DFT Assignment of International Summer School on Numerical Methods for Correlated Systems in Condensed Matter

Effect of U on Density of States(DOS) in NiO

We will study in this assignment the effect of U on the DOS. You can use the input files from the LDA+U tutorial for this assignment that you will have to modified sightly. In that tutorial you had to use non converged parameters in order for the runs to finish in a short time. In this assignment, it is preferable to use the converged parameters.

You should always check the convergence. For sake of time, here are the parameters needed to obtain converged values:

ecut 30 Ha
pawecutdg 60 Ha
ngkpt 10 10 10

With these parameters, each run will take several hours.

For this assignment, you have to plot the DOS while varying the U value. At the end of the tutorial PAW1, you have seen how to output the DOS, namely by including the option prtdos in the input file. For this assignment, use the tetrahedron method for the DOS, so prtdos 2.

Report the DOS for U=0, J=0; U=2, J=0.2; and U=8, J=0.8 eV. How does the electronic gap change?

No more than about one page. You can send your report to André-Marie at tremblay@physique.usherbrooke.ca .