Calculating bulk properties with SFHIngX

- Session E2 -

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Outline

- Introduction to SFHIngX
  - The program package and file structure
  - Set up the parameters for this calculation
  - Compute the total energy
  - Example run
- Determination of bulk properties
  - Theoretical lattice constant
  - The Murnaghan Equation of State
  - Convergence tests with respect to cutoff energy and k-point mesh
- Introduction to Session E2

Motivation

- How to calculate the bulk properties of a system

  → **optimize cutoff energy and k-point mesh**
- How to influence the convergence speed & accuracy and the memory demand

  → **use different electronic minimization schemes**
- How to influence the accuracy of a calculation

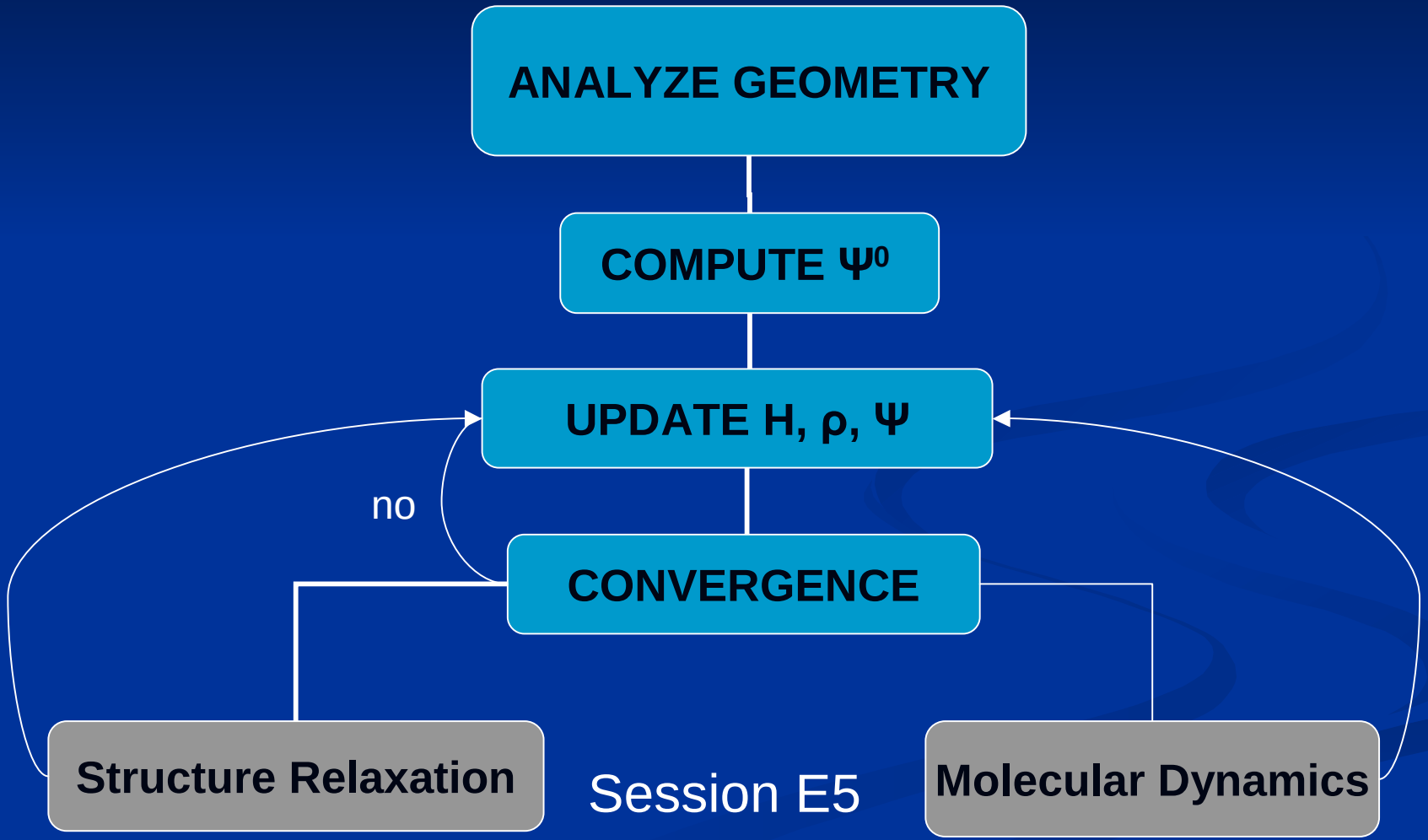
  → **use of LDA and GGA functional**

Tasks of session E2:

