

A calorimetric study of hydrogen storage on graphene functionalized with Titanium

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Since its discovery in 2004 [1], research on graphene has achieved remarkable results. In the last years, a huge research effort has been devoted to engineering carbon-based nanomaterials able to adsorb hydrogen molecules with high storage capacity and easy release of them. Monolayer graphene (MLG) represents an appealing material, owing to its favourable physical-chemical properties and its high specific surface area, which makes it ideal for functionalization. Thus, metal-functionalized MLG [2-6] has been widely investigated both theoretically and experimentally. The purpose of our work is to provide 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 realised. Thermometric measurements are performed monitoring its resistance variation with temperature. After a careful thermometer characterization and calibration, a thermal signal during hydrogen loading on a Ti-functionalized MLG has been detected. These results represent the first direct measurements of Enthalpy (H_r) released during hydrogen loading process in functionalized graphene. In two successive experiments, temperature increases of $\Delta T = 0.065$ K and $\Delta T = 0.25$ K have been measured, corresponding to $H_r = (23.4 \pm 4.7) \mu\text{J}$ and $H_r = (58 \pm 12) \mu\text{J}$. Each measurement has been cross-checked through Thermal Desorption Spectroscopy (TDS), extracting the loaded hydrogen amount and the binding energy using the Redhead equation. TDS spectra gave an average binding energy $E_b = (1.32 \pm 0.07)$ eV/molecule and a desorbed hydrogen amount of $N = (1.03 \pm 0.10) \times 10^{14}$ molecules, which corresponds to $H_r = (21.8 \pm 1.3) \mu\text{J}$ for the first experiment. Similarly, we obtain $E_b = (1.24 \pm 0.09)$ eV/molecule and $N = (2.71 \pm 0.03) \times 10^{14}$ molecules, which correspond to $H_r = (53.8 \pm 4.3) \mu\text{J}$, for the second exposure. Results are in good agreement with thermometric measurements. This represents the first direct measurement of heat release in metal-decorated graphene during hydrogen adsorption.

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