Karlsruhe Institute of Technology

The ABC of DFT: hands-on training AIMS 2

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Getting started

- The input files for and descriptions of the exercises are contained in a tar file
  `handsonsession.7.tar`
  under `/net/intact/home/dft20>`
- Please copy them to your account and unpack

```
> cp ~/../dft20/handsonsession.7.tar ~/ABC_of_DFT/hands-on-sessions/
> cd ~/ABC_of_DFT/hands-on-sessions
> tar -xvf handsonsession.7.tar
```

- If you did not do this laast time:

```
> cp ~/../dft20/setupaims .
> ./setupaims
```

- AIMS can now be executed by typing

```
> aims
```

Or better

```
> aims | tee outputfilename
```

Exercises

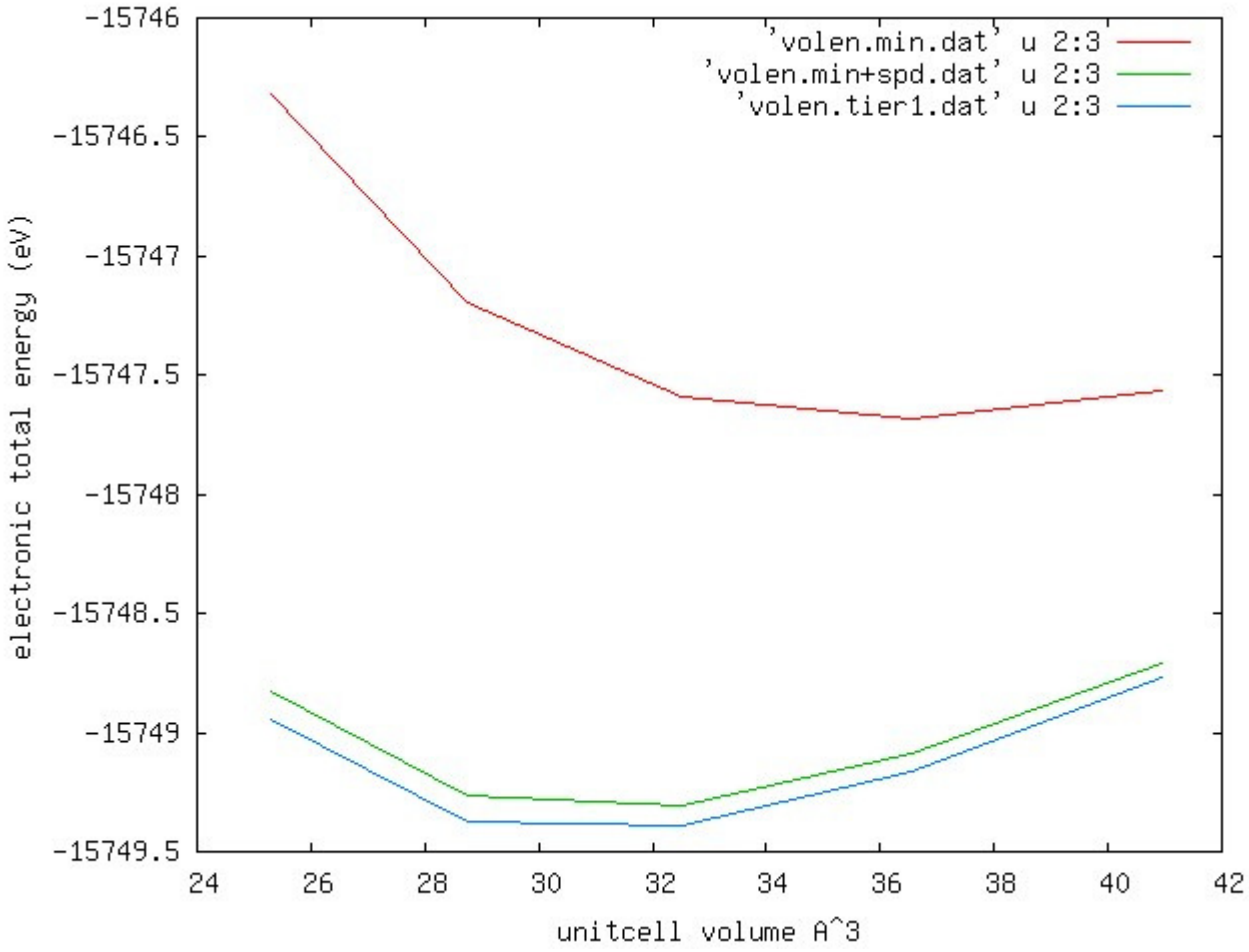
- Silicon :
  - Convergency of the energy v.s. volume curve
  - Phase stability
  - Cohesive energy
  - Equation of state
  - Phase transition

