An in-depth study of the formation of graphene/Si(111) interface from the electrochemical reduction of graphene oxide nanosheets

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A combined experimental and theoretical investigation approach has been applied electrochemical reduction to the of graphene oxide (GO) in order to unravel the corresponding reaction mechanism, so far scarcely addressed in the literature. Reduced graphene oxide (rGO) layers were prepared via electrochemical reduction of GO drop-casted onto hydrogenated Si(111) wafers in aqueous medium.[1,2] A cyclic potential variation programme was applied at different scan rates, followed by an ex-situ characterization of the obtained rGO deposits by means of X-ray photoelectron spectroscopy (XPS). By means of density functional theory (DFT) based calculations, focused on the fate of epoxyl and carbonyl groups upon electrochemical reduction, interpretation the reduction an of mechanism of the GO layers has been proposed for the first time, consistently with both XPS and CV results. Such mechanism is based on the sequential reduction of epoxyl and carbonyl moieties of GO through a two-electron and one-electron mechanism, respectively.[1]

References

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Figures



Figure 1: (Lower panel) Deconvolution analysis of a typical cyclic voltammogram associated to the electrochemical reduction of GO. (Upper panel) DFT model of GO depicting the most relevant oxygenated functional groups.