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Electronic properties of graphene nanoflakes: energy gap engineering CARLOS RAMOS, EDUARDO CIFUENTES, ROMEO DE COSS, Cinvestav Unidad Merida, EDGAR MARTINEZ, Universidad Autonoma de Nuevo Leon — Graphene nanostructures show an energy gap resulting of the finite size, and are of current interest because of the potential applications in electronic devices. Thus, we discuss some recent progress in the synthesis of graphene nanoflakes obtained from the reaction of polyaromatic hydrocarbons. We are presenting ab-initio results for the electronic properties of graphene nanoflakes with a hexagonal-zigzag (HZ) structure and different effective radius (R). The calculations were performed using the Density Functional Theory as implemented in the pseudopotential-LCAO method. We find that the, Kohn-Sham gap decreases with size as R^{-1}, while the quasi-particle energy gap follow the $R^{-0.8}$ scaling rule. A formula to evaluate the energy gap of a HZ graphene nanoflake of arbitrary size is provided. This research was supported by Conacyt-México under Grant No. 83604.

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