- Theoretical lattice constant
  - **Example calculation for GaAs with aLat =10.68 Bohr**
  - **Calculations for 9.6 – 11.6 Bohr, Murnaghan Fit**
- Convergence test for Ecut = 6-35 Ry and LDA/PBE
  - **For theoretical lattice constant**
  - **For several lattice constants, Murnghan fit**
- Convergence for k-point sampling for LDA and PBE
  - **At theoretical lattice constant and for best cutoff value**
- Electronic minimization schemes
  - **Steepest Descent**
  - **Williams-Soler algorithm**
  - **Damped Joannopoulos**
  - **All-state-conjugate-gradient**
  - **State-by-state-conjugate-gradient**
- Initialization of trial wave functions and charge density
  - **LCAO - Ansatz**
  - **Random numbers**

SFHIngX

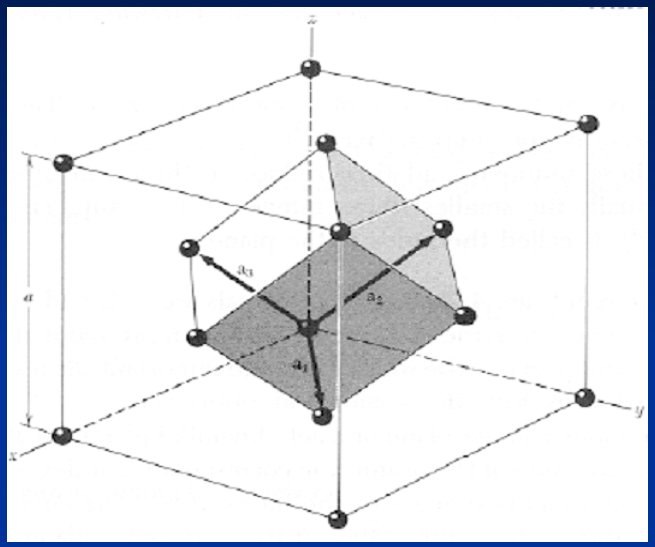
- Program Package –

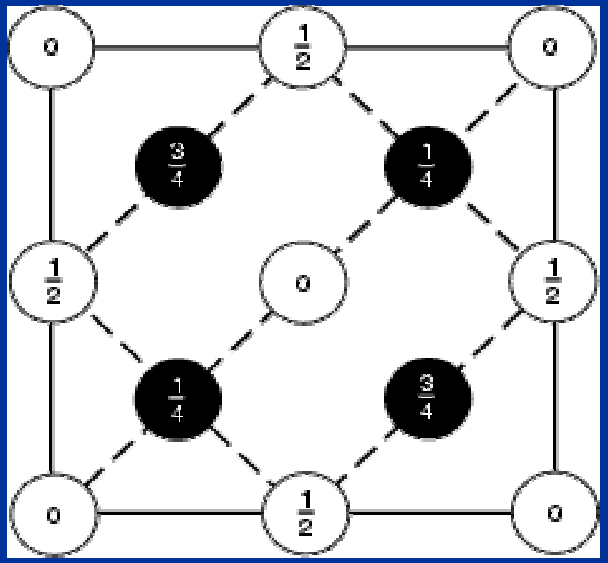


Set up of calculation
- the input file -

- The geometry
  - The lattice constant
  - The structure
  - The species
- The Basis
  - The cutoff energy
  - The k-point set
- The Hamiltonian
  - The exchange-correlation functional
- The trial wave functions and the initial charge density
- The main loop
  - Different minimization schemes

The Crystal Structure of GaAs





- Structure = Lattice + Basis
- Zincblend crystal structure
- Two interpenetrating fcc lattices with 2-atom basis
- 2nd fcc displaced by (¼ ¼ ¼) along body diagonal
- III-IV semiconductor
- 8 atoms per cubic cell in conventional cell :

  (0,0,0), (0, ½, ½), (½, 0, ½), (½, ½, 0),

  (¼/, ¼, ¼), (¼, ¾, ¾), (¾, ¼, ¾), (¾, ¾, ¼)

