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Chemical structure of multilayer oxidized epitaxial graphene SI ZHOU, ANGELO BONGIORNO, Georgia Institute of Technology — In this work, density functional theory (DFT) calculations are used to interpret new X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and atomic force microscope (AFM) measurements of the oxide of epitaxial graphene. This layered carbon material is obtained by Hummers oxidation of 6- to 17-layer graphene films grown epitaxially at high temperature on a silicon carbide substrate. The extensive DFT calculations carried out to solve the inverse problem posed by the aforementioned measurements show that a most plausible molecular structure for the oxide of epitaxial graphene consists of mildly oxidized graphene layers covalently bridged by short polyoxymethylene chains. Possible chemical reactions leading to this form of graphene derivative are discussed.

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