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Edge states and magnetism in carbon nanotubes with line defects HELIO CHACHAM, MARIO S. C. MAZZONI, SIMONE S. ALEXANDRE, Universidade Federal de Minas Gerais — Under certain conditions, magnetic ordering has been predicted to occur in carbon nanostructures even in the absence of transition metal impurities. These conditions involve situations in which electronic localization takes place, such as at zig-zag edges or defects in graphene sheets and ribbons or in topological defects in carbon nanostructures. In the present work, we apply first-principles calculations to investigate the interplay between electronic and magnetic properties of carbon nanotubes with line defects. We consider three types of defects: lines of C-O-C epoxy groups, and defects resulting from the substitution of the oxygen atoms by CH_2 or C_2H_4 divalent radicals. We find that the line defects behave as pairs of coupled graphene edge states, and a variety of electronic and magnetic ground states is predicted as a function of defect type, nanotube diameter, and a possibly applied transverse electric field.

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