

ERATO



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# *Hydrogen Storage on Graphene*

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# Hydrogen Storage on Graphene

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The realization of new and innovative hydrogen storage materials has worldwide strategic importance. In this context, 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 of the material, thus enabling fine tuning of the adsorption/desorption-properties of hydrogen on graphene. Theoretical studies suggest that graphene can adsorb up to 8 wt% by chemisorption and up to 10 wt% by physisorption of hydrogen. However, experimental demonstrations of these numbers have yet to be reported.

The energetics of the chemisorption of hydrogen on graphene can be modified by the local curvature of the graphene sheet. This effect is proposed as the basis of hydrogen storage systems in which the storage and release of hydrogen are obtained by exploiting and controlling the corrugation of individual layers of graphene. Testing these predictions we performed scanning tunneling microscopy experiments of hydrogenated graphene grown on SiC(0001). For the first time, we atomically resolved the hexagonal lattice of the buffer layer verifying that it is topologically identical to graphene [1]. We studied the positions of the hydrogen atoms on the atomically resolved lattice of monolayer graphene as a function of curvature by hydrogenating the sample in situ. We found that atomic hydrogen binds to the carbon atoms in the convexly curved areas of the supercell, indicating a  $\sim 0.15\text{eV}$  increase in the binding energy as compared to flat graphene ( $0.7\text{eV}$ ). We measured the carbon-hydrogen bond height to be  $\sim 1\text{\AA}$ , close to the calculated bond length of  $1.1\text{\AA}$ .

Theoretical studies regarding metal atoms (e.g. Ti) deposited on graphene suggest that such materials can adsorb up to 10 wt% gravimetric density of hydrogen. Each adsorbed Ti atom is predicted bind up to 4  $\sim$  5  $\text{H}_2$  molecules. Given the large number of theoretical papers on this subject, it is surprising that experimental demonstrations of the effect of such modifications on graphene have yet to be reported. Experimental work is under way in our group in order to evaluate the feasibility of graphene as a hydrogen storage medium. We have first experimental evidence that Ti atoms can store hydrogen molecules and release them at around  $250\text{ }^\circ\text{C}$ .

- [1] S. Goler, C. Coletti, V. Piazza, P. Pingue, F. Colangelo, V. Pellegrini, K. V. Emtsev, S. Forti, U. Starke, F. Beltram, and S. Heun, *Carbon* 51, 249 (2013).