Practical 7 – Exchange-Correlation

Example 1 – Silicon

1. Run a band structure calculation of silicon for LDA using the files `Si_LDA.cell` and `Si_LDA.param`. Plot the band structure using `dispersion.pl` and note the band gap. Modify the `.param` input file to do the same for the GGA functional by setting **`xc_functional= PBE`**
2. Now do the same calculation except using Kohn-Sham Hartree-Fock and the hybrid functional HSE06 (these input files are named `Si_HF.*` and `Si_HSE.*`). Compare the band structures and note the significant differences. Can you explain the differences?

Example 2 - Graphite

A basic set of input files for graphite is supplied, named `Graphite.cell` and `Graphite.param`. Modify them appropriately to obtain converged geometries using the LDA and PBE exchange-correlation functionals. Explain your result.

Extension

Take any small unit cell you like (e.g. the Si runs above). Run LDA and HSE05 single point energy calculations as a function of increasing k—point grid size (in the `.cell` file use **`kpoint_mp_grid`**) and note the run time for the calculations. Plot a graph of k-point set size against run time for both functionals and note the scaling. Do the same for plane wave cutoff energy (**`cutoff_energy`** in the `.param` file).

Example 3 – TD-DFT of N2

Perform a time-dependent DFT calculation using the input files `N2-LDA.*` and examine the output in detail, particularly noting the details in the `.castep` file and the `.tddft` file.

Extension

Pick another molecule (e.g. benzene, a simple amino acid, water, methane, etc), construct an appropriate `.cell` file, obtain a relaxed geometry and use TD-DFT with the PBE functional to examine the excitation spectrum of the molecule. Compare with experimental results.