Lab6 - *Magnetic graphene nanoribbons*

Simulation of Nanometric Systems – *Nanoscience and Nanotechnology - 22/23*

Daniel Bedmar Romero 1565494

In this practice, we aimed to reproduce the results obtained by Soon et. al [1] with the objective of getting more familiar with the operation of the SIESTA program and the sisl Python library. The code used for the practice can be found in my repository [2].

1 Day 1

On the first day, our objectives were to create the input for the simulation, think about which direction we needed to sample the k-space, and perform a simulation with this input to ensure everything was working correctly.
We can create the structure with the following sisl command (also plotting its unit cell), obtaining what we see in Figure 1.

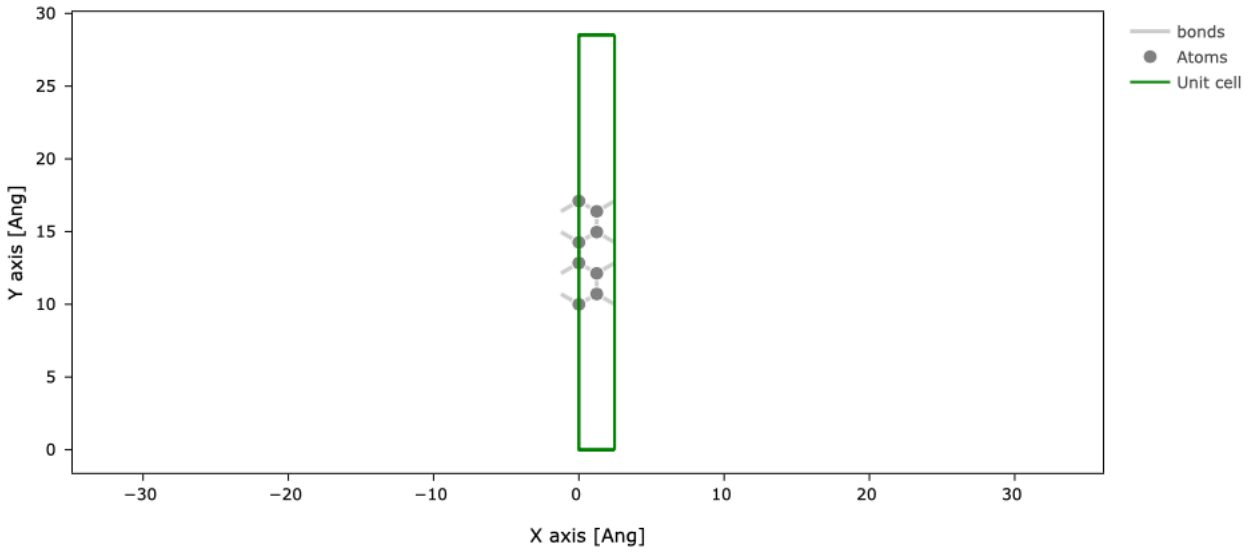


Figure 1

To create the input file, we create the file *RUN.fdf*, specifying that the structure is included and a 10x1x1 k-grid (x,y,z), as we want to sample the reciprocal space in the x-direction. In the input file, we also include saving the Hamiltonian and the electron density to later study its band structure. We also need to have a file ready with the pseudopotential of Carbon.

2 Day 2

When plotting the fatbands, we see localized states at the Fermi level that should not be there, these energy levels correspond to the outermost atoms of the ribbon. The appearance of these levels is due

to the fact that the natural state of the ribbon has these Carbons saturated with Hydrogen. To add these Hydrogens, we need to modify the structure of the generated ribbon by editing our *STRUCT.fdf* file. In Figure 2, we can see how we have modified the code to write the file correctly, it should be noted that to know where to place the Hydrogens I have looked for the bond distance between sp2 Carbon and Hydrogen and I have also added a file with the pseudopotential of Hydrogen.

```
open('RUN.fdf', 'w').write("""%include STRUCT.fdf
SystemLabel siesta_2
PAO.BasisSize DZP
MeshCutoff 250. Ry
SaveHS true
SaveRho true
%block kgrid.MonkhorstPack
  10  1 1 0.
   1 1 1 0.
   0  0 1 0.
%endblock
""")
rib.write('STRUCT.fdf')
```

