Prospects for Hydrogen Storage in Graphene

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Graphene is an intriguing material that shows promises for hydrogen storage [1]. We shall present in this talk theoretical and experimental evidence that by changing the curvature of graphene, the energy barrier for adsorbing and desorbing atomic hydrogen attached to the pi-bonds of graphene can be removed making it possible to attach and release hydrogen at room temperature, a mechanism that can be exploited for room temperature hydrogen storage applications.

By means of calculations based on density-functional theory, we demonstrate a tunability of the binding energies of more than 2 eV by changing the sheet out-of-plane deformation up to +-0.2Å, with the convex regions allocating the energetically favored hydrogen binding sites. We simulate the process of hydrogen chemisorption on corrugated graphene and release under the application of time-dependent mechanical deformations. Our results show that the corrugation of the graphene sheet and the controlled inversion of its curvature yield fast and efficient storage and release of hydrogen [2]. Our corrugated graphene device can potentially reach gravimetric capacities up to 8%wt and reversibly store and release hydrogen by external control of the local curvature at room conditions and with fast kinetics.

Experimental tests of the capacity of corrugated graphene to bind hydrogen are carried out on epitaxial graphene grown on SiC(0001). The initial carbon layer (also known as the interface, zerolayer or buffer layer) below the monolayer graphene has been theoretically predicted to have a high curvature with an amplitude of 1.2Å over a length of ~2nm making it an optimal laboratory for testing the interaction between hydrogen and graphene as a function of curvature [3]. To this end we shall discuss scanning tunneling microscopy experiments of hydrogenated graphene sheets grown on the silicon face of silicon carbide. In these experiments we were able to atomically resolve, for the first time, the hexagonal lattice of the zerolayer verifying that it is topologically identical to monolayer graphene [4]. Upon obtaining atomic resolution, we hydrogenated the sample in situ obtaining up to 1%wt and studied the position of hydrogen atoms on the graphene lattice as a function of curvature [5]. We found that atomic hydrogen binds to the carbon atoms in the convexly curved areas, in agreement with our theoretical evaluations based on DFT calculations [2], which indicates an increase of ~0.15eV in binding energy with respect to flat graphene (0.7eV). We resolved dimer, paradimer, and tetramer configurations. We finally measured the carbon hydrogen bond height to be ~1Å, in agreement with the expected bond length of 1.1Å [4,5].

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