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Confinement effect on spin-polarized edge states in graphene nanostructures CARLOS RAMOS-CASTILLO, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico — One of the most intriguing phenomena in condensed matter physics is the existence of edge states on the boundary of a 2D system. In graphene, the edge states have distinct properties from the bulk states and play important roles in the physicochemical properties of the material. In this work, we show ab-initio results of spin-polarized electronic edge states in graphene quantum dots of different sizes and shape. We found a critical size at which the singlet nonmagnetic ground state becomes singlet open-shell with antiferromagnetic order. We found that the critical size is strongly influenced by the shape of the quantum dot. We discuss this behavior based on energetics and electronic structure of the system under study. The calculations are base on the Density functional Theory (DFT). The Linear Combination of Atomic Orbital (LCAO) method for bases functions it was used. For exchange-correlation functional has been used the Generalized Gradient Approximation (GGA).

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