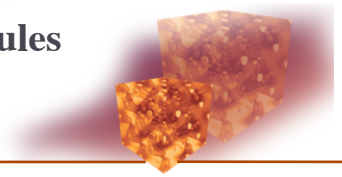

Structural optimizations within DFT (Abinit Code)

Richard Hennig, Ronald Cohen

1. Installation of Abinit

- Excellent website with documentation, tutorials, source code and precompiled executables at http://www.abinit.org/
- Choices of installation:
  (1) Download binary serial executable
  (2) Download binary parallel executable
  (3) Compile binary and parallel program from source code
- Copy the serial and parallel executable from ~train03/bin/abinis and ~/train/bin/abinip to your ~/bin directory

1.1 Compiling Abinit

- **Do not attempt this during the lab, it takes a long time to compile Abinit!**
- You can copy the source file from ~train03/Abinit/
- Make a directory where you want to compile Abinit
- Untar the file listed above in that directory
- Follow the steps in the file INSTALL
  (1) ./config/scripts/makemake
  (2) ./configure (or first create a build directory, then cd build, then ../configure)
  (3) ./make
  (4) ./make install

- To improve performance you might want to link to the Intel MKL libraries instead of using the standard BLAS library of Abinit
- To compile the MPI version of Abinit using the MPICH library, change step (2):
  ```
  soft add +mpich-tcp-1.2.6-intel9
  ./configure --with-mpi-prefix=/usr/apps/mpi/mpich-126
  ```
- While Abinit compiles you can already read ahead in Section 2 how to set up a calculation or look through the documentation and tutorial at http://www.abinit.org/

1.2 Running the Abinit tests

- After compiling abinit, you should find the executable at opt/abinis
- To run the basic abinit tests, type: make test1 and make tests_in
- Everything is fine if you get an output like

  ```
  OK for total energy
  OK for nuclei positions
  OK for forces
  OK for stresses
  ```
- If you are interested in the speed of your computer, you can run the performance tests using make tests_speed (not for Abinit 5.4.2)
- Performance data for a variety of machines can be found at http://www.abinit.org/documentation/?text=benchmarks

2. Setting up your first calculation

2.1 Input and output files

- Abinit requires several *input* files
  - Main input file
  - Input wave functions (if needed)
  - Pseudopotential data file(s)
- Abinit will create a number of *output* files
  - Main output file
  - Wave function files

- Temporary files

- The *filenames* for all these files are given in a separate file in the following order

```
abinit_input
abinit_output
abinit_input_wavefunctions
abinit_output_wavefunctions
temporary_files
Pseudopotential.psp
```

- Main input file
  - Controls the calculation
  - Geometry
  - Plane wave basis set
  - k-point integration
  - Self-consistency cycle
  - Choice of exchange-correlation functional
  - Ionic relaxations
  - Electronic band structure
  - Many other properties
  - For more information, see input variable description at http://www.abinit.org/Infos_v5.3/input_variables/keyhr.html

2.2 Sample calculations for silicon

- Follow lesson 3 from the tutorial for crystalline silicon: http://www.abinit.org/Infos_v5.3/tutorial/lesson_3.html
- You will learn the format of the input files, convergence with respect to plane wave basis and k-point mesh size and how to calculate lattice parameters, total energies and band structures
- The input files can be found in ~/train03/Abinit/abinitbin-5.4.2/tests/tutorial/Input/t3*

Remember: Always check convergence of your calculation with respect to k-point integration and basis set convergence!

3. Equation of state for the stishovite phase of SiO_2

- Modify the input file from the Silicon example for the stishovite phase of SiO_2
  - The crystal structure of stishovite is tetragonal
  - At p = 0 the lattice parameters are a = 7.90 a_0 and c = 5.03 a_0
  - The atom positions in unit cell coordinates are

Si	0.000	0.000	0.000
Si	0.500	0.500	0.500
O	0.310	0.310	0.000
O	-0.310	-0.310	0.000
O	0.810	0.190	0.500
O	0.190	0.810	0.500

- Use the Wu-Cohen exchange-correlation functional (ixc = 23)
  Phys. Rev. B 73, 235116 (2006)
- Converge the plane wave basis and the k-point mesh to an accuracy of 0.1 mHa
- Relax the atom positions and the unit cell shape (see optcell and ionmov)
- Calculate the total energy for unit cell volumes of 240 – 340 a_0^3 in steps of 5 a_0^3
- Share the work with the other groups:
  - Each group should calculate one volume
  - Combine the results and graph the equation of state (energy vs. volume)

4. Phase transformation from stishovite to the $CaCl_2$ phase

- Under pressure the stishovite phase transforms into the $CaCl_2$ phase by a symmetry breaking that rotates the oxygen octahedra of the structure
- Break the symmetry of the oxygen octahedra such that the atom positions are

Si	0.000	0.000	0.000
Si	0.500	0.500	0.500
O	0.320	0.270	0.000
O	-0.320	-0.270	0.000
O	0.820	0.230	0.500
O	0.180	0.770	0.500

- Relax this structure for the same volume you used for stishovite to check if the stishovite phase or the $CaCl_2$ phase is the stable phase at these volumes
- Combine all the data for the two phases and determine the phase transformation pressure