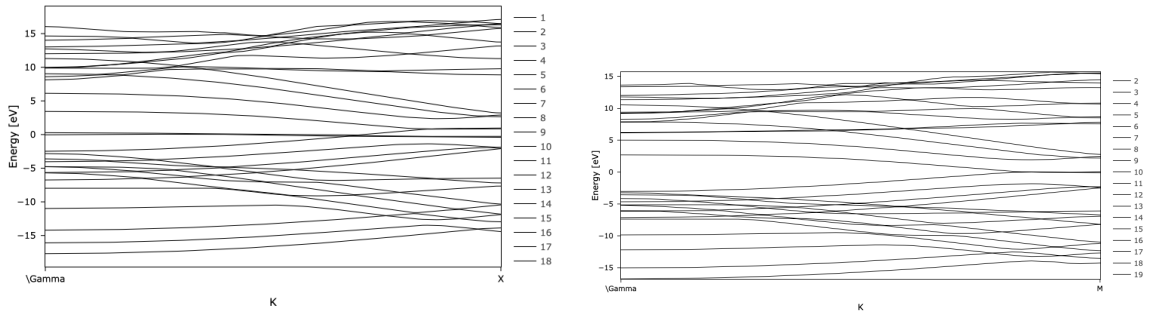
(a)

```
open('RUN.fdf', 'w').write("""%include STRUCT.fdf
SystemLabel siesta_2
PAO.BasisSize DZP
MeshCutoff 250. Ry
SaveHS true
SaveRho true
%block kgrid.MonkhorstPack
  10  1 1 0.
   1 1 1 0.
   0  0 1 0.
%endblock
""")
rib.write('STRUCT.fdf')
open('STRUCT.fdf', 'w').write("""LatticeConstant 1.0 Ang
%block LatticeVectors
 2.45951215 0.00000000 0.00000000
 0.00000000 28.52000000 0.00000000
 0.00000000 0.00000000 14.20000000
%endblock LatticeVectors

NumberOfAtoms 10
AtomicCoordinatesFormat Ang
%block AtomicCoordinatesAndAtomicSpecies
  0.00000000 10.00000000  0.00000000 1 # 1: C
  0.00000000 12.84000000  0.00000000 1 # 2: C
  0.00000000 14.26000000  0.00000000 1 # 3: C
  0.00000000 17.10000000  0.00000000 1 # 4: C
  1.22975607 10.71000000  0.00000000 1 # 5: C
  1.22975607 12.13000000  0.00000000 1 # 6: C
  1.22975607 14.97000000  0.00000000 1 # 7: C
  1.22975607 16.39000000  0.00000000 1 # 8: C
  0.00000000 8.912000000  0.00000000 2 # 9: H
  0.00000000 18.18800000  0.00000000 2 # 10: H

%endblock AtomicCoordinatesAndAtomicSpecies

NumberOfSpecies 2
%block ChemicalSpeciesLabel
 1 6 C
 2 1 H
%endblock ChemicalSpeciesLabel

""")
```

(b)

Figure 2: In (a), we can see the old version of the code, while in (b), we see the new version.

The difference between the band structures can be found in Figure 3.



(a) **(b)**

Figure 3: In (a), we can appreciate the states localized at the Fermi level, while in (b), these states are no longer there thanks to saturation with Hydrogens.

By adding spin polarization, we expected the states to separate, and as we can see in Figure 4, we can observe how in the fatbands the states corresponding to spin Up and spin Down split, and in the PDOS we can also appreciate this shift in the levels. SIESTA has achieved a spin polarization of 0.44, so this net polarization indicates that we have a ferromagnetic configuration, a configuration that does not quite fit with the output.
To force SIESTA to give us the antiferromagnetic configuration, we will force atoms 1 and 4 (remember that they are the outermost atoms of the ribbon and which play an important role in its physical properties) to have opposite spins. Once this is done, our system ends up having a zero magnetization and the states no longer separate between SpinUp and SpinDown. The results can also be seen in Figure 4