Performing a calculation

- the Structure and Basis of GaAs -

- The header
- The lattice constant
- The pseudopotentials
- zinc blende crystal structure
- fcc Bravais lattice
- Ga: [0, 0, 0]
- As : [¼, ¼, ¼]
- pw basis
- k-point set

```
format sfhingx;
include <parameters.sx>;

aLat = 10.68;
species_1 = <species/ga-lda-ham.sx>;
species_2 = <species/as-lda-ham.sx>;

structure  {
  include <structures/zincblend.sx>;
}
basis  {
  eCut      = 8 ;  // Ry
  kPoint {coords = [1/2, 1/2, 1/2];
          weight = 1; relative;}
  folding   = [4, 4, 4];
}
```

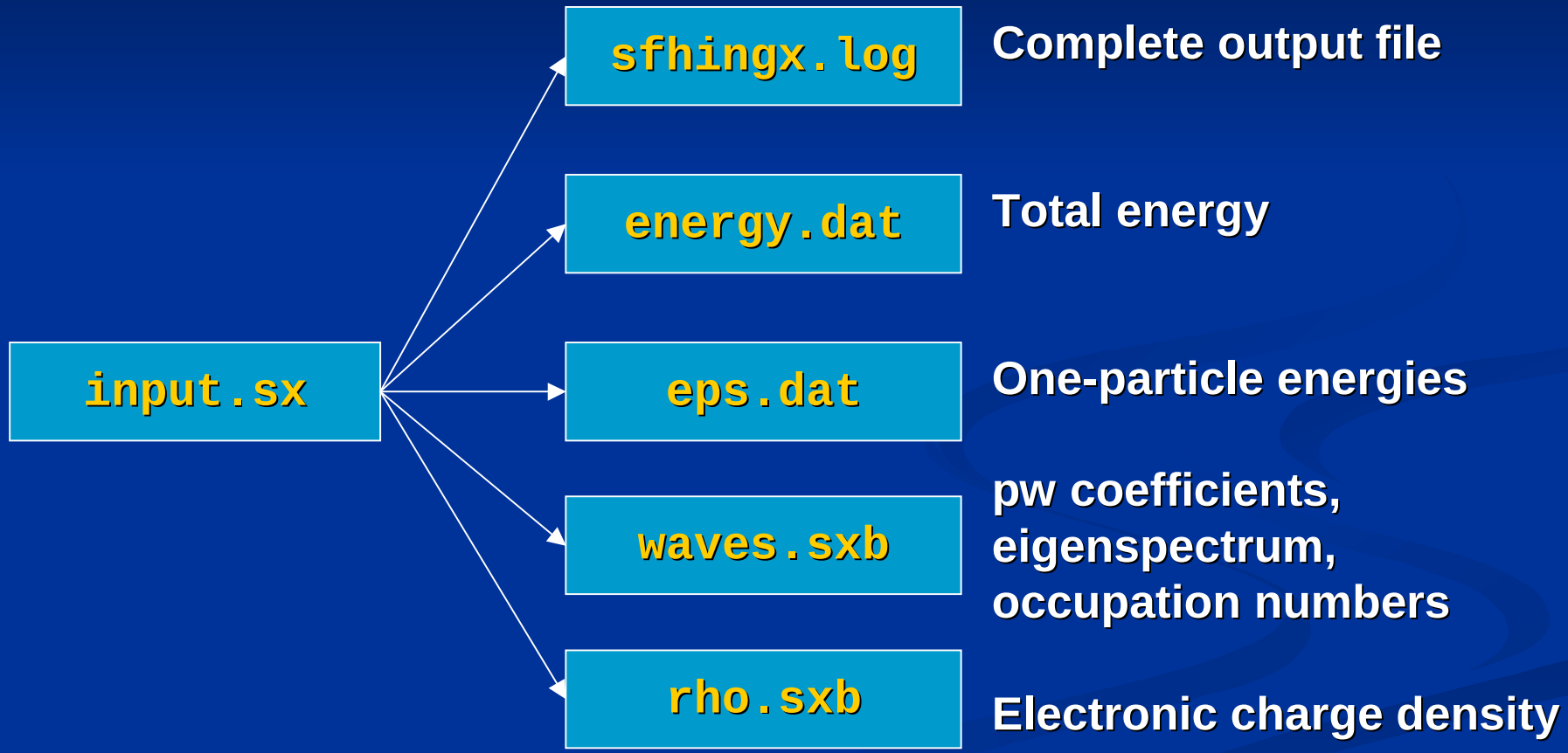
Performing a calculation

- Exchange-correlation: LDA
- Initialization of Ψ: LCAO
- Initialization of ρ: atomic orbitals
- Electronic minimization

