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Multilayer epitaxial graphene oxide: structural and chemical properties from a combined theoretical and experimental XPS study SI ZHOU, SUENNE KIM, ELISA RIEDO, ANGELO BONGIORNO, Georgia Inst of Tech — Multilayer graphene oxide (GO) is a material holding great promise in future energy storage and nano-electronic technologies. This material remains qualitatively known to date. In this work, we present a combined density functional theory (DFT) and experimental X-ray photo-emission spectroscopy (XPS) study of the structural, chemical, and thermal stability of multilayer GO grown epitaxially on silicon carbide. This investigation shows that at room temperature multilayer GO is a metastable material. GO films undergo spontaneous modifications and chemical reduction with a relaxation time of about one month. These processes lead multilayer GO toward a longer-living quasi-equilibrium state, consisting a structure deprived of epoxide groups, rich of hydroxyl groups, and with a O/C ratio of 0.38. Our study suggests that the presence of excess H chemisorbed on the graphitic sheets is the origin of the metastable character of multilayer GO. These H species favor the reduction of epoxide groups and the consequent transformation of hydroxyls into water molecules intercalated between the graphitic layers. Our DFT calculations show that these molecular transformations are controlled by diffusion processes.

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