

ABINIT assignment

Calculations of GaAs properties

Using what you have done for silicon, we will now calculate the properties of GaAs.

Use the pseudopotentials:

Psp_s_for_tests/HGH/31ga.3.hgh

Psp_s_for_tests/HGH/33as.5.hgh

- Determine the ecut necessary for a convergence of the total energy to 10^{-3} Ha. Present a graph or a table.
- Determine the ngkpt necessary for a convergence of the total energy to 10^{-3} Ha. Present a graph or a table.
- Determine the optimized lattice parameter and compare it to the experimental value of 5.65 Å.
- Using the example provided in:
/opt/pitp/abinit/example/Si-spin-orbit-coupling/
determine the DFT energy band gap, it is at Gamma, and compare it to the experimental value of 1.42 eV at room temperature. A GW calculation will be required to obtain a value closer to experiment but you do not have to do that for this assignment.
- Determine the Split-off energy, that is to say, the gap between the last occupied bands and the one below at Gamma, and compare it to the experimental value of 0.34 eV. We could show the band structure but it is not mandatory.