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Hydrogen Saturation of Graphene Nanoribbons: edge states suppression and gap behavior[1] THIAGO MARTINS, ANTONIO J. R. DA SILVA, ADALBERTO FAZZIO, Physics Institute - University of Sao Paulo — Di-hydrogenated zigzag edges Graphene Nanoribbons (2H-ZZ-GNR) are more stable than the usually studied mono-hydrogenated [1] passivation (H-ZZ-GNR). Using density functional theory, we studied a variety of 2H-ZZ-GNR configurations. We investigated how the interaction between the CH_2 units depends on their separation at the same edge as well as on the width of the ribbon. We observe, in agreement with previous studies [1], that the 2H-ZZ-GNR passivation suppresses the presence of edge states, thus eliminating the magnetic instability of H-ZZ-GNR that is responsible for the gap opening in the anti-ferromagnetic ground state configuration. Moreover, there is a reduction of coupling between edge and bulk carbon atoms, resulting in a band structure whose gap is dominated by bulk bands and confinement effects. We also studied the behavior of the gap as a function of the ribbon's width, and we observed that it quickly closes as the width is increased.

[1] T. Wassmann, A. P. Seitsonen, A. M. Saitta, M. Lazzeri, and F. Mauri, Phys. Rev. Lett. **101**, 096402 (2008).

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