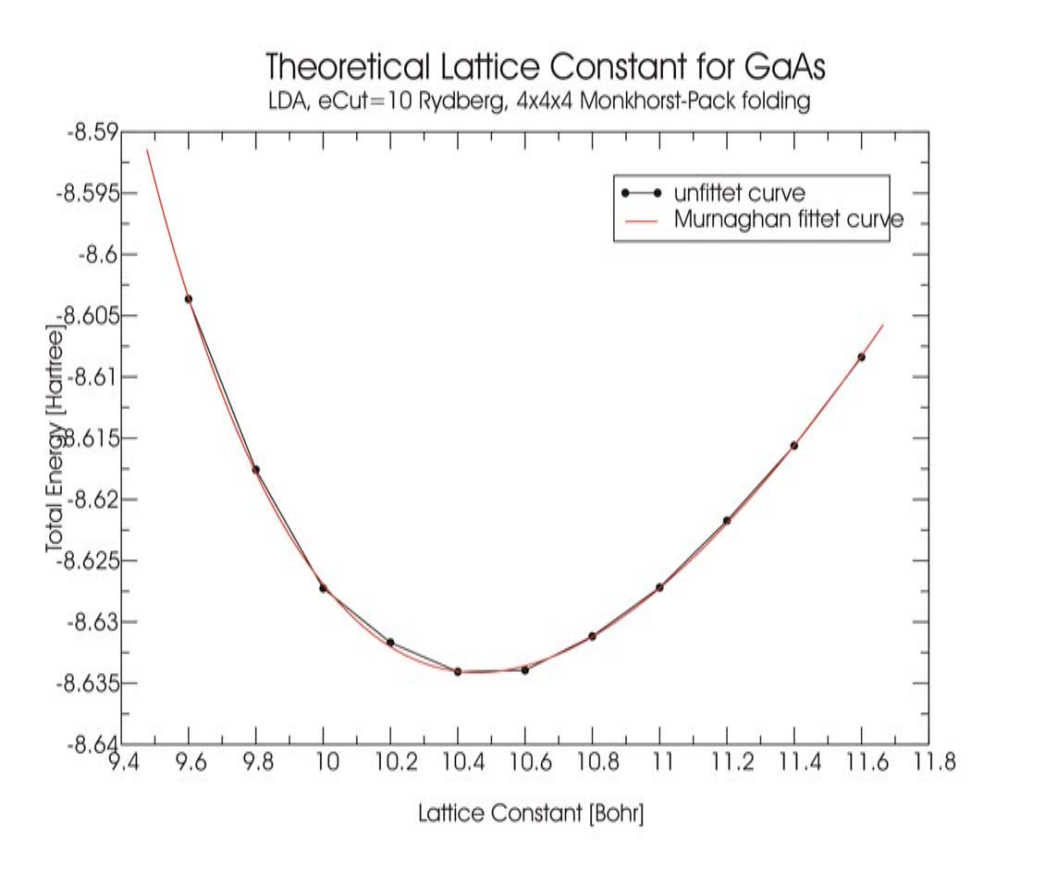
```
Hamiltonian  {
   ekt         = 0;
   xc          = LDA;
}

initialGuess  {
   waves {lcao{maxIt=1;rhoMixing=0.05;}}
   rho {atomicOrbitals;}
}

main  {
   CCG  {
      maxSteps      = 50;
      dEnergy       = 1e-06;  // Hartree
      printSteps    = 5;
         }
}
```

