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Edge-Saturation Effect on Finite Size 0-D Carbon Nano-Ribbons — a Density Functional Theory Study LI CHEN, Massachesetts College of Pharmacy and Health Sciences, LOUIS CIRELLO, Rhode Island College — Using computational simulation and Density Functional Theory, we have studied the absorption of various foreign molecular/atomic groups saturated at the edge of semiconducting, finite-size armchair carbon nano-ribbons (ACNR). The effect of this edge-saturation was studied in terms of its impact on HOMO-LUMO gap, electronic structure and spin distribution. A comparison was made between the non-saturated pristine ACNRs and saturated ones, as well as, between different saturation species, different doping sites, different doping concentration and ACNR length. Our results suggest that the type of elements play a more important role than the concentration and/or doping sites in terms of the change in HOMO-LUMO gap, which leads to the possibilities of using CNBs as nano-scale chemical sensors. The doping of some elements also introduces a spin distribution different from the pristine CNBs.

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