

ABINIT assignment (2024)

Calculations of GaAs properties

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

The tar file for this assignment is located:

/project/doc/abinit_tutorial/ABINIT_assignment.tar

Use the pseudopotentials provided in the tar file:

For Gallium: Ga.psp8

For Arsenic: As.psp8

- 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 for Si, 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 the 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.

Where to deposit your lab report:

Copy your lab report in PDF format on the school server. Name it "Surname_ABINIT.pdf", where "Surname" is your Surname!

```
[userXXX@ ] cp "Surname_ABINIT.pdf" /project/lab_reports/userXX/
```

To produce a band structure, you can use two tools:

Abipy

Adapt what you have done in the Tutorial Base 3 for Silicon.

GRACE

```
[lect19@login1] module load StdEnv/2020 intel/2020.1.217  
[lect19@login1] module load grace/5.99.0  
[lect19@login1] xmgrace-5.99.0 sio_DS2_EBANDS.agr
```

The last command will open the GUI of Grace where you can interact with the program. In the above example, we are plotting the 2nd dataset band structure. You will have to adapt to plot the correct file for the GaAs case.