Metal-functionalized graphene for hydrogen storage

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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.

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 [1]. 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 (TDS). 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 [2]. 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 [3]. We also explore the use of amorphous graphene for this purpose. Furthermore, we have developed a new experimental tool to directly measure the heat released during the hydrogen loading of functionalized graphene. For this purpose, a sensitive gold film thermometer has been realized. After a careful thermometer characterization and calibration, a thermal signal during hydrogen loading on Ti-functionalized graphene has been detected. Each measurement has been cross-checked through TDS. Results are in good agreement with thermometric measurements. This represents the first direct measurement of enthalpy release in metal-decorated graphene during hydrogen adsorption.

Finally, I will discuss first results on Li-functionalized graphene [4].

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[4] S. Fiori, Y. Murata, S. Veronesi, A. Rossi, C. Coletti, and S. Heun, Phys. Rev. B, in press; arXiv:1706.01386.