Performing a calculation

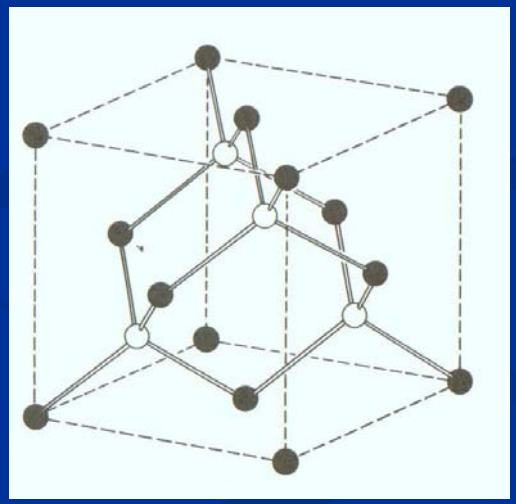
- the output files -



Determination of Theoretical Lattice constant



- Compute a series of E_{tot} for several lattice constants
- Murnaghan Equation

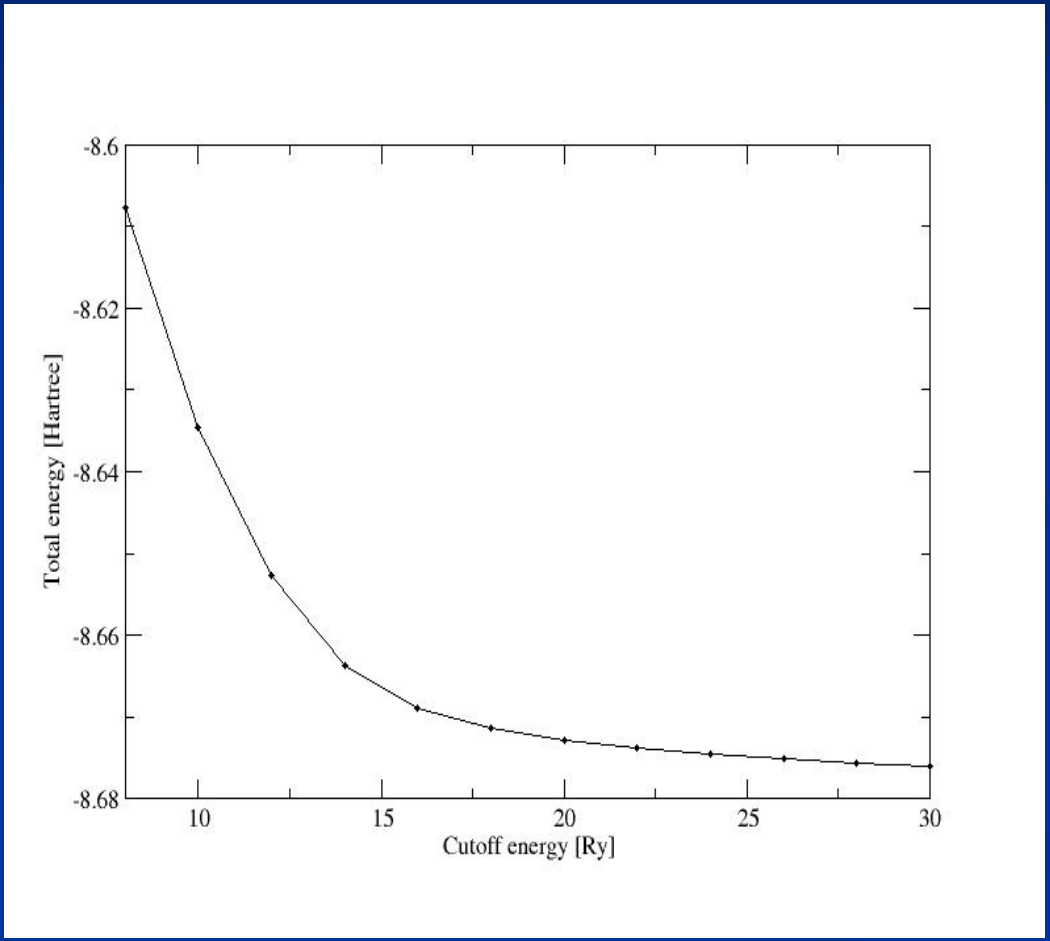


$$E_{tot}(V) - E_0(V_0) = \frac{B_0 V}{B_0'(B_0'-1)}\left[B_0'\left(1-\frac{V_0}{V}\right)+\left(\frac{V_0}{V}\right)^{B'_0}-1\right]$$

⇒ sxmurn

Convergence test for cutoff energy for GaAs (LDA)

