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Engineering of Ferromagnetic Graphite and Graphene ROBSON R. DA SILVA, Instituto de Física "Gleb Wataghin," Universidade Estadual de Campinas, UNICAMP 13083-970, Campinas, São Paulo, Brasil, YAKOV KOPELEVICH, IVAN N. NAUMOV, ALEXANDER M. BRATKOVSKY, Hewlett-Packard Laboratories, 1501 Page Mill Road, Palo Alto, California 94304, USA — In the present work, we demonstrate both experimentally and by ab-initio simulations that room-temperature ferromagnetism can be induced in graphitic materials by means of adsorbed oxygen or sulfur. The results show that oxygen/sulfur-induced edges of graphitic fragments (via unzipping effect) play an essential role in this phenomenon, and that the finite magnetic moment takes place if zig-zag edges in a graphitic ribbon are terminated asymmetrically, i.e. with a different oxygen/sulfur occupation at opposite edges. In particular, our ab-initio calculations performed within the local spin density approximation showed that in the case of pure graphene ribbon, its edge carbon atoms carry large magnetic moment ($\sim$0.72 μ_B/C). In an oxidized graphene, however, the magnetic moment at the edge with absorbed oxygen atoms vanishes, leading to effective ferro(ferri)-magnetic behavior of the sample.

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