1 Convergency of the energy v.s. volume curve

- Study the basis-set dependence of the energy v.s. curve for the beta-Tin structure of Si
- We uses a 12x12x12 K-point mesh
  (we should have tested that as well obviously)
- Look at the run.lploop script
- Calculate the curve of the minimal, minimal+spd, and full tier 1 basis sets

1 Convergency of the energy v.s. volume curve

Beta-Tin

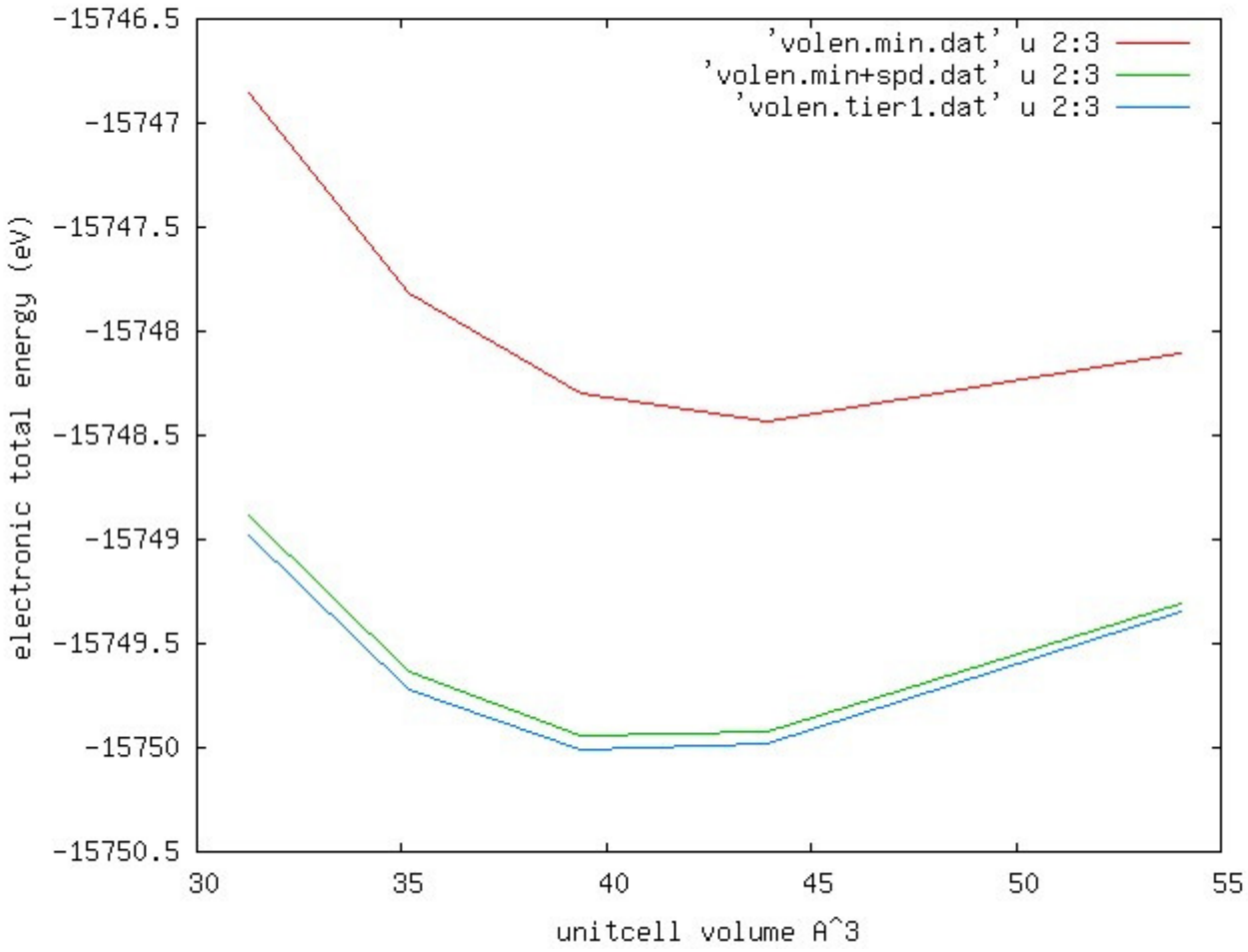


1 Convergency of the energy v.s. volume curve

- Study the basis-set dependence of the energy v.s. curve for the diamond structure of Si
- Look at the run.lploop script
- Calculate the curve of the minimal, minimal+spd, and full tier 1 basis sets
- Compare the two structures by visualizing them with VESTA

