Perovskite $SrTiO_3$

Introduction: The topic of this project corresponds to the perovskite material $SrTiO_3$ (STO) and to look at the effect of a dopant atom (Lanthanum or Vanadium) on the density of states.

The preliminary work is mandatory as well as the more advanded task.

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 lattice cell of STO which is a simple cubic structure.

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). Moreover, you are going to use the Murnaghan equation of state to predict the bulk modulus of the material. For this aim, you must repeat your calculation for several values of the lattice parameter close to the optimal value. Be aware that the calculation type (keyword `calculation`) must turn to `scf` and no more `vc-relax`. A simple tool to compute the bulk modulus (called ev.x) is available within the quantum espresso package. This tool is taking as input a text file with two column. The first column being the unit cell volume (a.u^3 or Å^3) of each of your calculations, the second column being the corresponding total energy (Ry). A lot of tutorial are available on internet for this. The predicted value for the bulk modulus should be compared with the experimental one.The optimal lattice vector may also be compared with the experimental value.

Doping:

In this part you are going to introduce a dopant atom in substitution to either Sr or Ti. For instance, Lanthanum in substitution to Sr lead to a n type doping. Vanadium in substitution to Ti is also leading to n type doping but with a specific impurity band. It is requested to study one of them. If you're interested, you can investigate another substitution (Ytrium in substitution to Sr lead to a n type doping as well as Niobium in substitution to Ti).

To study the effect of a dopant atom, you will have to consider a supercell (a repetition of the primitive cell) and you will have to replace one atom (Sr or Ti) by the dopant one. An example of a $2 \times 2 \times 1$ supercell with La doping is given in the directory of the project. The size of the supercell will define the doping concentration. The structure has been optimized and you will just need to perform a `scf` calculation.

You may look at the density of states to observe the effect of the dopant on the occupation of the bands (the Fermi level is given in the output of all the calculation and should be shifted toward the conduction band). You may also look at the projected density of states (PDOS) to pinpoint the occurrence of localized states. The pdos is computed using the code called `projwfc.x`. It gives as ouptut the DOS on each atoms. A set of files with explicit nanimg convention is created containing the PDOS on each atom.

You may also want to check the electron/hole concentration (or carrier concentration) by integrating the DOS from the bottom of the conduction band up to the Fermi level for n doping or from the top of the valence band down to the Fermi level for p doping. For this you will need to write by yourself a program which integrate the DOS. For instance microsoft excel may be used for that.

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.