Step 1: Wave function calculation

- Inspect the input file “bulk_Si_pwscf.in”
- Set outdir = “./outdir”
- Set pseudo = ../../pseudo

- Inspect the script file “job.sh”
- Set outdir and pseudo as in “bulk_Si_pwscf.in”
- Modify the path to Quantum Espresso pw.x
- Run the “job.sh” script file

NOTE: Make another copy of the completed step 1 folder so you don’t re-run in case there is a problem later.

Step 2: Create k-points

- Use a dense grid k-points.
- To do this modify the “KPOINTS_prim_cell.in” file by increasing the k grid in the second line of this file.
- “prim_cell_lattice.in” and “supercell_lattice.in” file demand some careful generation, see table below:

	prim_cell_lattice.in	sup_cell_lattice.in
2nd line = lattice conts. in Angstrom	value available in “pwscf.out” in step1 (only unit conversion is required)	same value as prim_cell_lattice.in
3rd to 5th lines = the array of the cell dimensions	open “pwscf.out” in step 1 and divide by the supercell factor	same values with those in “pwscf.out” in step 1 DON’T divide

- Run the script file
- Copy the kpoints generated in the KPOINT_supercell.out file to be used in step 3

Step 3: Band calculation

- Inspect the input file “bulk_Si_pwscf_bands.in”
- Paste the kpoints obtained from Step 2 in the “bulk_Si_pwscf_bands.in” file
- Inspect the “job.sh” file and make sure that the outdir and pseudo is set to same path as in step 1
- Run the script file

Step 4: Unfolding and plotting

- Inspect the script file
- Is emin, emax, and dE values appropriate for your calculation?
- Run the script file
- NOTE: dE is very important for the sharpness of the plot
  cmap and vmax should be controlled adequately to give a fine figure.
  For cmap options see the link:
  https://matplotlib.org/examples/color/colormaps_reference.html