- aLat=10.42 Bohr, LDA
- 4x4x4 mesh



eCut [Ry]	ΔE [%]
8	0.07
10	0.04
16	0.007
26	0.001
30	0

Convergence tests for GaAs bulk

LDA, 4x4x4 mesh
CCG minimizer

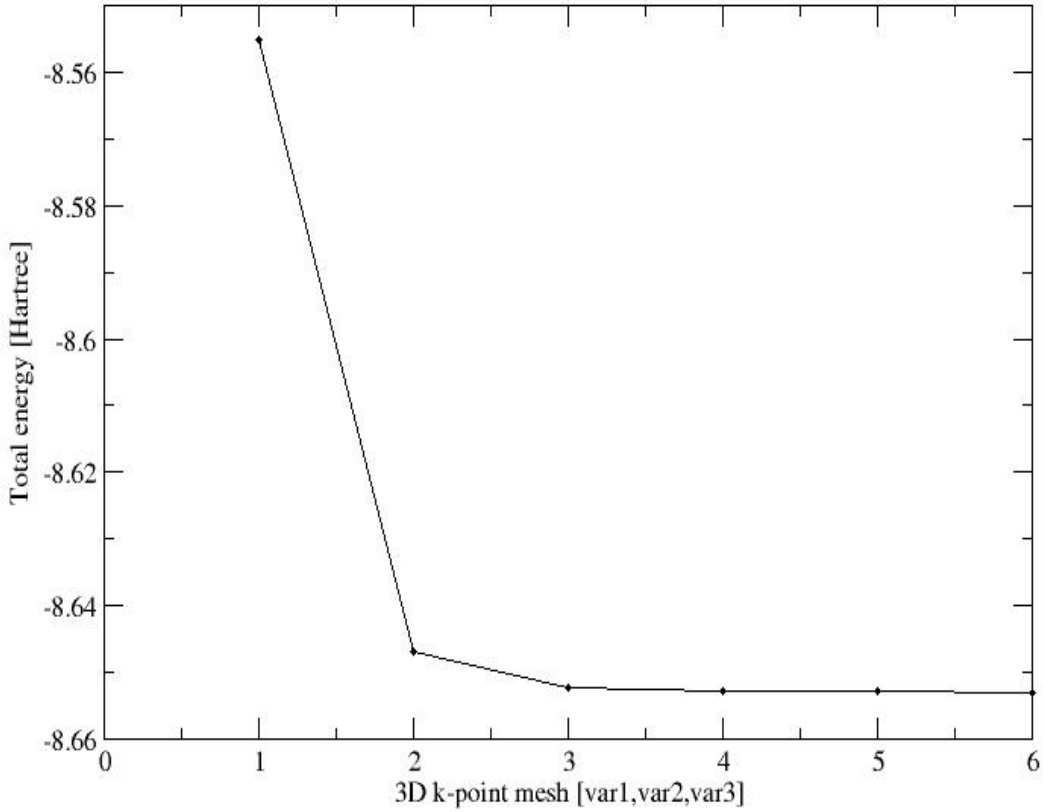
E_{cut} (Ryd)	a_0 (Bohr)	B_0 (GPa)
6	10.40	80.50
8	10.44	73.22
10	10.46	71.03
16	10.46	72.54
20	10.46	72.79
Exp. [1]	10.68	74.8

[1] Handbook of Chemistry and Physics, ed. By David R. Lide, 76th edition, 1995-1996, CRC Press, Inc. (1996)

The k-point mesh for GaAs

- (LDA, eCut=10 Ry) -

#of k-points	ΔE[%]
1	0.098
2	0.0061
6	0.0007
10	0.0002
19	0.0001
28	0



Minimization Methods

Iterative Diagonalization

Direct Set Methods

- Steepest Descent
- Williams-Soler
- Damped Joannopoulos

Conjugate Gradient Approach

- All-state conjugate gradient
- State-by-state conjugate gradient

Session E2

- Calculation of E_{tot} of a GaAs bulk within LDA
  - **Setting up the input file**
  - **Execution of SFHIngX**
  - **Analyze of the output files**
- Calculation of theoretical lattice constant
  - **Calculating a series of E_{tot}**
  - **Performing a Murnaghan Fit**
- Convergence tests for eCut and k-point mesh
- Controlling electronic minimization
- GGA versus LDA
- Initialization of Ψ and ρ