THE CHARACTERIZATION OF A NEW 2-D CARBON ALLOTROPE CALLED POPGRAPHENE UNDER A BIAS VOLTAGE APPLICATION

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Abstract

Graphene is a structure formed by hexagons with a thickness of 1 atom, and this two-dimensional aspect gives it wide theoretical surfaces and allows the insertion of a large number of molecules by adsorption or doping in it, giving the graphene new properties or the improvement of existing properties. Because of these features, graphene its widely use in the construction of batteries, catalysts, biosensors, among other applications. Graphene originally has a zero gap energy, and this can be see in its band structure, who presents two cones connected, knowledge's as Dirac cones. The insertions of defects or a bias voltage application could causes a semiconductor behavior in it, because it could causes the disconnection of the Dirac cones causing the appearance of a gap. There is a possibility of inserting defects in graphene through changes in its aromatic rings, which gives rise to other two-dimensional allotrope forms of carbon with new properties. For example, the insertion of defects 5-6-7 in graphene can give rise to Phagraphene or Ψ-graphene, and the insertion of defects 5-8-5 originates the Popgraphene. Among the two-dimensional forms of carbon, the Popgraphene stands out for having attractive characteristics in the manufacture of anode materials for the preparation of batteries, since it is a good conductor, has good adsorption capacity for lithium atoms and a high thermal stability, occurring the deformation of the structure only for temperatures of approximately 1500K. As Popgraphene also presents a zero gap energy, a theoretical study of its properties under the application of a bias voltage using DFT methodology its promising, since the bias voltage could create a gap energy and a semiconductor behavior in it, to possibility its application in molecular electronics. The results show that popgraphene is a new nanodevice that can be applied in molecular electronics, because despite being somewhat unstable when subjected to the action of an external agent, it presents a higher conductance and a well define I-V characteristic curve of a Field Effect Transistor (FET).

Palavras-chave: Molibdatos, Expansão Térmica Negativa, Espectroscopia Raman.