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Vibrational and Electronic Properties of Carbon Dioxide Absorbed in Graphene Nanosheets

João Paulo Cascudo Rodrigues, Wiliam Ferreira da Cunha, Pedro Henrique de Oliveira Neto, Ricardo Gargano

Institute of Physics, University of Brasília – UnB, Brasília, Brazil

Abstract: Graphene has turned into a key material in chemistry, condensed matter physics, and materials science in view of their unique structural features[1]. Acting as a platform for anchoring catalyst, photodetectors, solar cells, and battery devices, graphene systems have already found various applications[2]. In this work, we investigated the electronic and vibrational properties of multi-layers graphene sheets interacting with a CO2 molecule. Electronic structure calculations were performed by means of density functional theory (DFT). The possible equilibrium geometries and binding energies were evaluated using Gaussian09 at the B3LYP level using the 6-31G** basis set. In order to evaluate the potential energy curves, we performed several single points DFT calculations for varying distances between the Carbon-dioxide molecule and the graphene sheet, as in ref[3]. Using an extended Rydberg function[4], we fit the potential energy curve, thus obtaining an analytical expression. Following, through the application of the DVR methodology[5], we used the analytical expression in the solution of the Schrodinger nuclear equation in order to obtain rovibrational energies. The results presented here may provide guidance to the understanding of the underlying science of Carbon-dioxide absorption in graphene nanosheets.

Key-words: carbon dioxide absorption, potential energy curve, density functional theory

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