PANDASCIENCE.NET

1 Ground state calculation using GPAW

1. Prepare two cell objects, one in conventional and the other in primitive configuration.

2. Set GPAW as calculator for both cells with some reasonable settings like:
   https://wiki.fysik.dtu.dk/gpaw/tutorialsexercises/electronic/bandstructures/bandstructures.html

   - Plane wave (PW) mode with an energy cut-off of $400\,\text{eV}$ (~30 Ry)

   - Monkhorst-Pack k-point grid of $8 \times 8 \times 8$ points

   - Exchange-correlation functional PBE (= version of GGA) or LDA

   - File where text output is written to

3. Find help text, then ask GPAW to calculate the ground state of your system

4. Repeat the calculation and time it

5. Compare the total energy of both setups. Can you find a reason for the huge difference in energy? How much is the difference exactly? What would be a reasonable quantity to be used for comparing both calculations?

2 Calculate and plot ground state density

DFT is based on the Hohenberg-Kohn theorem, which states that all information about the quantum mechanical system is contained within one essential quantity: the ground state charge density $n(\boldsymbol{x})$. In the following, we will calculate this quantity and plot it using the already familiar VESTA tool.

https://wiki.fysik.dtu.dk/gpaw/tutorialsexercises/wavefunctions/plotting/plot_wave_functions.html
https://wiki.fysik.dtu.dk/gpaw/tutorialsexercises/wavefunctions/all-electron/all_electron_density.html

1. Write wave functions to file for later reference (CUBE format)
   Optional: Write all WFs to different files

2. Get pseudo and all-electron density

3. Integrate both densities numerically and interpret the output

4. Write densities to file and plot them using VESTA:

   a) Compute volumetric data (e. g. wave function or density) for plotting (task 1 and 2).

   b) In VESTA, load CIF/Structure first.

   c) Import plot data via:
      `Edit → Edit Data → Volumetric Data → Isosurfaces → Import`

   d) Set iso value to a number that results in a nice plot:
      `Style Tab → Properties… → Isosurfaces → Isosurface Level → +0.5`