Guide To QuantumAtk

Steps involved in studying the band structure of Silicon.

* Firstly, we go to the Builder.
* There we go to the database to select the desired element which is Graphene in this case.
* After this we go to script generator
* There we select the things we are interested in finding out: -

1. We select the LCAO calculator.

* Here we need to make sure during setting of parameters that the sampling has been set to an odd integer (in this case we took it as 13\*13)
* Another thing to be noted is if we are dealing with a unit cell that has two atoms in the case of graphene, its reciprocal (Brillouin zone) would be bigger than that of its supercell. So, while dealing with a unit cell we require more k sampling points than in the case of supercell due to its reciprocal being smaller.
* Now, when we are taking parameters like mesh parameter and k points sampling parameter, we need to optimise these. Here, optimising means reducing the computational expense. In this step from the analysis section, we choose chemical potential. To optimise these parameters, we need to bring in the change in the python code. While changing the code, we need to select the range for the for loop and also decide upon an appropriate no. of iterations.
* After bringing about the change in code, we get some coordinates in the end of the log file which needs to be plotted. After plotting we are supposed to select the appropriate value, as there should not be much of a variation in the chemical potential after the value we have selected. From the graph we get a value for k sampling and mesh grid.
* In LCAO Basis set we select Dispersion Correction and there ‘Grimme DFT-D2’ is selected to bring into consider the Vander waal’s forces.
* Counterpoise => for adsorbing
* Poisson => FFT
* Spin: Unpolarised and polarised (both of these cases have been taken into consideration)

Note: While we took polarised into consideration we selected the following from the analysis block:-

1. Density of states
2. Electron density
3. Electron localisation Function
4. Fat band structure (for both spin up/ down and elements and orbitals)
5. Total energy

* Exchange Correlation: GGA
* Pseudo Potential: Pseudodojo
* From the graph after optimisation: (For our case)

1. Density Mesh Cut-Off: 60
2. Sampling: 6\*6\*1
3. Then we select optimisation which opens several options and we again select geometry optimisation in there. (the acceptable value for force tolerance is 0.01 to 0.05, we generally stick to 0.01) Reason being optimisation is required to bring stability to the system. By optimising we have selected the lowest potential system and we have made it follow the second theorem of Density Functional Theorem (DFT) which is based on the variational principle by the means of which we can find the lowest energy of the system and hence making it more stable.