1 Convergency of the energy v.s. volume curve

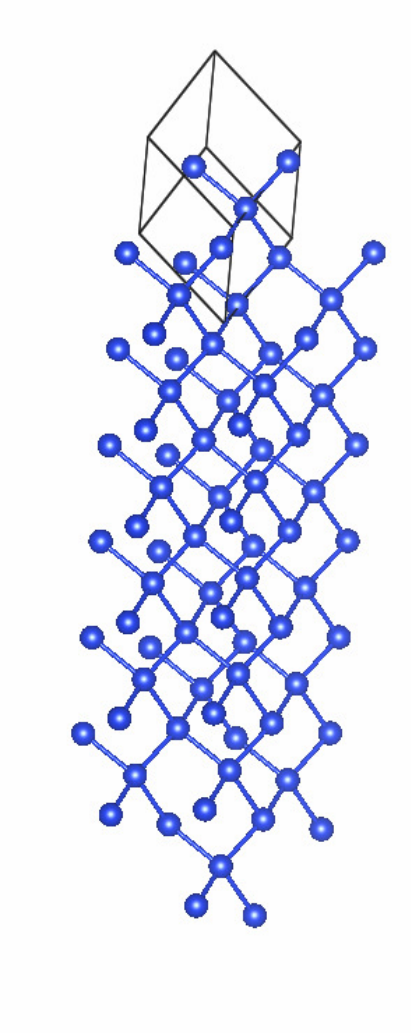
Diamond

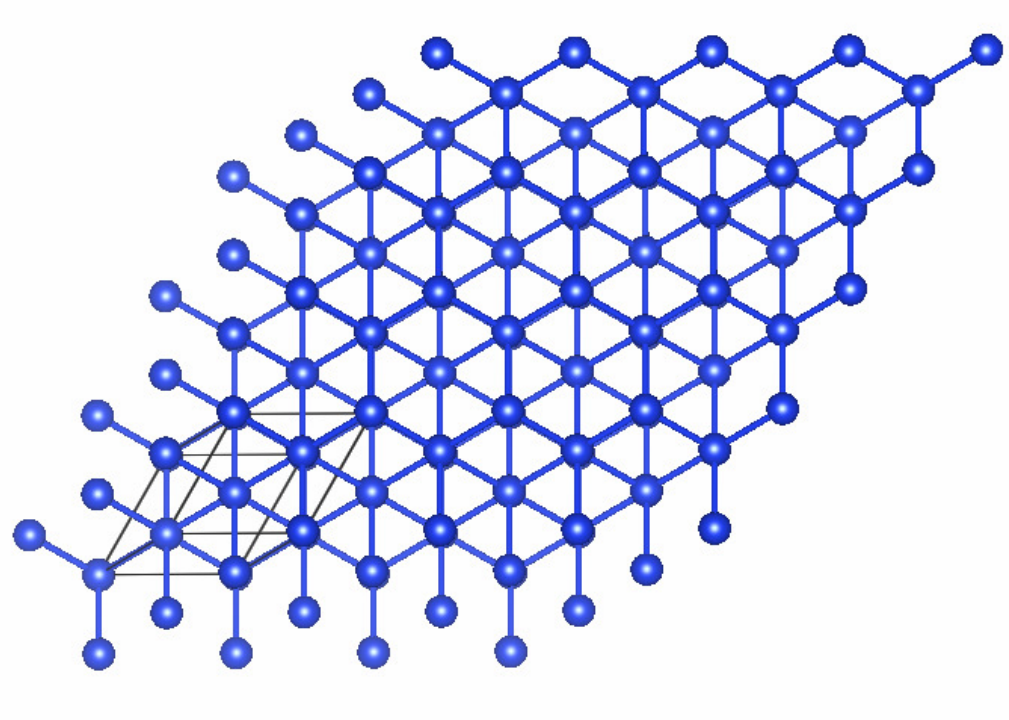


2 Comparing the two structures

