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A TD-DFT study on the Optical and dielectric properties of graphene nanoflakes CARLOS RAMOS, EDUARDO CIFUENTES, ROMEO DE COSS, CINVESTAV Unidad Merida — Optical and dielectric properties of graphene nanostructures are of current interest because the potential applications in electronic and photonics devices. Recently, it has been reported important progress in the synthesis of graphene nanoflakes and their applications as quantum dots. In this work, the size and geometric shape effects on the optical spectrum and dielectric constant of graphene nanoflakes are studied by using an ab-initio approach. The calculations were performed using the Time-Dependent Density Functional Theory (TD-DFT) as implemented in the plane wave method and the results provide insights about controlling the optical properties of graphene using the size and shape of the nanostructure. This research was supported by Conacyt-México under Grant No. 83604.

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