nearest neighbour atoms along the bond); Δ_σ is a promotion integral (transfer between hybrid orbitals on the same site): $\Delta_\sigma = (E_s - E_p)/(\nu + 1)$.

For an infinite three dimensional crystal (bulk), the gap between valence and conduction band (forbidden band) is $g = |-2\beta_\sigma + (\nu+1)\Delta_\sigma|$ (for VIb elements) and β_σ may be derived from the values of g [5].

The Hamiltonian for the π bonds is:

$$H_\pi = E_p \sum_i |i><i| + \beta_\pi \sum_{i,i' \neq i} |i><i'| \tag{3}$$

with $|i>$ the π orbitals centered on atoms i and β_π is the hopping integral for π levels.

The β_π value for C was chosen in order to get the correct positions for C_2 energy levels in comparison to the results of the Verhaegen's ab initio calculations [6].

We need only three parameters:β_σ, β_π and Δ_σ for the homonuclear model which represent in fact the average potential $V(r)$ and which take into account the nuclear attraction and the dielectronic attraction [5]. The values of these three parameters are given in table I.

III. RESULTS

We computed the density of states of pure and doped graphene nanoflakes. The nanoflakes have boundaries represented in figure 1. We studied nanoflakes containing 480, 720 and 960 atoms: we obtained their geometry by reproducing figure 1 in the y direction.

In figure 2, one may see the density of states of nanoflakes of graphene containing 480 atoms. The nanoflakes are isolated, i.e. they are not connected to any other conducting material or connected to any substrate. The 3 graphs in figure 2 representing the DOS (density of states) correspond to: (a) pure graphene nanoflake (b) 5% of Si atoms randomly introduced in the graphene nanoflake and (c) 5% of sp^3 hybridized carbon atoms randomly distributed within the nanoflake. , 10%, 15% and 20%. The boundaries of the nanoflakes correspond to the armchair geometry.

Figure 3 corresponds to the same nanoflakes (i.e. pure, with 5% of Si atoms and with 5% of sp^3 hybridized carbon atoms) but in this case for 720 atoms.

Figure 4 corresponds also to 3 DOS with the same nanoflakes but this time containing 960 atoms.