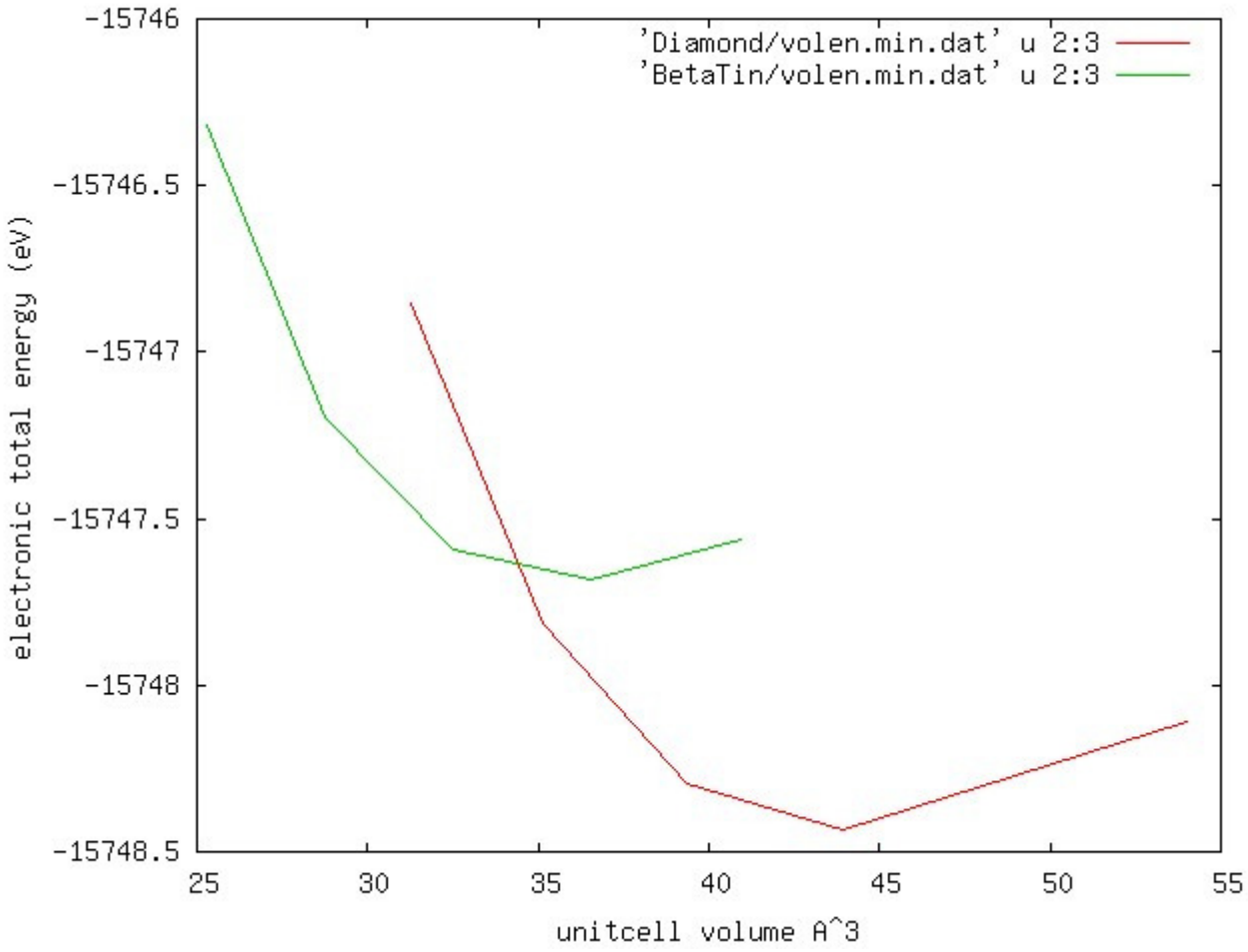
- Compare the two structures by visualizing them with VESTA
- Compare bond lengths, they can be measured in VESTA
- bond angles
- Compare the total energy curves

