2D graphene

Introduction: For this project, you will investigate a 2 dimensions (2D) material which is Graphene (you may suggest another 2D if you want for your project). We propose you to look at the properties of different kind of defects within graphene: Potassium adsorbed dopant, the so called 5-7 defect and a vacancy defect.

The preliminary work is mandatory as well as one of the more advanded task as Potassium doping, 5-7 defect or vacancy defect.

Preliminary work:

All the work proposed in this section may be done on a small computer (laptop). You may want to reserve the use of the cluster for the second part of this project.

At first your are going to look at the convergence of a calculation on bulk material, *i.e.* you are going to consider the primitive cell of graphene which is a 2D hexagonal cell. There is 2 carbon atoms within the primitive cell. You must be aware that graphene is a 2D material and thus a vacuum gap has to be introduce in the out of plane direction. As quantum espresso is using periodic conditions the dimension of the unit cell in this direction must be chosen large enough to ensure that the graphene sheet is not interacting with itself.

The two main physical parameters which have to be tuned carefully are the energy cut-off (mainly the plane wave cut-off) corresponding to the parameter `ecutwfc` and the k-points sampling of the Brillouin zone (parameter `K_POINTS`). Basically, you will have to redo the same calculation for increasing values of these parameters and look at the total energy of the system which is the the key physical quantity. The convergence is reached when the total energy is not varying anymore. Be aware that you need to relax the cell (the lattice parameter may also be monitored for the convergence) for each of your calculation (parameter `calculation = 'vc-relax'`).

Once the optimal plane wave cut-off and k-points sampling have been found, you may compute and plot the Band structure and the density of states (DOS). Furthermore, you may check the dimension of the cell in the direction perpendicular to the graphene plane to check that the vaccum is large enough. The c dimension of the cell is given by the parameter `celldm(3)`. Its value in Bohr corresponds to `celldm(3)*celldm(1)`. For this task, you should reduce the cell dimension in this direction step by step and look at the total energy and at the hydrostatic pressure and see, at which point, a significant change is observed.

Defect:

In this part you are going to introduce a defect in the graphene sheet. For this study you will need to consider a supercell. A 4×4 supercell is actually proposed for this project. However, if you have limited access to a supercomputer,you may consider to define a smaller supercell in order to reduce the computational time. Three different kinds of defect have been selected for you:

- Potassium atoms, when adsorbed on the graphene sheet, is leading to n type doping. A charge transfer between the Potassium atom and the graphene sheet is occurring leading to a shift of the Fermi level toward the conduction band. You may look at the projected density of states to investigate the localization effect induced by the dopant and also to quantify the charge transfer. Indeed, the charge tranfert (or charge carrier) is not an integer number of electron. To quantify the carrier density, it is mandatory to integrate the DOS from the top of the valence band (for graphene it is corresponds to the tip of the dirac cone) to the Fermi level. You will need to write your own code for that.

- The 5-7 defect (also called Stone-Wales) corresponds to a rotation of 2 carbon atoms leading to the occurrence of 2 pentagons and 2 heptagones. This is a very common defect within graphene. For

this defect you may compute the DOS and the projected density of states (PDOS) to observe some localization effect for the atoms close to the defect.

- Another common defect within graphene corresponds to vacancies. We propose to study the effect of a single vacancy within the graphene sheet. Single vacancy is not the most stable one (di-vacancy is actually more stable and its leading to a pentagon reconstruction). You may investigate this reconstruction and look at the variation of the bond lengths. you may also compute the DOS and the projected density of states (PDOS) to observe some localization effect for the atoms close to the defect.

All endeavours/initiatives are strongly encouraged. If you need help, you may request a zoom meeting with myself. Just email me `christophe.adessi@univ-lyon1.fr` to make an appointment.