Graphene has recently attracted attention as a promising hydrogen storage medium. Indeed, graphene is lightweight, chemically stable, and exhibits attractive physico-chemical properties for hydrogen adsorption. Furthermore, the interaction between hydrogen and graphene can be controlled by chemical functionalization.

The energetics of the chemisorption of hydrogen on graphene can be modified by the local curvature of the graphene sheet. Based on scanning tunneling microscopy (STM) we report on site-selective adsorption of atomic hydrogen on convexly warped regions of monolayer graphene grown on SiC(0001). This system exhibits an intrinsic curvature owing to the interaction with the substrate [1]. We show that at low coverage hydrogen is found on convex areas of the graphene lattice [2]. No hydrogen is detected on concave regions. These findings are in agreement with theoretical models which suggest that both binding energy and adsorption barrier can be tuned by controlling the local curvature of the graphene lattice. This curvature-dependence combined with the known graphene flexibility may be exploited for storage and controlled release of hydrogen at room temperature.

Theoretical studies regarding metal atoms (e.g. Ti, Li) deposited on graphene suggest that such materials can adsorb up to 8 wt% gravimetric density of hydrogen. We investigate the deposition of Ti on graphene and its potential for hydrogen storage [3]. The Ti atoms form small islands (diameter ~ 10 nm). The Ti-covered graphene was exposed to molecular hydrogen, and the hydrogen desorption dynamics was measured by thermal desorption spectroscopy. Our data demonstrate the stability of hydrogen binding at room temperature and show that the hydrogen desorbs at moderate temperatures – both ideally matching technical requirements for hydrogen storage. First principle calculations clarify the multi-bonding state between hydrogen and the graphene-supported Ti clusters [4]. To further increase the hydrogen uptake of these samples, we employ controlled surface modifications to increase the active surface for hydrogen adsorption by decreasing the size of the Ti-islands and increasing their density [5].

References

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