2 Beta-Tin and Diamond structures

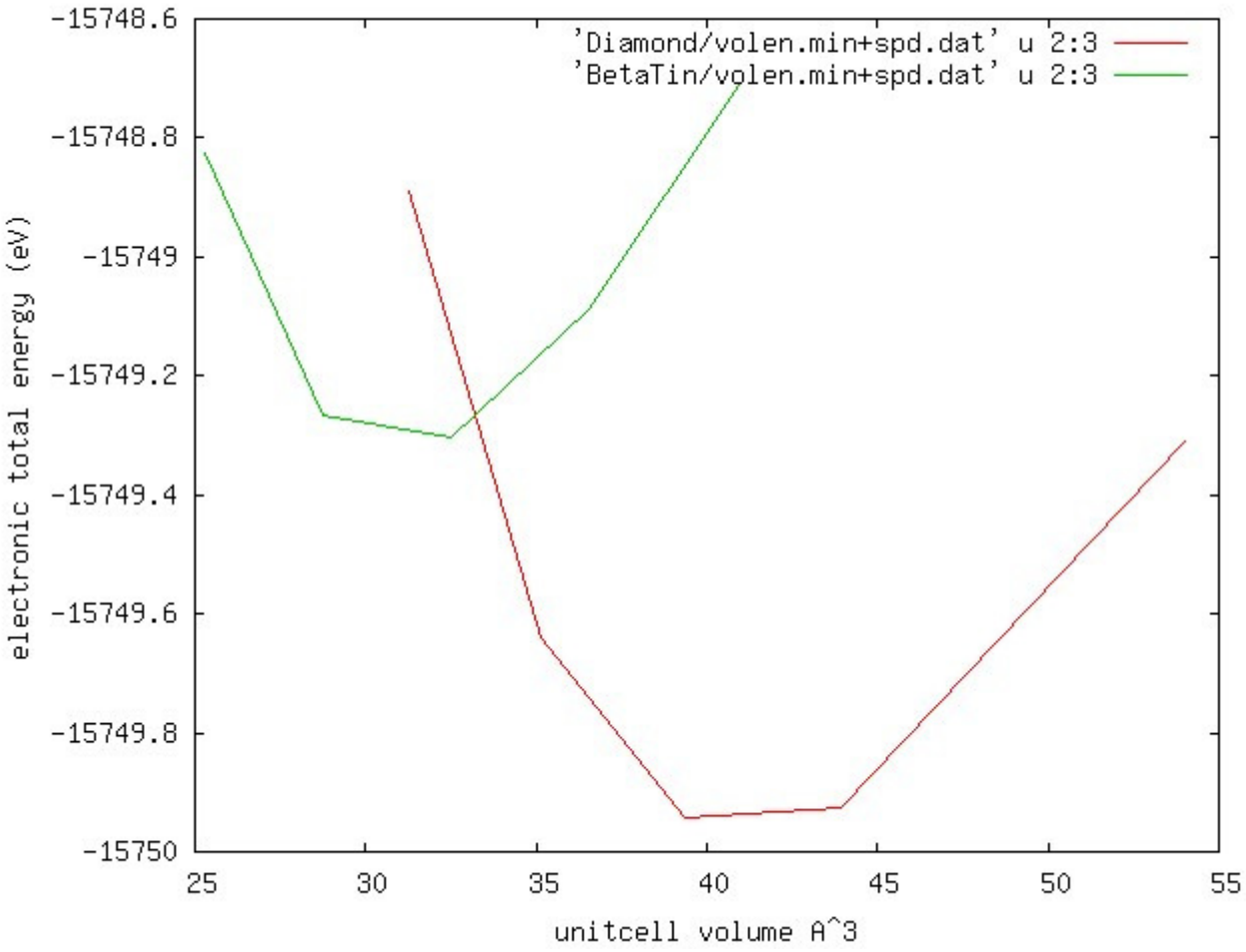




2 Comparison with minimal basis sets



2 Comparison with minimal + spd basis sets



3 Cohesive energy

- What does the energy we calculate actually mean?
- What “should” we compare to?

3 Cohesive energy

- What does the energy we calculate actually mean?
- What “should” we compare to?
- Calculate the total energy of a single atom as a reference
  - `spin collinear`
  - `default_initial_moment hund`
  - `tier 3 basis`
  - `cut_pot 8. 3. 1.`
  - `basis_dep_cutoff 0.`

4.601 eV

4 Equation of state

- Xmgrace
  - Data, Transformations, nonlinear curve fitting

$$E(V) = E_0 + \frac{B_0 V}{B_0'}\left(\frac{(V_0/V)^{B_0'}}{B_0' - 1} + 1\right) - \frac{B_0 V_0}{B_0' - 1}$$

  - Extract the optimal lattice parameter
  - Extract the bulk modulus

- B_0, B_0' and V_0 now give, to first order, the volume pressure relation:

$$P(V) = \frac{B_0}{B_0'}\left(\left(\frac{V_0}{V}\right)^{B_0'} - 1\right)$$

4 Equation of state

- Beta-Tin

- E_0 = -15749.4 eV
- B_0 = 0.655741eV / A^3
- B_0' = 4.98048
- V_0 = 30.7478 A^3

