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**Oxygen- and Sulfur- driven Ferromagnetism in Graphitic Fragments: Ab-Initio Study** IVAN NAUMOV, Hewlett-Packard Laboratories, YAKOV KOPELEVICH, Instituto de Física “Gleb Wataghin,” Universidade Estadual de Campinas, UNICAMP 13083-970, Campinas, São Paulo, Brasil, ALEXANDER BRATKOVSKY, Hewlett-Packard Laboratories, HEWLETT-PACKARD LABORATORIES COLLABORATION — We study the origins of high-temperature ferromagnetic behavior in graphite by means of unbiased ab-initio calculations and compare them with our data. The experimental 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 appears if edges in a graphitic ribbon are occupied asymmetrically by either oxygen or sulphur. In particular, our ab-initio calculations performed within the LDA and GGA approximations showed that in the case of pure graphene ribbon, its zig-zag edge carbon atoms carry large magnetic moment ( $\sim 1 \mu_B/C$ ). In an oxidized or sulfurized graphene, however, the magnetic moment at the edge with absorbed atoms gets considerably reduced, leading to effective ferromagnetic (more precisely, ferri-magnetic) behavior of the sample.

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