

Abstract Submitted
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Gap opening due to topological defects in graphene¹ RICARDO NUNES, JOICE ARAÚJO, HELIO CHACHAM, UFMG - Brazil — Stone-Wales defects (SWD = two adjacent pentagon-heptagon pairs) are common low-energy defects in carbon nanotubes. Previously, Crespi et al.[**PRB**, **53**, **1996**] have proposed a purely-carbon covalent metal sheet called “pentaheptite,” consisting entirely of SWDs, with a relatively low formation energy of 0.32 eV/atom, with respect to graphene. In this work, we consider three different families of periodic carbon sheets containing topological defects (TDs = pentagons and heptagons). The families differ by the density of TDs in a seed structure. In each family, we generate periodic structures in which isolated pentagons and heptagons are surrounded only by hexagons. By means of ab initio calculations, we propose that, depending on the density and distribution of TDs, these carbon sheets may behave as a semiconductor, a metal or a semimetal. In the range of TD concentrations we examine, the sheets are stable in a planar form, but, allowing for the corrugation generated by the curvature fields associated with the isolated TDs, leads to lower formation energies and to either a reduction of the density of states or to gap opening at the Fermi level. Formation energies can be very small: in particular, we obtain a semiconducting structure with a formation energy of only 92 meV/atom with respect to graphene.

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