- Diamond

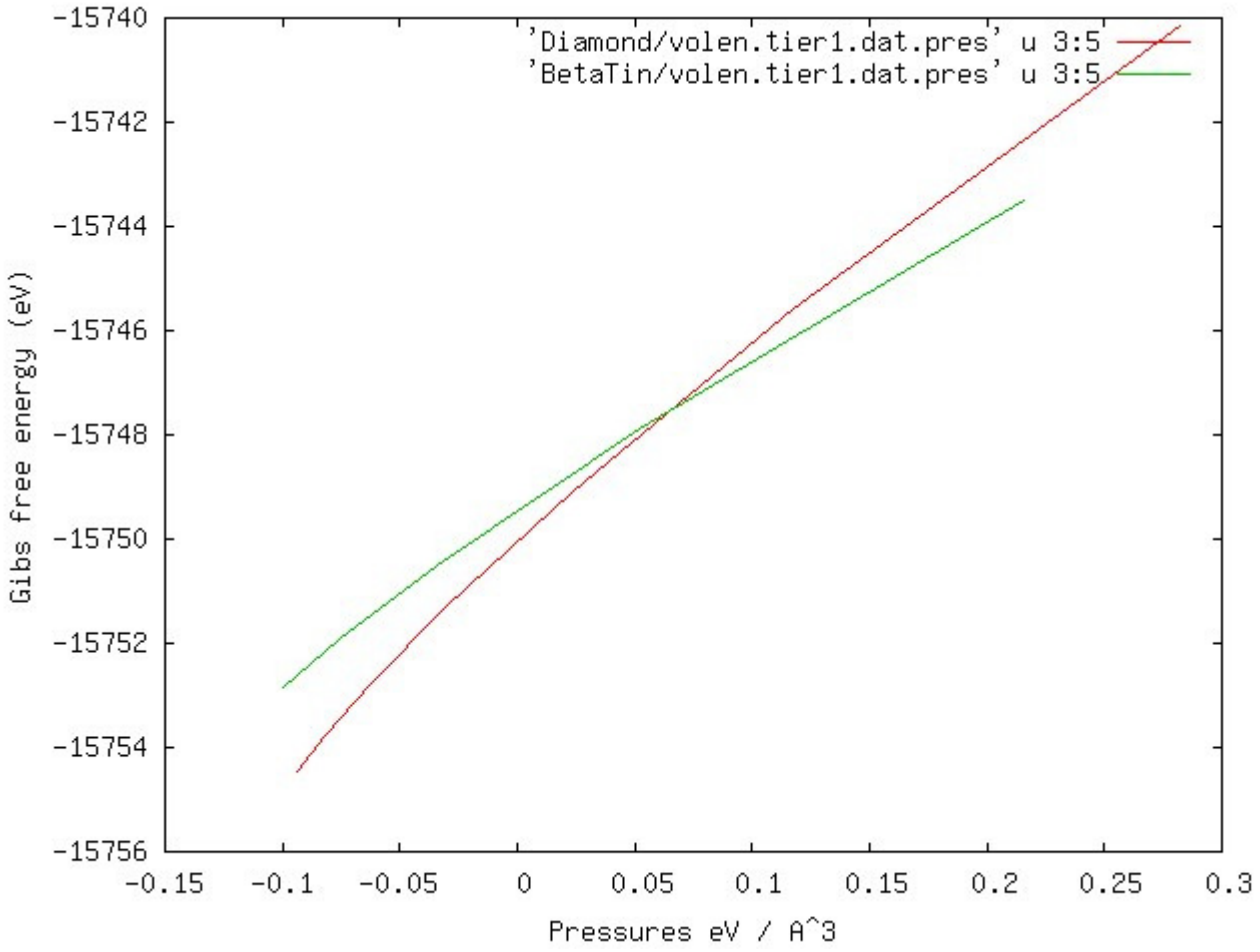
- E_0 = -15750 eV
- B_0 = 0.522452 eV / A^3
- B_0' = 4.56235
- V_0 = 41.0388 A^3

$$P(V) = \frac{B_0}{B_0'}\left(\left(\frac{V_0}{V}\right)^{B_0'} - 1\right)$$

Script: `v2p.pl filename B0 B0p V0`

Adds a pressure and a H = E + PV collumn

5 Comparing Gibbs (Helmholz) Free energies



Experimental and DFT@pbe values

- a = 5.430 (5.48) A
- B_0 = 98.8 (83.5) GPa
- E_{coh} = 4.63 (4.601) eV
- Diamond > beta-Tin 12 (10.75) GPa