Tuning of the electronic properties of *armchair* graphene nanoribbons by mild functionalization. Theoretical study of the $^1\Delta_g$ O_2 border addition.

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Armchair graphene nanoribbons (*a*-GNRs) are finite strips of graphite sheets cut along a specific direction with a width < 10 nm and a length/width ratio > 10.[1] They feature peculiar electronic and optical properties so they have been touted as a promising material for everything from solar cells to computers.[2] The energies of their HOMOs and LUMOs, along with their difference (gap) are some of the most important parameters to be controlled in the design of organic electronic devices mechanisms.[3] In this this work we propose a modification of their electronic properties through the oxidation of *a*-GNRs with $^1\Delta_g$ O_2 in mild conditions.[4] This process should bring about a decoration with vicinal dialdehydic groups (Figure 1) of the border of the *a*-GNRs via endoperoxide "1,2".

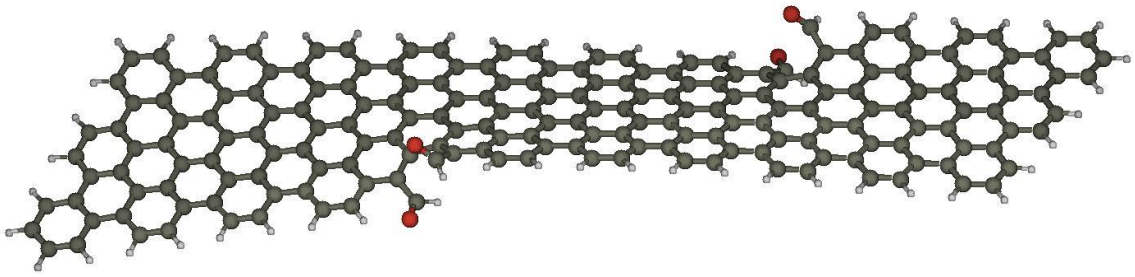

Figure 1

The new material should present LUMO energies lowered by 0.3 – 0.5 eV with respect to the original material. As a consequence, the HOMO-LUMO gap should be reduced by almost the same amount, being the HOMO energy less sensitive to the oxidation. This method is intended to be alternative or complementary to the simple tuning of the *a*-GNRs size.

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