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Physisorption of Fullerenes in Graphene layers and carbon Nanoribbons¹ MONICA PACHECO, PEDRO ORELLANA, Universidad Tecnica Federico Santa Maria, JULIAN CORREA, Universidad de Medellin — The study of nanostructures based on carbon allotropes has captured the interest of the scientific community in the last two decades, due to its great versatility. In such structures a simple change of geometry leads to important changes in their physicochemical properties. In this context it has been studied different carbon allotropes complexes in particular for the development of photovoltaic systems. In this paper we show a study of opto-electronic properties of fullerenes physisorbed on graphene nanoribbons. Our calculations are carried out within the framework of density functional theory (DFT) using the SIESTA package. Our results show that effectively the fullerenes bind both to the layer of graphene as well as to the nanoribbons, with binding energies of about 0.5eV. We find that when the complex is formed, the physical properties of fullerenes, graphene and nanoribbons are preserved and when graphene is functionalized with various fullerenes the electronic spectrum is composed of bands of energy which increases the intensity of the optical absorption spectrum of the complex.

¹Conicyt ACT 1204, USM 11.14.68

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