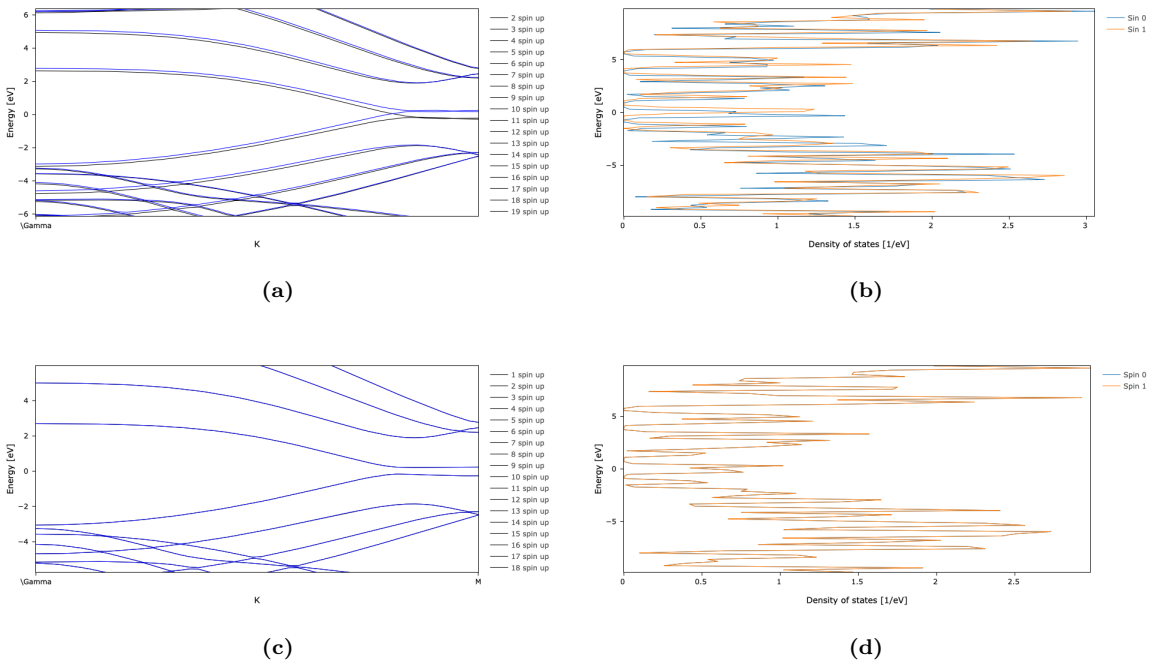
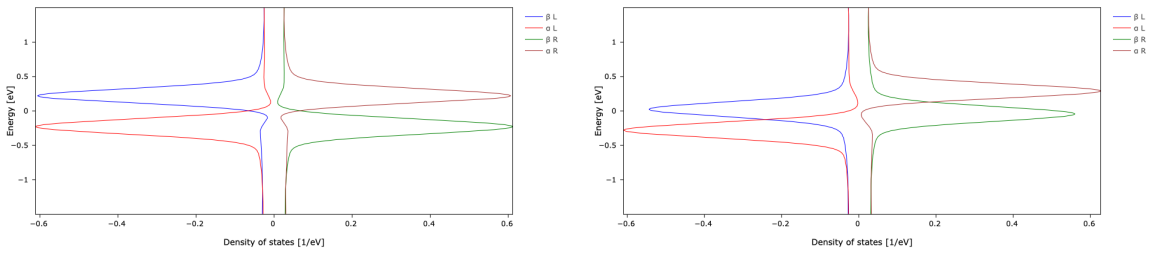


Figure 4: In (a) and (b), the fatbands and the PDOS, respectively, of the system when we do not induce any initial magnetization, while in (c) and (d), the fatbands and the PDOS, respectively, of the system when we induce the initial magnetization.

3 Day 3

Once we have obtained the system we wanted, we need to recreate Figure 3 (a) and 3 (b) from the paper. In Figure (a), there is no electric field, and in (b), there is. My recreation of these figures can be seen in Figure 5



(a) **(b)**

Figure 5: In (a), we can see how this kind of GAP is formed between the states with spin Up and down, both on the left and on the right, while in (b), we clearly have states at the Fermi level, both on the left and on the right.

References

[1] M. L. C. . S. G. L. Young-Woo Son, "Half-metallic graphene nanoribbons," *nature*, vol. 444, no. 1, pp. 347—-349, 2006.

[2] "Repositori github." https://github.com/DaniBedmar/Lab9.